Instructors' Solution Manual
Introduction to Quantum Mechanics, 3rd ed.

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Preface

These are our own solutions to the problems in *Introduction to Quantum Mechanics, 3rd ed.* We have made every effort to insure that they are clear and correct, but errors are bound to occur, and for this we apologize in advance. We would like to thank the many people who pointed out mistakes in the solution manual for the second edition, and encourage anyone who finds defects in this one to alert us (griffith@reed.edu or schroetd@reed.edu). We especially thank Kenny Scott, Alain Thys, and Sergei Walter, who found many errors in the 2nd edition solution manual. We maintain a list of errata on the web page (http://academic.reed.edu/physics/faculty/griffiths.html), and incorporate corrections in the manual itself from time to time. We also thank our students for many useful suggestions, and Neelaksh Sadhoo, who did much of the typesetting for the second edition.

David Griffiths and Darrell Schroeter

Chapter 1

The Wave Function

Problem 1.1

(a)

$$\langle j\rangle^2 = 21^2 = \boxed{441.}$$

$$\langle j^2\rangle = \frac{1}{N}\sum j^2 N(j) = \frac{1}{14}\left[(14^2) + (15^2) + 3(16^2) + 2(22^2) + 2(24^2) + 5(25^2)\right]$$
$$= \frac{1}{14}(196 + 225 + 768 + 968 + 1152 + 3125) = \frac{6434}{14} = \boxed{459.571.}$$

(b)

j	$\Delta j = j - \langle j\rangle$
14	$14 - 21 = -7$
15	$15 - 21 = -6$
16	$16 - 21 = -5$
22	$22 - 21 = 1$
24	$24 - 21 = 3$
25	$25 - 21 = 4$

$$\sigma^2 = \frac{1}{N}\sum(\Delta j)^2 N(j) = \frac{1}{14}\left[(-7)^2 + (-6)^2 + (-5)^2\cdot 3 + (1)^2\cdot 2 + (3)^2\cdot 2 + (4)^2\cdot 5\right]$$
$$= \frac{1}{14}(49 + 36 + 75 + 2 + 18 + 80) = \frac{260}{14} = \boxed{18.571.}$$

$$\sigma = \sqrt{18.571} = \boxed{4.309.}$$

(c)

$$\langle j^2\rangle - \langle j\rangle^2 = 459.571 - 441 = 18.571. \quad \text{[Agrees with (b).]}$$

Problem 1.2

(a)

$$\langle x^2\rangle = \int_0^h x^2 \frac{1}{2\sqrt{hx}}dx = \frac{1}{2\sqrt{h}}\left(\frac{2}{5}x^{5/2}\right)\Big|_0^h = \frac{h^2}{5}.$$

$$\sigma^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{h^2}{5} - \left(\frac{h}{3}\right)^2 = \frac{4}{45}h^2 \;\Rightarrow\; \sigma = \boxed{\frac{2h}{3\sqrt{5}} = 0.2981h.}$$

(b)

$$P = 1 - \int_{x_-}^{x_+} \frac{1}{2\sqrt{hx}}dx = 1 - \frac{1}{2\sqrt{h}}(2\sqrt{x})\Big|_{x_-}^{x_+} = 1 - \frac{1}{\sqrt{h}}\left(\sqrt{x_+} - \sqrt{x_-}\right).$$

$$x_+ \equiv \langle x\rangle + \sigma = 0.3333h + 0.2981h = 0.6315h; \quad x_- \equiv \langle x\rangle - \sigma = 0.3333h - 0.2981h = 0.0352h.$$

$$P = 1 - \sqrt{0.6315} + \sqrt{0.0352} = \boxed{0.393.}$$

Problem 1.3

(a)

$$1 = \int_{-\infty}^{\infty} Ae^{-\lambda(x-a)^2}dx. \qquad \text{Let } u \equiv x-a,\ du = dx,\ u: -\infty \to \infty.$$

$$1 = A\int_{-\infty}^{\infty} e^{-\lambda u^2}du = A\sqrt{\frac{\pi}{\lambda}} \quad \Rightarrow \quad \boxed{A = \sqrt{\frac{\lambda}{\pi}}.}$$

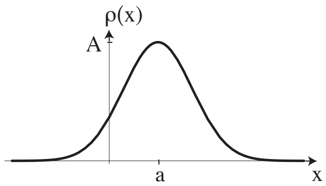
(b)

$$\begin{aligned}\langle x\rangle &= A\int_{-\infty}^{\infty} xe^{-\lambda(x-a)^2}dx = A\int_{-\infty}^{\infty}(u+a)e^{-\lambda u^2}du \\ &= A\left[\int_{-\infty}^{\infty} ue^{-\lambda u^2}du + a\int_{-\infty}^{\infty} e^{-\lambda u^2}du\right] = A\left(0 + a\sqrt{\frac{\pi}{\lambda}}\right) = \boxed{a.}\end{aligned}$$

$$\begin{aligned}\langle x^2\rangle &= A\int_{-\infty}^{\infty} x^2 e^{-\lambda(x-a)^2}dx \\ &= A\left\{\int_{-\infty}^{\infty} u^2 e^{-\lambda u^2}du + 2a\int_{-\infty}^{\infty} ue^{-\lambda u^2}du + a^2\int_{-\infty}^{\infty} e^{-\lambda u^2}du\right\} \\ &= A\left[\frac{1}{2\lambda}\sqrt{\frac{\pi}{\lambda}} + 0 + a^2\sqrt{\frac{\pi}{\lambda}}\right] = \boxed{a^2 + \frac{1}{2\lambda}.}\end{aligned}$$

$$\sigma^2 = \langle x^2\rangle - \langle x\rangle^2 = a^2 + \frac{1}{2\lambda} - a^2 = \frac{1}{2\lambda}; \qquad \boxed{\sigma = \frac{1}{\sqrt{2\lambda}}.}$$

(c)



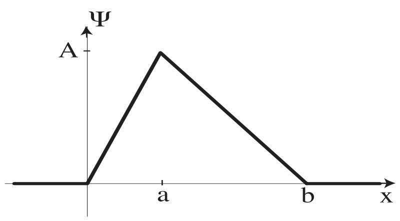
Problem 1.4

(a)

$$1 = \frac{|A|^2}{a^2}\int_0^a x^2 dx + \frac{|A|^2}{(b-a)^2}\int_a^b (b-x)^2 dx = |A|^2 \left\{ \frac{1}{a^2}\left(\frac{x^3}{3}\right)\Big|_0^a + \frac{1}{(b-a)^2}\left(-\frac{(b-x)^3}{3}\right)\Big|_a^b \right\}$$

$$= |A|^2\left[\frac{a}{3} + \frac{b-a}{3}\right] = |A|^2\frac{b}{3} \ \Rightarrow \ \boxed{A = \sqrt{\frac{3}{b}}.}$$

(b)



(c) At $\boxed{x = a.}$

(d)

$$P = \int_0^a |\Psi|^2 dx = \frac{|A|^2}{a^2}\int_0^a x^2 dx = |A|^2\frac{a}{3} = \boxed{\frac{a}{b}.} \begin{cases} P = 1 & \text{if } \ b = a, \ \checkmark \\ P = 1/2 & \text{if } \ b = 2a. \ \checkmark \end{cases}$$

(e)

$$\langle x \rangle = \int x|\Psi|^2 dx = |A|^2 \left\{ \frac{1}{a^2}\int_0^a x^3 dx + \frac{1}{(b-a)^2}\int_a^b x(b-x)^2 dx \right\}$$

$$= \frac{3}{b}\left\{ \frac{1}{a^2}\left(\frac{x^4}{4}\right)\Big|_0^a + \frac{1}{(b-a)^2}\left(b^2\frac{x^2}{2} - 2b\frac{x^3}{3} + \frac{x^4}{4}\right)\Big|_a^b \right\}$$

$$= \frac{3}{4b(b-a)^2}\left[a^2(b-a)^2 + 2b^4 - 8b^4/3 + b^4 - 2a^2b^2 + 8a^3b/3 - a^4\right]$$

$$= \frac{3}{4b(b-a)^2}\left(\frac{b^4}{3} - a^2b^2 + \frac{2}{3}a^3b\right) = \frac{1}{4(b-a)^2}(b^3 - 3a^2b + 2a^3) = \boxed{\frac{2a+b}{4}.}$$

Problem 1.5

(a)

$$1 = \int |\Psi|^2 dx = 2|A|^2 \int_0^\infty e^{-2\lambda x} dx = 2|A|^2 \left(\frac{e^{-2\lambda x}}{-2\lambda} \right)\Bigg|_0^\infty = \frac{|A|^2}{\lambda}; \quad \boxed{A = \sqrt{\lambda}.}$$

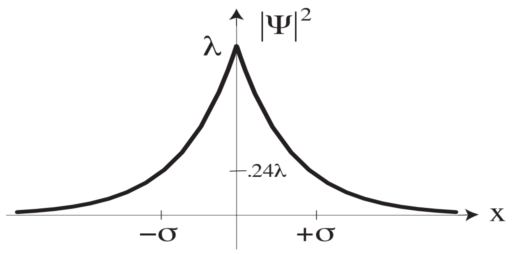
(b)

$$\langle x \rangle = \int x|\Psi|^2 dx = |A|^2 \int_{-\infty}^{\infty} x e^{-2\lambda|x|} dx = \boxed{0.} \qquad \text{[Odd integrand.]}$$

$$\langle x^2 \rangle = 2|A|^2 \int_0^\infty x^2 e^{-2\lambda x} dx = 2\lambda \left[\frac{2}{(2\lambda)^3} \right] = \boxed{\frac{1}{2\lambda^2}.}$$

(c)

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{1}{2\lambda^2}; \qquad \boxed{\sigma = \frac{1}{\sqrt{2}\lambda}.} \qquad |\Psi(\pm\sigma)|^2 = |A|^2 e^{-2\lambda\sigma} = \lambda e^{-2\lambda/\sqrt{2}\lambda} = \lambda e^{-\sqrt{2}} = 0.2431\lambda.$$



Probability outside:

$$2\int_\sigma^\infty |\Psi|^2 dx = 2|A|^2 \int_\sigma^\infty e^{-2\lambda x} dx = 2\lambda \left(\frac{e^{-2\lambda x}}{-2\lambda} \right)\Bigg|_\sigma^\infty = e^{-2\lambda\sigma} = \boxed{e^{-\sqrt{2}} = 0.2431.}$$

Problem 1.6

For integration by parts, the differentiation has to be with respect to the *integration* variable – in this case the differentiation is with respect to t, but the integration variable is x. It's true that

$$\frac{\partial}{\partial t}(x|\Psi|^2) = \frac{\partial x}{\partial t}|\Psi|^2 + x\frac{\partial}{\partial t}|\Psi|^2 = x\frac{\partial}{\partial t}|\Psi|^2,$$

but this does *not* allow us to perform the integration:

$$\int_a^b x\frac{\partial}{\partial t}|\Psi|^2 dx = \int_a^b \frac{\partial}{\partial t}(x|\Psi|^2) dx \neq (x|\Psi|^2)\Big|_a^b.$$

Problem 1.7

From Eq. 1.33, $\frac{d\langle p\rangle}{dt} = -i\hbar\int \frac{\partial}{\partial t}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)dx$. But, noting that $\frac{\partial^2\Psi}{\partial x\partial t} = \frac{\partial^2\Psi}{\partial t\partial x}$ and using Eqs. 1.23-1.24:

$$\frac{\partial}{\partial t}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right) = \frac{\partial\Psi^*}{\partial t}\frac{\partial\Psi}{\partial x} + \Psi^*\frac{\partial}{\partial x}\left(\frac{\partial\Psi}{\partial t}\right) = \left[-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*\right]\frac{\partial\Psi}{\partial x} + \Psi^*\frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi\right]$$
$$= \frac{i\hbar}{2m}\left[\Psi^*\frac{\partial^3\Psi}{\partial x^3} - \frac{\partial^2\Psi^*}{\partial x^2}\frac{\partial\Psi}{\partial x}\right] + \frac{i}{\hbar}\left[V\Psi^*\frac{\partial\Psi}{\partial x} - \Psi^*\frac{\partial}{\partial x}(V\Psi)\right]$$

The first term integrates to zero, using integration by parts twice, and the second term can be simplified to $V\Psi^*\frac{\partial\Psi}{\partial x} - \Psi^*V\frac{\partial\Psi}{\partial x} - \Psi^*\frac{\partial V}{\partial x}\Psi = -|\Psi|^2\frac{\partial V}{\partial x}$. So

$$\frac{d\langle p\rangle}{dt} = -i\hbar\left(\frac{i}{\hbar}\right)\int -|\Psi|^2\frac{\partial V}{\partial x}dx = \langle -\frac{\partial V}{\partial x}\rangle. \qquad \text{QED}$$

Problem 1.8

Suppose Ψ satisfies the Schrödinger equation *without* V_0: $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$. We want to find the solution Ψ_0 *with* V_0: $i\hbar\frac{\partial\Psi_0}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_0}{\partial x^2} + (V+V_0)\Psi_0$.

Claim: $\Psi_0 = \Psi e^{-iV_0t/\hbar}$.

Proof: $i\hbar\frac{\partial\Psi_0}{\partial t} = i\hbar\frac{\partial\Psi}{\partial t}e^{-iV_0t/\hbar} + i\hbar\Psi\left(-\frac{iV_0}{\hbar}\right)e^{-iV_0t/\hbar} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi\right]e^{-iV_0t/\hbar} + V_0\Psi e^{-iV_0t/\hbar}$
$= -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_0}{\partial x^2} + (V+V_0)\Psi_0.$ QED

This has *no* effect on the expectation value of a dynamical variable, since the extra phase factor, being independent of x, cancels out in Eq. 1.36.

Problem 1.9

(a)

$$1 = 2|A|^2\int_0^\infty e^{-2amx^2/\hbar}dx = 2|A|^2\frac{1}{2}\sqrt{\frac{\pi}{(2am/\hbar)}} = |A|^2\sqrt{\frac{\pi\hbar}{2am}}; \qquad \boxed{A = \left(\frac{2am}{\pi\hbar}\right)^{1/4}.}$$

(b)

$$\frac{\partial\Psi}{\partial t} = -ia\Psi; \quad \frac{\partial\Psi}{\partial x} = -\frac{2amx}{\hbar}\Psi; \quad \frac{\partial^2\Psi}{\partial x^2} = -\frac{2am}{\hbar}\left(\Psi + x\frac{\partial\Psi}{\partial x}\right) = -\frac{2am}{\hbar}\left(1 - \frac{2amx^2}{\hbar}\right)\Psi.$$

Plug these into the Schrödinger equation, $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$:

$$V\Psi = i\hbar(-ia)\Psi + \frac{\hbar^2}{2m}\left(-\frac{2am}{\hbar}\right)\left(1 - \frac{2amx^2}{\hbar}\right)\Psi$$
$$= \left[\hbar a - \hbar a\left(1 - \frac{2amx^2}{\hbar}\right)\right]\Psi = 2a^2mx^2\Psi, \quad \text{so} \quad \boxed{V(x) = 2ma^2x^2.}$$

(c)

$$\langle x\rangle = \int_{-\infty}^{\infty} x|\Psi|^2 dx = \boxed{0.} \qquad \text{[Odd integrand.]}$$

$$\langle x^2\rangle = 2|A|^2\int_0^{\infty} x^2 e^{-2amx^2/\hbar}dx = 2|A|^2\frac{1}{2^2(2am/\hbar)}\sqrt{\frac{\pi\hbar}{2am}} = \boxed{\frac{\hbar}{4am}.}$$

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = \boxed{0.}$$

$$\begin{aligned}\langle p^2\rangle &= \int \Psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2\Psi dx = -\hbar^2\int\Psi^*\frac{\partial^2\Psi}{\partial x^2}dx \\ &= -\hbar^2\int\Psi^*\left[-\frac{2am}{\hbar}\left(1-\frac{2amx^2}{\hbar}\right)\Psi\right]dx = 2am\hbar\left\{\int|\Psi|^2dx - \frac{2am}{\hbar}\int x^2|\Psi|^2dx\right\} \\ &= 2am\hbar\left(1-\frac{2am}{\hbar}\langle x^2\rangle\right) = 2am\hbar\left(1-\frac{2am}{\hbar}\frac{\hbar}{4am}\right) = 2am\hbar\left(\frac{1}{2}\right) = \boxed{am\hbar.}\end{aligned}$$

(d)

$$\sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{\hbar}{4am} \Longrightarrow \boxed{\sigma_x = \sqrt{\frac{\hbar}{4am}}}; \quad \sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2 = am\hbar \Longrightarrow \boxed{\sigma_p = \sqrt{am\hbar}.}$$

$\sigma_x\sigma_p = \sqrt{\frac{\hbar}{4am}}\sqrt{am\hbar} = \frac{\hbar}{2}$. This *is* (just barely) consistent with the uncertainty principle.

Problem 1.10

From Math Tables: $\pi = 3.141592653589793238462643\cdots$

(a) $\boxed{\begin{array}{lllll} P(0)=0 & P(1)=2/25 & P(2)=3/25 & P(3)=5/25 & P(4)=3/25 \\ P(5)=3/25 & P(6)=3/25 & P(7)=1/25 & P(8)=2/25 & P(9)=3/25\end{array}}$

In general, $P(j) = \frac{N(j)}{N}$.

(b) *Most probable*: $\boxed{3.}$ *Median*: 13 are ≤ 4, 12 are ≥ 5, so median is $\boxed{4.}$

Average: $\langle j\rangle = \frac{1}{25}[0\cdot0+1\cdot2+2\cdot3+3\cdot5+4\cdot3+5\cdot3+6\cdot3+7\cdot1+8\cdot2+9\cdot3]$

$= \frac{1}{25}[0+2+6+15+12+15+18+7+16+27] = \frac{118}{25} = \boxed{4.72.}$

(c) $\langle j^2\rangle = \frac{1}{25}[0+1^2\cdot2+2^2\cdot3+3^2\cdot5+4^2\cdot3+5^2\cdot3+6^2\cdot3+7^2\cdot1+8^2\cdot2+9^2\cdot3]$

$= \frac{1}{25}[0+2+12+45+48+75+108+49+128+243] = \frac{710}{25} = \boxed{28.4.}$

$\sigma^2 = \langle j^2\rangle - \langle j\rangle^2 = 28.4 - 4.72^2 = 28.4 - 22.2784 = 6.1216;\quad \sigma = \sqrt{6.1216} = \boxed{2.474.}$

Problem 1.11

(a)

$$\frac{1}{2}mv^2 + V = E \quad \rightarrow \quad \boxed{v(x) = \sqrt{\frac{2}{m}\left(E - V(x)\right)}.}$$

(b)

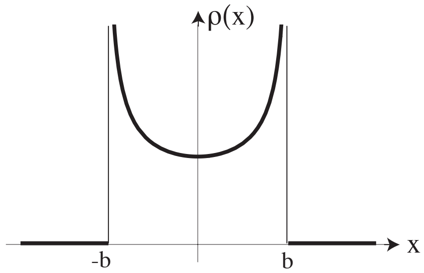
$$T = \int_a^b \frac{1}{\sqrt{\frac{2}{m}\left(E - \frac{1}{2}kx^2\right)}}\, dx = \sqrt{\frac{m}{k}} \int_a^b \frac{1}{\sqrt{(2E/k) - x^2}}\, dx.$$

Turning points: $v = 0 \Rightarrow E = V = \frac{1}{2}kb^2 \Rightarrow b = \sqrt{2E/k}$; $\quad a = -b$.

$$T = 2\sqrt{\frac{m}{k}} \int_0^b \frac{1}{\sqrt{b^2 - x^2}}\, dx = 2\sqrt{\frac{m}{k}} \sin^{-1}\left(\frac{x}{b}\right)\Big|_0^b = 2\sqrt{\frac{m}{k}} \sin^{-1}(1)$$
$$= 2\sqrt{\frac{m}{k}}\left(\frac{\pi}{2}\right) = \pi\sqrt{\frac{m}{k}}.$$

$$\rho(x) = \frac{1}{\pi\sqrt{\frac{m}{k}}\sqrt{\frac{2}{m}\left(E - \frac{1}{2}kx^2 1\right)}} = \boxed{\frac{1}{\pi\sqrt{b^2 - x^2}}.}$$

$$\int_a^b \rho(x)\, dx = \frac{2}{\pi}\int_0^b \frac{1}{\sqrt{b^2 - x^2}}\, dx = \frac{2}{\pi}\left(\frac{\pi}{2}\right) = 1. \checkmark$$



(c) $\boxed{\langle x \rangle = 0.}$

$$\langle x^2 \rangle = \frac{1}{\pi}\int_{-b}^b \frac{x^2}{\sqrt{b^2 - x^2}}\, dx = \frac{2}{\pi}\int_0^b \frac{x^2}{\sqrt{b^2 - x^2}}\, dx$$
$$= \frac{2}{\pi}\left[-\frac{x}{2}\sqrt{b^2 - x^2} + \frac{b^2}{2}\sin^{-1}\left(\frac{x}{b}\right)\right]\Big|_0^b = \frac{b^2}{\pi}\sin^{-1}(1) = \frac{b^2}{\pi}\frac{\pi}{2} = \frac{b^2}{2} = \boxed{\frac{E}{k}.}$$

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\langle x^2 \rangle} = \frac{b}{\sqrt{2}} = \boxed{\sqrt{\frac{E}{k}}.}$$

Problem 1.12

(a)

$$\rho(p)\, dp = \frac{dt}{T} = \frac{|dt/dp|\, dp}{T}$$

where dt is now the time it spends with momentum in the range dp (dt is intrinsically positive, but $dp/dt = F = -kx$ runs negative—hence the absolute value). Now

$$\frac{p^2}{2m} + \frac{1}{2}kx^2 = E \Rightarrow x = \pm\sqrt{\frac{2}{k}\left(E - \frac{p^2}{2m}\right)},$$

so

$$\rho(p) = \frac{1}{\pi\sqrt{\frac{m}{k}}\, k\sqrt{\frac{2}{k}\left(E - \frac{p^2}{2m}\right)}} = \boxed{\frac{1}{\pi\sqrt{2mE - p^2}}} = \frac{1}{\pi\sqrt{c^2 - p^2}},$$

where $c \equiv \sqrt{2mE}$. This is the same as $\rho(x)$ (Problem 1.11(b)), with c in place of b (and, of course, p in place of x).

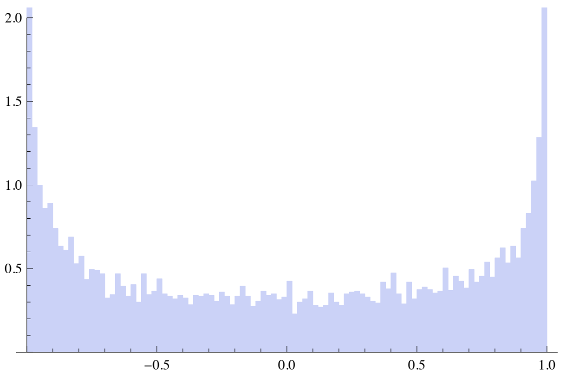
(b) From Problem 1.11(c), $\boxed{\langle p \rangle = 0,\ \langle p^2 \rangle = \frac{c^2}{2},\ \sigma_p = \frac{c}{\sqrt{2}} = \sqrt{mE}\,.}$

(c) $\sigma_x \sigma_p = \sqrt{\frac{E}{k}}\sqrt{mE} = \boxed{\sqrt{\frac{m}{k}}\,E} = \frac{E}{\omega}$. If $E \geq \frac{1}{2}\hbar\omega$, then $\sigma_x\sigma_p \geq \frac{1}{2}\hbar$, which is precisely the Heisenberg uncertainty principle!

Problem 1.13

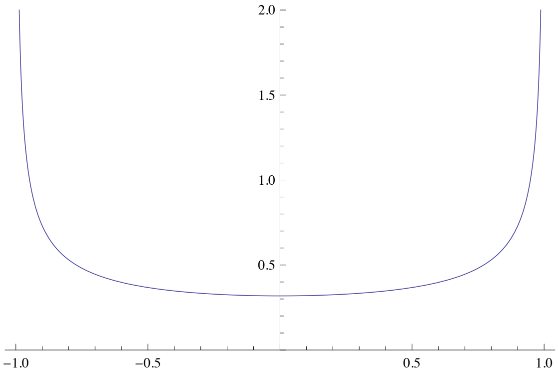
```
x[t_] := Cos[t]
snapshots = Table[x[π RandomReal[j]], {j, 10 000}]
```

```
Histogram[snapshots, 100, "PDF", PlotRange → {0, 2}]
```

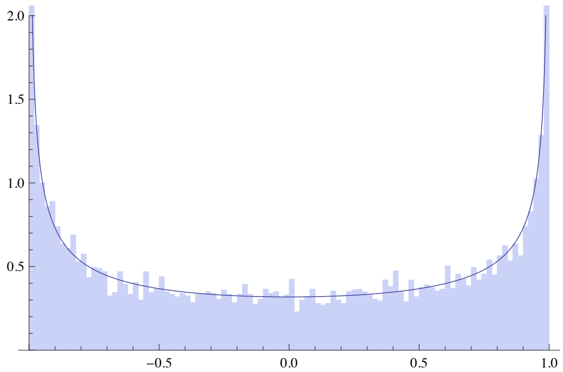


```
r[x_] := 1/(π Sqrt[1 - x^2])

Plot[ r[x], {x, -1, 1}, PlotRange -> {0, 2}]
```




```
Show[Histogram[snapshots, 100, "PDF", PlotRange → {0, 2}],
 Plot[ r[x], {x, -1, 1}, PlotRange -> {0, 2}]]
```



Problem 1.14

(a) $P_{ab}(t) = \int_a^b |\Psi(x,t)|^2 dx$, so $\frac{dP_{ab}}{dt} = \int_a^b \frac{\partial}{\partial t}|\Psi|^2 dx$. But (Eq. 1.25):

$$\frac{\partial|\Psi|^2}{\partial t} = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right] = -\frac{\partial}{\partial x}J(x,t).$$

$$\therefore \frac{dP_{ab}}{dt} = -\int_a^b \frac{\partial}{\partial x}J(x,t)dx = -\left[J(x,t)\right]\Big|_a^b = J(a,t) - J(b,t). \qquad \text{QED}$$

Probability is dimensionless, so J has the dimensions 1/time, and units $\boxed{\text{seconds}^{-1}.}$

(b) Here $\Psi(x,t) = f(x)e^{-iat}$, where $f(x) \equiv Ae^{-amx^2/\hbar}$, so $\Psi\frac{\partial\Psi^*}{\partial x} = fe^{-iat}\frac{df}{dx}e^{iat} = f\frac{df}{dx}$, and $\Psi^*\frac{\partial\Psi}{\partial x} = f\frac{df}{dx}$ too, so $\boxed{J(x,t) = 0.}$

Problem 1.15

Use Eqs. [1.23] and [1.24], and integration by parts:

$$
\begin{aligned}
\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2\,dx &= \int_{-\infty}^{\infty}\frac{\partial}{\partial t}\left(\Psi_1^*\Psi_2\right)dx = \int_{-\infty}^{\infty}\left(\frac{\partial\Psi_1^*}{\partial t}\Psi_2 + \Psi_1^*\frac{\partial\Psi_2}{\partial t}\right)dx \\
&= \int_{-\infty}^{\infty}\left[\left(\frac{-i\hbar}{2m}\frac{\partial^2\Psi_1^*}{\partial x^2} + \frac{i}{\hbar}V\Psi_1^*\right)\Psi_2 + \Psi_1^*\left(\frac{i\hbar}{2m}\frac{\partial^2\Psi_2}{\partial x^2} - \frac{i}{\hbar}V\Psi_2\right)\right]dx \\
&= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left(\frac{\partial^2\Psi_1^*}{\partial x^2}\Psi_2 - \Psi_1^*\frac{\partial^2\Psi_2}{\partial x^2}\right)dx \\
&= -\frac{i\hbar}{2m}\left[\frac{\partial\Psi_1^*}{\partial x}\Psi_2\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{\partial\Psi_1^*}{\partial x}\frac{\partial\Psi_2}{\partial x}dx - \Psi_1^*\frac{\partial\Psi_2}{\partial x}\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\frac{\partial\Psi_1^*}{\partial x}\frac{\partial\Psi_2}{\partial x}dx\right] = 0.\ \text{QED}
\end{aligned}
$$

Problem 1.16

(a)

$$
\begin{aligned}
1 &= |A|^2\int_{-a}^{a}\left(a^2-x^2\right)^2dx = 2|A|^2\int_{0}^{a}\left(a^4-2a^2x^2+x^4\right)dx = 2|A|^2\left[a^4x - 2a^2\frac{x^3}{3}+\frac{x^5}{5}\right]\Big|_0^a \\
&= 2|A|^2a^5\left(1-\frac{2}{3}+\frac{1}{5}\right) = \frac{16}{15}a^5|A|^2,\ \text{so}\ \boxed{A=\sqrt{\frac{15}{16a^5}}.}
\end{aligned}
$$

(b)

$$
\langle x\rangle = \int_{-a}^{a}x|\Psi|^2\,dx = \boxed{0.}\quad \text{(Odd integrand.)}
$$

(c)

$$
\langle p\rangle = \frac{\hbar}{i}A^2\int_{-a}^{a}\left(a^2-x^2\right)\underbrace{\frac{d}{dx}\left(a^2-x^2\right)}_{-2x}dx = \boxed{0.}\quad \text{(Odd integrand.)}
$$

Since we only know $\langle x\rangle$ at $t=0$ we cannot calculate $d\langle x\rangle/dt$ directly.

(d)

$$
\begin{aligned}
\langle x^2\rangle &= A^2\int_{-a}^{a}x^2\left(a^2-x^2\right)^2dx = 2A^2\int_{0}^{a}\left(a^4x^2-2a^2x^4+x^6\right)dx \\
&= 2\frac{15}{16a^5}\left[a^4\frac{x^3}{3}-2a^2\frac{x^5}{5}+\frac{x^7}{7}\right]\Big|_0^a = \frac{15}{8a^5}\left(a^7\right)\left(\frac{1}{3}-\frac{2}{5}+\frac{1}{7}\right) \\
&= \frac{\cancel{15}a^2}{8}\left(\frac{35-42+15}{\cancel{3}\cdot\cancel{5}\cdot 7}\right) = \frac{a^2}{8}\cdot\frac{8}{7} = \boxed{\frac{a^2}{7}.}
\end{aligned}
$$

(e)

$$\langle p^2\rangle = -A^2\hbar^2\int_{-a}^{a}\left(a^2-x^2\right)\underbrace{\frac{d^2}{dx^2}\left(a^2-x^2\right)}_{-2}dx = 2A^2\hbar^2 2\int_0^a\left(a^2-x^2\right)dx$$

$$= 4\cdot\frac{15}{16a^5}\hbar^2\left(a^2x-\frac{x^3}{3}\right)\Big|_0^a = \frac{15\hbar^2}{4a^5}\left(a^3-\frac{a^3}{3}\right) = \frac{15\hbar^2}{4a^2}\cdot\frac{2}{3} = \boxed{\frac{5}{2}\frac{\hbar^2}{a^2}.}$$

(f)

$$\sigma_x = \sqrt{\langle x^2\rangle-\langle x\rangle^2} = \sqrt{\frac{1}{7}a^2} = \boxed{\frac{a}{\sqrt{7}}.}$$

(g)

$$\sigma_p = \sqrt{\langle p^2\rangle-\langle p\rangle^2} = \sqrt{\frac{5}{2}\frac{\hbar^2}{a^2}} = \boxed{\sqrt{\frac{5}{2}}\frac{\hbar}{a}.}$$

(h)

$$\sigma_x\sigma_p = \frac{a}{\sqrt{7}}\cdot\sqrt{\frac{5}{2}}\frac{\hbar}{a} = \sqrt{\frac{5}{14}}\hbar = \sqrt{\frac{10}{7}}\frac{\hbar}{2} > \frac{\hbar}{2}.\ \checkmark$$

Problem 1.17

(a) Eq. 1.24 now reads $\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V^*\Psi^*$, and Eq. 1.25 picks up an extra term:

$$\frac{\partial}{\partial t}|\Psi|^2 = \cdots + \frac{i}{\hbar}|\Psi|^2(V^*-V) = \cdots + \frac{i}{\hbar}|\Psi|^2(V_0+i\Gamma-V_0+i\Gamma) = \cdots - \frac{2\Gamma}{\hbar}|\Psi|^2,$$

and Eq. 1.27 becomes $\frac{dP}{dt} = -\frac{2\Gamma}{\hbar}\int_{-\infty}^{\infty}|\Psi|^2dx = -\frac{2\Gamma}{\hbar}P.$ QED

(b)

$$\frac{dP}{P} = -\frac{2\Gamma}{\hbar}dt \Longrightarrow \ln P = -\frac{2\Gamma}{\hbar}t + \text{constant} \Longrightarrow \boxed{P(t) = P(0)e^{-2\Gamma t/\hbar},}\ \text{so}\ \boxed{\tau = \frac{\hbar}{2\Gamma}.}$$

Problem 1.18

$$\frac{h}{\sqrt{3mk_BT}} > d \ \Rightarrow\ T < \frac{h^2}{3mk_Bd^2}.$$

(a) Electrons ($m = 9.1\times10^{-31}$ kg):

$$T < \frac{(6.6\times10^{-34})^2}{3(9.1\times10^{-31})(1.4\times10^{-23})(3\times10^{-10})^2} = \boxed{1.3\times10^5\ \text{K.}}$$

Silicon nuclei ($m = 28m_p = 28(1.7\times10^{-27}) = 4.8\times10^{-26}$ kg):

$$T < \frac{(6.6\times10^{-34})^2}{3(4.8\times10^{-26})(1.4\times10^{-23})(3\times10^{-10})^2} = \boxed{2.4\ \text{K.}}$$

(b) $PV = Nk_BT$; volume occupied by one molecule ($N = 1,\ V = d^3$) $\Rightarrow d = (k_BT/P)^{1/3}$.

$$T < \frac{h^2}{3mk_B}\left(\frac{P}{k_BT}\right)^{2/3} \quad \Rightarrow\ T^{5/3} < \frac{h^2}{3m}\frac{P^{2/3}}{k_B^{5/3}} \ \Rightarrow T < \frac{1}{k_B}\left(\frac{h^2}{3m}\right)^{3/5} P^{2/5}.$$

For helium ($m = 4m_p = 6.8 \times 10^{-27}$ kg) at 1 atm $= 1.0 \times 10^5$ N/m^2:

$$T < \frac{1}{(1.4 \times 10^{-23})}\left(\frac{(6.6 \times 10^{-34})^2}{3(6.8 \times 10^{-27})}\right)^{3/5} (1.0 \times 10^5)^{2/5} = \boxed{2.8 \text{ K.}}$$

For atomic hydrogen ($m = m_p = 1.7 \times 10^{-27}$ kg) with $d = 0.01$ m:

$$T < \frac{(6.6 \times 10^{-34})^2}{3(1.7 \times 10^{-27})(1.4 \times 10^{-23})(10^{-2})^2} = \boxed{6.2 \times 10^{-14} \text{ K.}}$$

At 3 K it is definitely in the classical regime.

Chapter 2

The Time-Independent Schrödinger Equation

Problem 2.1

(a)

$$\Psi(x,t) = \psi(x)e^{-i(E_0+i\Gamma)t/\hbar} = \psi(x)e^{\Gamma t/\hbar}e^{-iE_0 t/\hbar} \Longrightarrow |\Psi|^2 = |\psi|^2 e^{2\Gamma t/\hbar}.$$

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = e^{2\Gamma t/\hbar}\int_{-\infty}^{\infty} |\psi|^2 dx.$$

The second term is independent of t, so if the product is to be 1 for all time, the first term ($e^{2\Gamma t/\hbar}$) must also be constant, and hence $\Gamma = 0$. QED

(b) If ψ satisfies Eq. 2.5, $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$, then (taking the complex conjugate and noting that V and E are real): $-\frac{\hbar^2}{2m}\frac{d^2\psi^*}{dx^2} + V\psi^* = E\psi^*$, so ψ^* *also* satisfies Eq. 2.5. Now, if ψ_1 and ψ_2 satisfy Eq. 2.5, so too does any linear combination of them ($\psi_3 \equiv c_1\psi_1 + c_2\psi_2$):

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2\psi_3}{dx^2} + V\psi_3 &= -\frac{\hbar^2}{2m}\left(c_1\frac{d^2\psi_1}{dx^2} + c_2\frac{d^2\psi_2}{dx^2}\right) + V(c_1\psi_1 + c_2\psi_2) \\ &= c_1\left[-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + V\psi_1\right] + c_2\left[-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2\right] \\ &= c_1(E\psi_1) + c_2(E\psi_2) = E(c_1\psi_1 + c_2\psi_2) = E\psi_3. \end{aligned}$$

Thus, $(\psi + \psi^*)$ and $i(\psi - \psi^*)$ – both of which are *real* – satisfy Eq. 2.5. *Conclusion:* From any complex solution, we can always construct two *real* solutions (of course, if ψ is already real, the second one will be zero). In particular, since $\psi = \frac{1}{2}[(\psi + \psi^*) - i(i(\psi - \psi^*))]$, ψ can be expressed as a linear combination of two real solutions. QED

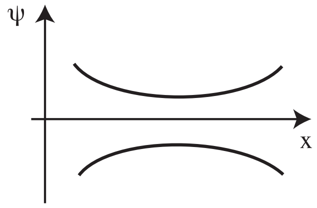
(c) If $\psi(x)$ satisfies Eq. 2.5, then, changing variables $x \to -x$ and noting that $d^2/d(-x)^2 = d^2/dx^2$,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + V(-x)\psi(-x) = E\psi(-x);$$

so if $V(-x) = V(x)$ then $\psi(-x)$ *also* satisfies Eq. 2.5. It follows that $\psi_+(x) \equiv \psi(x) + \psi(-x)$ (which is *even*: $\psi_+(-x) = \psi_+(x)$) and $\psi_-(x) \equiv \psi(x) - \psi(-x)$ (which is *odd*: $\psi_-(-x) = -\psi_-(x)$) both satisfy Eq. 2.5. But $\psi(x) = \frac{1}{2}(\psi_+(x) + \psi_-(x))$, so any solution can be expressed as a linear combination of even and odd solutions. QED

Problem 2.2

Given $\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[V(x) - E]\psi$, if $E < V_{\min}$, then ψ'' and ψ always have the same sign: If ψ is positive(negative), then ψ'' is also positive(negative). This means that ψ always curves away from the axis (see Figure). However, it has got to go to zero as $x \to -\infty$ (else it would not be normalizable). At some point it's got to *depart* from zero (if it *doesn't*, it's going to be identically zero *everywhere*), in (say) the positive direction. At this point its slope is positive, and *increasing*, so ψ gets bigger and bigger as x increases. It can't ever "turn over" and head back toward the axis, because that would require a negative second derivative—it always has to bend away from the axis. By the same token, if it starts out heading negative, it just runs more and more negative. In neither case is there any way for it to come back to zero, as it must (at $x \to \infty$) in order to be normalizable. QED



Problem 2.3

Equation 2.23 says $\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$; Eq. 2.26 says $\psi(0) = \psi(a) = 0$. If $E = 0$, $d^2\psi/dx^2 = 0$, so $\psi(x) = A + Bx$; $\psi(0) = A = 0 \Rightarrow \psi = Bx$; $\psi(a) = Ba = 0 \Rightarrow B = 0$, so $\psi = 0$. If $E < 0$, $d^2\psi/dx^2 = \kappa^2\psi$, with $\kappa \equiv \sqrt{-2mE}/\hbar$ real, so $\psi(x) = Ae^{\kappa x} + Be^{-\kappa x}$. This time $\psi(0) = A + B = 0 \Rightarrow B = -A$, so $\psi = A(e^{\kappa x} - e^{-\kappa x})$, while $\psi(a) = A\left(e^{\kappa a} - e^{-\kappa a}\right) = 0 \Rightarrow$ either $A = 0$, so $\psi = 0$, or else $e^{\kappa a} = e^{-\kappa a}$, so $e^{2\kappa a} = 1$, so $2\kappa a = \ln(1) = 0$, so $\kappa = 0$, and again $\psi = 0$. In all cases, then, the boundary conditions force $\psi = 0$, which is unacceptable (non-normalizable).

Problem 2.4

$$\begin{aligned}
\langle x \rangle &= \int x|\psi|^2 dx = \frac{2}{a}\int_0^a x\sin^2\left(\frac{n\pi}{a}x\right)dx. \qquad \text{Let } y \equiv \frac{n\pi}{a}x, \text{ so } dx = \frac{a}{n\pi}dy; \quad y: 0 \to n\pi. \\
&= \frac{2}{a}\left(\frac{a}{n\pi}\right)^2\int_0^{n\pi} y\sin^2 y\,dy = \frac{2a}{n^2\pi^2}\left[\frac{y^2}{4} - \frac{y\sin 2y}{4} - \frac{\cos 2y}{8}\right]\Bigg|_0^{n\pi} \\
&= \frac{2a}{n^2\pi^2}\left[\frac{n^2\pi^2}{4} - \frac{\cos 2n\pi}{8} + \frac{1}{8}\right] = \boxed{\frac{a}{2}.} \quad \text{(Independent of } n.\text{)}
\end{aligned}$$

$$\begin{aligned}
\langle x^2 \rangle &= \frac{2}{a}\int_0^a x^2\sin^2\left(\frac{n\pi}{a}x\right)dx = \frac{2}{a}\left(\frac{a}{n\pi}\right)^3\int_0^{n\pi} y^2\sin^2 y\,dy \\
&= \frac{2a^2}{(n\pi)^3}\left[\frac{y^3}{6} - \left(\frac{y^2}{4} - \frac{1}{8}\right)\sin 2y - \frac{y\cos 2y}{4}\right]_0^{n\pi} \\
&= \frac{2a^2}{(n\pi)^3}\left[\frac{(n\pi)^3}{6} - \frac{n\pi\cos(2n\pi)}{4}\right] = \boxed{a^2\left[\frac{1}{3} - \frac{1}{2(n\pi)^2}\right].}
\end{aligned}$$

$$\langle p \rangle = m\frac{d\langle x \rangle}{dt} = \boxed{0.} \quad (\textit{Note}: \text{Eq. 1.33 is much faster than Eq. 1.35.})$$

$$\langle p^2 \rangle = \int \psi_n^* \left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi_n\, dx = -\hbar^2 \int \psi_n^* \left(\frac{d^2\psi_n}{dx^2}\right) dx$$

$$= (-\hbar^2)\left(-\frac{2mE_n}{\hbar^2}\right)\int \psi_n^*\psi_n\, dx = 2mE_n = \boxed{\left(\frac{n\pi\hbar}{a}\right)^2.}$$

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = a^2\left(\frac{1}{3} - \frac{1}{2(n\pi)^2} - \frac{1}{4}\right) = \frac{a^2}{4}\left(\frac{1}{3} - \frac{2}{(n\pi)^2}\right); \quad \boxed{\sigma_x = \frac{a}{2}\sqrt{\frac{1}{3} - \frac{2}{(n\pi)^2}}.}$$

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 = \left(\frac{n\pi\hbar}{a}\right)^2; \quad \boxed{\sigma_p = \frac{n\pi\hbar}{a}.} \quad \therefore \sigma_x\sigma_p = \boxed{\frac{\hbar}{2}\sqrt{\frac{(n\pi)^2}{3} - 2}.}$$

The product $\sigma_x\sigma_p$ is $\boxed{\text{smallest for } n = 1;}$ in that case, $\sigma_x\sigma_p = \frac{\hbar}{2}\sqrt{\frac{\pi^2}{3} - 2} = (1.136)\hbar/2 > \hbar/2.$ ✓

Problem 2.5

(a)

$$|\Psi|^2 = \Psi^*\Psi = |A|^2(\psi_1^* + \psi_2^*)(\psi_1 + \psi_2) = |A|^2[\psi_1^*\psi_1 + \psi_1^*\psi_2 + \psi_2^*\psi_1 + \psi_2^*\psi_2].$$

$$1 = \int |\Psi|^2 dx = |A|^2 \int [|\psi_1|^2 + \psi_1^*\psi_2 + \psi_2^*\psi_1 + |\psi_2|^2] dx = 2|A|^2 \Rightarrow \boxed{A = 1/\sqrt{2}.}$$

(b)

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1 e^{-iE_1t/\hbar} + \psi_2 e^{-iE_2t/\hbar}\right] \quad \left(\text{but } \frac{E_n}{\hbar} = n^2\omega\right)$$

$$= \frac{1}{\sqrt{2}}\sqrt{\frac{2}{a}}\left[\sin\left(\frac{\pi}{a}x\right)e^{-i\omega t} + \sin\left(\frac{2\pi}{a}x\right)e^{-i4\omega t}\right] = \boxed{\frac{1}{\sqrt{a}}e^{-i\omega t}\left[\sin\left(\frac{\pi}{a}x\right) + \sin\left(\frac{2\pi}{a}x\right)e^{-3i\omega t}\right].}$$

$$|\Psi(x,t)|^2 = \frac{1}{a}\left[\sin^2\left(\frac{\pi}{a}x\right) + \sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}x\right)\left(e^{-3i\omega t} + e^{3i\omega t}\right) + \sin^2\left(\frac{2\pi}{a}x\right)\right]$$

$$= \boxed{\frac{1}{a}\left[\sin^2\left(\frac{\pi}{a}x\right) + \sin^2\left(\frac{2\pi}{a}x\right) + 2\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}x\right)\cos(3\omega t)\right].}$$

(c)

$$\langle x \rangle = \int x|\Psi(x,t)|^2 dx$$

$$= \frac{1}{a}\int_0^a x\left[\sin^2\left(\frac{\pi}{a}x\right) + \sin^2\left(\frac{2\pi}{a}x\right) + 2\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}x\right)\cos(3\omega t)\right] dx$$

$$\int_0^a x\sin^2\left(\frac{\pi}{a}x\right)dx = \left[\frac{x^2}{4} - \frac{x\sin\left(\frac{2\pi}{a}x\right)}{4\pi/a} - \frac{\cos\left(\frac{2\pi}{a}x\right)}{8(\pi/a)^2}\right]\Bigg|_0^a = \frac{a^2}{4} = \int_0^a x\sin^2\left(\frac{2\pi}{a}x\right)dx.$$

$$\int_0^a x\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}x\right)dx = \frac{1}{2}\int_0^a x\left[\cos\left(\frac{\pi}{a}x\right) - \cos\left(\frac{3\pi}{a}x\right)\right]dx$$

$$= \frac{1}{2}\left[\frac{a^2}{\pi^2}\cos\left(\frac{\pi}{a}x\right) + \frac{ax}{\pi}\sin\left(\frac{\pi}{a}x\right) - \frac{a^2}{9\pi^2}\cos\left(\frac{3\pi}{a}x\right) - \frac{ax}{3\pi}\sin\left(\frac{3\pi}{a}x\right)\right]_0^a$$

$$= \frac{1}{2}\left[\frac{a^2}{\pi^2}\big(\cos(\pi)-\cos(0)\big) - \frac{a^2}{9\pi^2}\big(\cos(3\pi)-\cos(0)\big)\right] = -\frac{a^2}{\pi^2}\left(1-\frac{1}{9}\right) = -\frac{8a^2}{9\pi^2}.$$

$$\therefore \langle x\rangle = \frac{1}{a}\left[\frac{a^2}{4} + \frac{a^2}{4} - \frac{16a^2}{9\pi^2}\cos(3\omega t)\right] = \boxed{\frac{a}{2}\left[1 - \frac{32}{9\pi^2}\cos(3\omega t)\right].}$$

Amplitude: $\boxed{\frac{32}{9\pi^2}\left(\frac{a}{2}\right) = 0.3603(a/2);}$ *angular frequency:* $\boxed{3\omega = \frac{3\pi^2\hbar}{2ma^2}.}$

(d)

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = m\left(\frac{a}{2}\right)\left(-\frac{32}{9\pi^2}\right)(-3\omega)\sin(3\omega t) = \boxed{\frac{8\hbar}{3a}\sin(3\omega t).}$$

(e) You could get either $\boxed{E_1 = \pi^2\hbar^2/2ma^2}$ or $\boxed{E_2 = 2\pi^2\hbar^2/ma^2,}$ with equal probability $\boxed{P_1 = P_2 = 1/2.}$

So $\langle H\rangle = \boxed{\frac{1}{2}(E_1+E_2) = \frac{5\pi^2\hbar^2}{4ma^2};}$ it's the *average* of E_1 and E_2.

Problem 2.6

From Problem 2.5, we see that

$$\Psi(x,t) = \boxed{\tfrac{1}{\sqrt{a}}e^{-i\omega t}\left[\sin\left(\tfrac{\pi}{a}x\right) + \sin\left(\tfrac{2\pi}{a}x\right)e^{-3i\omega t}e^{i\phi}\right];}$$

$$|\Psi(x,t)|^2 = \boxed{\tfrac{1}{a}\left[\sin^2\left(\tfrac{\pi}{a}x\right) + \sin^2\left(\tfrac{2\pi}{a}x\right) + 2\sin\left(\tfrac{\pi}{a}x\right)\sin\left(\tfrac{2\pi}{a}x\right)\cos(3\omega t-\phi)\right];}$$

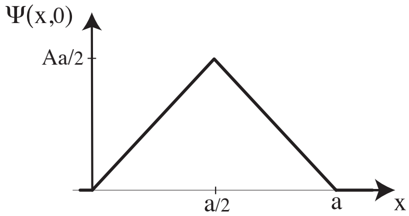
and hence $\boxed{\langle x\rangle = \frac{a}{2}\left[1 - \frac{32}{9\pi^2}\cos(3\omega t-\phi)\right].}$ This amounts physically to starting the clock at a different time (i.e., shifting the $t=0$ point).

If $\phi = \dfrac{\pi}{2}$, so $\Psi(x,0) = A[\psi_1(x) + i\psi_2(x)]$, then $\cos(3\omega t-\phi) = \sin(3\omega t)$; $\langle x\rangle$ starts at $\dfrac{a}{2}$.

If $\phi = \pi$, so $\Psi(x,0) = A[\psi_1(x) - \psi_2(x)]$, then $\cos(3\omega t-\phi) = -\cos(3\omega t)$; $\langle x\rangle$ starts at $\dfrac{a}{2}\left(1+\dfrac{32}{9\pi^2}\right)$.

Problem 2.7

(a)



$$1 = A^2\int_0^{a/2} x^2 dx + A^2\int_{a/2}^{a}(a-x)^2 dx = A^2\left[\left.\frac{x^3}{3}\right|_0^{a/2} - \left.\frac{(a-x)^3}{3}\right|_{a/2}^{a}\right]$$

$$= \frac{A^2}{3}\left(\frac{a^3}{8}+\frac{a^3}{8}\right) = \frac{A^2a^3}{12} \Rightarrow \boxed{A = \frac{2\sqrt{3}}{\sqrt{a^3}}.}$$

(b)

$$c_n = \sqrt{\frac{2}{a}}\frac{2\sqrt{3}}{a\sqrt{a}}\left[\int_0^{a/2} x\sin\left(\frac{n\pi}{a}x\right)dx + \int_{a/2}^{a}(a-x)\sin\left(\frac{n\pi}{a}x\right)dx\right]$$

$$= \frac{2\sqrt{6}}{a^2}\left\{\left[\left(\frac{a}{n\pi}\right)^2\sin\left(\frac{n\pi}{a}x\right) - \frac{xa}{n\pi}\cos\left(\frac{n\pi}{a}x\right)\right]\Bigg|_0^{a/2}\right.$$

$$\left. + a\left[-\frac{a}{n\pi}\cos\left(\frac{n\pi}{a}x\right)\right]\Bigg|_{a/2}^{a} - \left[\left(\frac{a}{n\pi}\right)^2\sin\left(\frac{n\pi}{a}x\right) - \left(\frac{ax}{n\pi}\right)\cos\left(\frac{n\pi}{a}x\right)\right]\Bigg|_{a/2}^{a}\right\}$$

$$= \frac{2\sqrt{6}}{a^2}\left[\left(\frac{a}{n\pi}\right)^2\sin\left(\frac{n\pi}{2}\right) - \cancel{\frac{a^2}{2n\pi}\cos\left(\frac{n\pi}{2}\right)} - \cancel{\frac{a^2}{n\pi}\cos n\pi} + \cancel{\frac{a^2}{n\pi}\cos\left(\frac{n\pi}{2}\right)}\right.$$

$$\left. + \left(\frac{a}{n\pi}\right)^2\sin\left(\frac{n\pi}{2}\right) + \cancel{\frac{a^2}{n\pi}\cos n\pi} - \cancel{\frac{a^2}{2n\pi}\cos\left(\frac{n\pi}{2}\right)}\right]$$

$$= \frac{2\sqrt{6}}{\cancel{a^2}}2\frac{\cancel{a^2}}{(n\pi)^2}\sin\left(\frac{n\pi}{2}\right) = \frac{4\sqrt{6}}{(n\pi)^2}\sin\left(\frac{n\pi}{2}\right) = \begin{cases} 0, & n \text{ even,} \\ (-1)^{(n-1)/2}\frac{4\sqrt{6}}{(n\pi)^2}, & n \text{ odd.}\end{cases}$$

So $\boxed{\Psi(x,t) = \frac{4\sqrt{6}}{\pi^2}\sqrt{\frac{2}{a}}\sum_{n=1,3,5,\dots}(-1)^{(n-1)/2}\frac{1}{n^2}\sin\left(\frac{n\pi}{a}x\right)e^{-iE_nt/\hbar},}$ where $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$.

(c)

$$P_1 = |c_1|^2 = \frac{16\cdot 6}{\pi^4} = \boxed{0.9855.}$$

(d)

$$\langle H\rangle = \sum |c_n|^2 E_n = \frac{96}{\pi^4}\frac{\pi^2\hbar^2}{2ma^2}\Bigg(\underbrace{\frac{1}{1}+\frac{1}{3^2}+\frac{1}{5^2}+\frac{1}{7^2}+\cdots}_{\pi^2/8}\Bigg) = \frac{48\hbar^2}{\pi^2 ma^2}\frac{\pi^2}{8} = \boxed{\frac{6\hbar^2}{ma^2}.}$$

Problem 2.8

$$A^2 \int_0^{a/2} dx = A^2(a/2) = 1 \Rightarrow A = \sqrt{\frac{2}{a}}.$$

From Eq. 2.37,

$$c_1 = A\sqrt{\frac{2}{a}} \int_0^{a/2} \sin\left(\frac{\pi}{a}x\right) dx = \frac{2}{a}\left[-\frac{a}{\pi}\cos\left(\frac{\pi}{a}x\right)\right]\Big|_0^{a/2} = -\frac{2}{\pi}\left[\cos\left(\frac{\pi}{2}\right) - \cos 0\right] = \frac{2}{\pi}.$$

$$P_1 = |c_1|^2 = \boxed{(2/\pi)^2 = 0.4053.}$$

Problem 2.9

$$\hat{H}\Psi(x,0) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[Ax(a-x)\right] = -A\frac{\hbar^2}{2m}\frac{\partial}{\partial x}(a-2x) = A\frac{\hbar^2}{m}.$$

$$\begin{aligned}\int \Psi(x,0)^* \hat{H}\Psi(x,0)\,dx &= A^2\frac{\hbar^2}{m}\int_0^a x(a-x)\,dx = A^2\frac{\hbar^2}{m}\left(a\frac{x^2}{2} - \frac{x^3}{3}\right)\Big|_0^a \\ &= A^2\frac{\hbar^2}{m}\left(\frac{a^3}{2} - \frac{a^3}{3}\right) = \frac{30}{a^5}\frac{\hbar^2}{m}\frac{a^3}{6} = \boxed{\frac{5\hbar^2}{ma^2}}\end{aligned}$$

(same as Example 2.3).

Problem 2.10

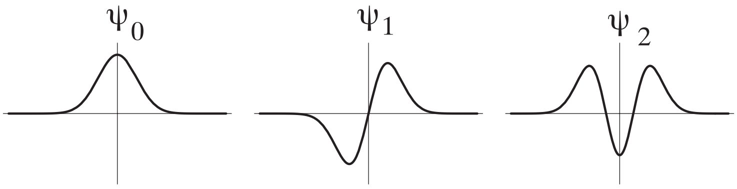
(a) Using Eqs. 2.48 and 2.60,

$$\begin{aligned}a_+\psi_0 &= \frac{1}{\sqrt{2\hbar m\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \\ &= \frac{1}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[-\hbar\left(-\frac{m\omega}{2\hbar}\right)2x + m\omega x\right] e^{-\frac{m\omega}{2\hbar}x^2} = \frac{1}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} 2m\omega x e^{-\frac{m\omega}{2\hbar}x^2}. \\ (a_+)^2\psi_0 &= \frac{1}{2\hbar m\omega}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} 2m\omega\left(-\hbar\frac{d}{dx} + m\omega x\right) x e^{-\frac{m\omega}{2\hbar}x^2} \\ &= \frac{1}{\hbar}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[-\hbar\left(1 - x\frac{m\omega}{2\hbar}2x\right) + m\omega x^2\right] e^{-\frac{m\omega}{2\hbar}x^2} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(\frac{2m\omega}{\hbar}x^2 - 1\right) e^{-\frac{m\omega}{2\hbar}x^2}.\end{aligned}$$

Therefore, from Eq. 2.68,

$$\psi_2 = \frac{1}{\sqrt{2}}(a_+)^2\psi_0 = \boxed{\frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(\frac{2m\omega}{\hbar}x^2 - 1\right) e^{-\frac{m\omega}{2\hbar}x^2}.}$$

(b)



(c) Since ψ_0 and ψ_2 are even, whereas ψ_1 is odd, $\int \psi_0^* \psi_1 dx$ and $\int \psi_2^* \psi_1 dx$ vanish automatically. The only one we need to check is $\int \psi_2^* \psi_0 \, dx$:

$$\begin{aligned}
\int \psi_2^* \psi_0 \, dx &= \frac{1}{\sqrt{2}} \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} \left(\frac{2m\omega}{\hbar} x^2 - 1 \right) e^{-\frac{m\omega}{\hbar} x^2} dx \\
&= -\sqrt{\frac{m\omega}{2\pi\hbar}} \left(\int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar} x^2} dx - \frac{2m\omega}{\hbar} \int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar} x^2} dx \right) \\
&= -\sqrt{\frac{m\omega}{2\pi\hbar}} \left(\sqrt{\frac{\pi\hbar}{m\omega}} - \frac{2m\omega}{\hbar} \frac{\hbar}{2m\omega} \sqrt{\frac{\pi\hbar}{m\omega}} \right) = 0. \checkmark
\end{aligned}$$

Problem 2.11

(a) Note that ψ_0 is even, and ψ_1 is odd. In either case $|\psi|^2$ is even, so $\langle x \rangle = \int x |\psi|^2 dx = \boxed{0.}$ Therefore $\langle p \rangle = m d\langle x \rangle / dt = \boxed{0.}$ (These results hold for *any* stationary state of the harmonic oscillator.)

From Eqs. 2.60 and 2.63, $\psi_0 = \alpha e^{-\xi^2/2}$, $\psi_1 = \sqrt{2} \alpha \xi e^{-\xi^2/2}$. So

<u>$n = 0$</u>**:**

$$\langle x^2 \rangle = \alpha^2 \int_{-\infty}^{\infty} x^2 e^{-\xi^2} dx = \alpha^2 \left(\frac{\hbar}{m\omega} \right)^{3/2} \int_{-\infty}^{\infty} \xi^2 e^{-\xi^2} d\xi = \frac{1}{\sqrt{\pi}} \left(\frac{\hbar}{m\omega} \right) \frac{\sqrt{\pi}}{2} = \boxed{\frac{\hbar}{2m\omega}}.$$

$$\begin{aligned}
\langle p^2 \rangle &= \int \psi_0 \left(\frac{\hbar}{i} \frac{d}{dx} \right)^2 \psi_0 \, dx = -\hbar^2 \alpha^2 \sqrt{\frac{m\omega}{\hbar}} \int_{-\infty}^{\infty} e^{-\xi^2/2} \left(\frac{d^2}{d\xi^2} e^{-\xi^2/2} \right) d\xi \\
&= -\frac{m\hbar\omega}{\sqrt{\pi}} \int_{-\infty}^{\infty} (\xi^2 - 1) e^{-\xi^2} d\xi = -\frac{m\hbar\omega}{\sqrt{\pi}} \left(\frac{\sqrt{\pi}}{2} - \sqrt{\pi} \right) = \boxed{\frac{m\hbar\omega}{2}}.
\end{aligned}$$

<u>$n = 1$</u>**:**

$$\langle x^2 \rangle = 2\alpha^2 \int_{-\infty}^{\infty} x^2 \xi^2 e^{-\xi^2} dx = 2\alpha^2 \left(\frac{\hbar}{m\omega} \right)^{3/2} \int_{-\infty}^{\infty} \xi^4 e^{-\xi^2} d\xi = \frac{2\hbar}{\sqrt{\pi} m\omega} \frac{3\sqrt{\pi}}{4} = \boxed{\frac{3\hbar}{2m\omega}}.$$

$$\begin{aligned}
\langle p^2 \rangle &= -\hbar^2 2\alpha^2 \sqrt{\frac{m\omega}{\hbar}} \int_{-\infty}^{\infty} \xi e^{-\xi^2/2} \left[\frac{d^2}{d\xi^2} (\xi e^{-\xi^2/2}) \right] d\xi \\
&= -\frac{2m\omega\hbar}{\sqrt{\pi}} \int_{-\infty}^{\infty} (\xi^4 - 3\xi^2) e^{-\xi^2} d\xi = -\frac{2m\omega\hbar}{\sqrt{\pi}} \left(\frac{3}{4}\sqrt{\pi} - 3\frac{\sqrt{\pi}}{2} \right) = \boxed{\frac{3m\hbar\omega}{2}}.
\end{aligned}$$

(b) $\underline{n=0}$**:**

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{\hbar}{2m\omega}};\ \sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\frac{m\hbar\omega}{2}};$$

$$\sigma_x\sigma_p = \sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{m\omega\hbar}{2}} = \frac{\hbar}{2}. \quad \text{(Right } \textit{at} \text{ the uncertainty limit.)}\checkmark$$

$\underline{n=1}$**:**

$$\sigma_x = \sqrt{\frac{3\hbar}{2m\omega}};\quad \sigma_p = \sqrt{\frac{3m\hbar\omega}{2}};\quad \sigma_x\sigma_p = 3\frac{\hbar}{2} > \frac{\hbar}{2}.\ \checkmark$$

(c)

$$\langle T\rangle = \frac{1}{2m}\langle p^2\rangle = \boxed{\left\{\begin{array}{l}\frac{1}{4}\hbar\omega\ \ (n=0)\\ \\ \frac{3}{4}\hbar\omega\ \ (n=1)\end{array}\right\}};\quad \langle V\rangle = \frac{1}{2}m\omega^2\langle x^2\rangle = \boxed{\left\{\begin{array}{l}\frac{1}{4}\hbar\omega\ \ (n=0)\\ \\ \frac{3}{4}\hbar\omega\ \ (n=1)\end{array}\right\}}.$$

$$\langle T\rangle + \langle V\rangle = \langle H\rangle = \left\{\begin{array}{l}\frac{1}{2}\hbar\omega\ \ (n=0)\ = E_0\\ \\ \frac{3}{2}\hbar\omega\ \ (n=1)\ = E_1\end{array}\right\}, \text{ as expected.}$$

Problem 2.12

From Eq. 2.70,

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-),\quad p = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-),$$

so

$$\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\int \psi_n^*(a_+ + a_-)\psi_n\,dx.$$

But (Eq. 2.67)

$$a_+\psi_n = \sqrt{n+1}\psi_{n+1},\quad a_-\psi_n = \sqrt{n}\psi_{n-1}.$$

So

$$\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\int \psi_n^*\psi_{n+1}\,dx + \sqrt{n}\int \psi_n^*\psi_{n-1}\,dx\right] = \boxed{0} \text{ (by orthogonality).}$$

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = \boxed{0.}\quad x^2 = \frac{\hbar}{2m\omega}(a_+ + a_-)^2 = \frac{\hbar}{2m\omega}\left(a_+^2 + a_+a_- + a_-a_+ + a_-^2\right).$$

$$\langle x^2\rangle = \frac{\hbar}{2m\omega}\int \psi_n^*\left(a_+^2 + a_+a_- + a_-a_+ + a_-^2\right)\psi_n. \quad \text{But}$$

$$\left\{\begin{array}{llll}
a_+^2\psi_n & = a_+\left(\sqrt{n+1}\psi_{n+1}\right) & = \sqrt{n+1}\sqrt{n+2}\psi_{n+2} & = \sqrt{(n+1)(n+2)}\psi_{n+2}.\\
a_+a_-\psi_n & = a_+\left(\sqrt{n}\psi_{n-1}\right) & = \sqrt{n}\sqrt{n}\psi_n & = n\psi_n.\\
a_-a_+\psi_n & = a_-\left(\sqrt{n+1}\psi_{n+1}\right) & = \sqrt{n+1)}\sqrt{n+1}\psi_n & = (n+1)\psi_n.\\
a_-^2\psi_n & = a_-\left(\sqrt{n}\psi_{n-1}\right) & = \sqrt{n}\sqrt{n-1}\psi_{n-2} & = \sqrt{(n-1)n}\psi_{n-2}.
\end{array}\right.$$

So

$$\langle x^2\rangle = \frac{\hbar}{2m\omega}\left[0 + n\int|\psi_n|^2dx + (n+1)\int|\psi_n|^2\,dx + 0\right] = \frac{\hbar}{2m\omega}(2n+1) = \boxed{\left(n+\frac{1}{2}\right)\frac{\hbar}{m\omega}.}$$

$$p^2 = -\frac{\hbar m\omega}{2}(a_+ - a_-)^2 = -\frac{\hbar m\omega}{2}\left(a_+^2 - a_+a_- - a_-a_+ + a_-^2\right) \Rightarrow$$

$$\langle p^2\rangle = -\frac{\hbar m\omega}{2}\left[0 - n - (n+1) + 0\right] = \frac{\hbar m\omega}{2}(2n+1) = \boxed{\left(n+\frac{1}{2}\right)m\hbar\omega.}$$

$$\langle T\rangle = \langle p^2/2m\rangle = \boxed{\frac{1}{2}\left(n+\frac{1}{2}\right)\hbar\omega}.$$

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{n+\frac{1}{2}}\sqrt{\frac{\hbar}{m\omega}}; \quad \sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{n+\frac{1}{2}}\sqrt{m\hbar\omega}; \quad \sigma_x\sigma_p = \left(n+\frac{1}{2}\right)\hbar \geq \frac{\hbar}{2}. \checkmark$$

Problem 2.13

(a)

$$1 = \int |\Psi(x,0)|^2 dx = |A|^2 \int \left(9|\psi_0|^2 + 12\psi_0^*\psi_1 + 12\psi_1^*\psi_0 + 16|\psi_1|^2\right) dx$$
$$= |A|^2(9+0+0+16) = 25|A|^2 \Rightarrow \boxed{A = 1/5.}$$

(b)

$$\Psi(x,t) = \frac{1}{5}\left[3\psi_0(x)e^{-iE_0t/\hbar} + 4\psi_1(x)e^{-iE_1t/\hbar}\right] = \boxed{\frac{1}{5}\left[3\psi_0(x)e^{-i\omega t/2} + 4\psi_1(x)e^{-3i\omega t/2}\right]}.$$

(Here ψ_0 and ψ_1 are given by Eqs. 2.60 and 2.63; E_0 and E_1 by Eq. 2.62.)

$$|\Psi(x,t)|^2 = \frac{1}{25}\left[9\psi_0^2 + 12\psi_0\psi_1 e^{i\omega t/2}e^{-3i\omega t/2} + 12\psi_0\psi_1 e^{-i\omega t/2}e^{3i\omega t/2} + 16\psi_1^2\right]$$
$$= \boxed{\frac{1}{25}\left[9\psi_0^2 + 16\psi_1^2 + 24\psi_0\psi_1\cos(\omega t)\right].}$$

(With ψ_2 in place of ψ_1 the frequency would be $(E_2 - E_0)/\hbar = [(5/2)\hbar\omega - (1/2)\hbar\omega]/\hbar = 2\omega$.)

(c)

$$\langle x\rangle = \frac{1}{25}\left[9\int x\psi_0^2\,dx + 16\int x\psi_1^2\,dx + 24\cos(\omega t)\int x\psi_0\psi_1\,dx\right].$$

But $\int x\psi_0^2\,dx = \int x\psi_1^2\,dx = 0$ (see Problem 2.11 or 2.12), while

$$\int x\psi_0\psi_1\,dx = \sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{2m\omega}{\hbar}}\int xe^{-\frac{m\omega}{2\hbar}x^2}xe^{-\frac{m\omega}{2\hbar}x^2}dx = \sqrt{\frac{2}{\pi}}\left(\frac{m\omega}{\hbar}\right)\int_{-\infty}^{\infty}x^2e^{-\frac{m\omega}{\hbar}x^2}dx$$
$$= \sqrt{\frac{2}{\pi}}\left(\frac{m\omega}{\hbar}\right)2\sqrt{\pi}2\left(\frac{1}{2}\sqrt{\frac{\hbar}{m\omega}}\right)^3 = \sqrt{\frac{\hbar}{2m\omega}}.$$

So

$$\langle x\rangle = \boxed{\frac{24}{25}\sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t);} \quad \langle p\rangle = m\frac{d}{dt}\langle x\rangle = \boxed{-\frac{24}{25}\sqrt{\frac{m\omega\hbar}{2}}\sin(\omega t).}$$

Ehrenfest's theorem says $d\langle p\rangle/dt = -\langle \partial V/\partial x\rangle$. Here

$$\frac{d\langle p\rangle}{dt} = -\frac{24}{25}\sqrt{\frac{m\omega\hbar}{2}}\omega\cos(\omega t), \quad V = \frac{1}{2}m\omega^2x^2 \Rightarrow \frac{\partial V}{\partial x} = m\omega^2 x,$$

so

$$-\langle\frac{\partial V}{\partial x}\rangle = -m\omega^2\langle x\rangle = -m\omega^2\frac{24}{25}\sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t) = -\frac{24}{25}\sqrt{\frac{\hbar m\omega}{2}}\omega\cos(\omega t),$$

so Ehrenfest's theorem holds.

(d) You could get $\boxed{E_0 = \frac{1}{2}\hbar\omega,}$ with probability $|c_0|^2 = \boxed{9/25,}$ or $\boxed{E_1 = \frac{3}{2}\hbar\omega,}$ with probability $|c_1|^2 = \boxed{16/25.}$

Problem 2.14

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}, \text{ so } P = 2\sqrt{\frac{m\omega}{\pi\hbar}}\int_{x_0}^{\infty} e^{-\xi^2}dx = 2\sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{\hbar}{m\omega}}\int_{\xi_0}^{\infty} e^{-\xi^2}d\xi.$$

Classically allowed region extends out to: $\frac{1}{2}m\omega^2x_0^2 = E_0 = \frac{1}{2}\hbar\omega$, or $x_0 = \sqrt{\frac{\hbar}{m\omega}}$, so $\xi_0 = 1$.

$$P = \frac{2}{\sqrt{\pi}}\int_1^{\infty} e^{-\xi^2}d\xi = 2(1-F(\sqrt{2})) \text{ (in notation of CRC Table)} = \boxed{0.157.}$$

Problem 2.15

<u>$n=5$:</u> $j=1 \Rightarrow a_3 = \frac{-2(5-1)}{(1+1)(1+2)}a_1 = -\frac{4}{3}a_1$; $j=3 \Rightarrow a_5 = \frac{-2(5-3)}{(3+1)(3+2)}a_3 = -\frac{1}{5}a_3 = \frac{4}{15}a_1$; $j=5 \Rightarrow a_7 = 0$. So $H_5(\xi) = a_1\xi - \frac{4}{3}a_1\xi^3 + \frac{4}{15}a_1\xi^5 = \frac{a_1}{15}(15\xi - 20\xi^3 + 4\xi^5)$. By convention the coefficient of ξ^5 is 2^5, so $a_1 = 15\cdot 8$, and $\boxed{H_5(\xi) = 120\xi - 160\xi^3 + 32\xi^5}$ (which agrees with Table 2.1).

<u>$n=6$:</u> $j=0 \Rightarrow a_2 = \frac{-2(6-0)}{(0+1)(0+2)}a_0 = -6a_0$; $j=2 \Rightarrow a_4 = \frac{-2(6-2)}{(2+1)(2+2)}a_2 = -\frac{2}{3}a_2 = 4a_0$; $j=4 \Rightarrow a_6 = \frac{-2(6-4)}{(4+1)(4+2)}a_4 = -\frac{2}{15}a_4 = -\frac{8}{15}a_0$; $j=6 \Rightarrow a_8 = 0$. So $H_6(\xi) = a_0 - 6a_0\xi^2 + 4a_0\xi^4 - \frac{8}{15}\xi^6 a_0$. The coefficient of ξ^6 is 2^6, so $2^6 = -\frac{8}{15}a_0 \Rightarrow a_0 = -15\cdot 8 = -120$. $\boxed{H_6(\xi) = -120 + 720\xi^2 - 480\xi^4 + 64\xi^6.}$

Problem 2.16

(a)

$$\frac{d}{d\xi}(e^{-\xi^2}) = -2\xi e^{-\xi^2}; \quad \left(\frac{d}{d\xi}\right)^2 e^{-\xi^2} = \frac{d}{d\xi}(-2\xi e^{-\xi^2}) = (-2+4\xi^2)e^{-\xi^2};$$

$$\left(\frac{d}{d\xi}\right)^3 e^{-\xi^2} = \frac{d}{d\xi}\left[(-2+4\xi^2)e^{-\xi^2}\right] = \left[8\xi + (-2+4\xi^2)(-2\xi)\right]e^{-\xi^2} = (12\xi - 8\xi^3)e^{-\xi^2};$$

$$\left(\frac{d}{d\xi}\right)^4 e^{-\xi^2} = \frac{d}{d\xi}\left[(12\xi - 8\xi^3)e^{-\xi^2}\right] = \left[12 - 24\xi^2 + (12\xi - 8\xi^3)(-2\xi)\right]e^{-\xi^2} = (12 - 48\xi^2 + 16\xi^4)e^{-\xi^2}.$$

$$H_3(\xi) = -e^{\xi^2}\left(\frac{d}{d\xi}\right)^3 e^{-\xi^2} = \boxed{-12\xi + 8\xi^3;}\; H_4(\xi) = e^{\xi^2}\left(\frac{d}{d\xi}\right)^4 e^{-\xi^2} = \boxed{12 - 48\xi^2 + 16\xi^4.}$$

(b)

$$H_5 = 2\xi H_4 - 8H_3 = 2\xi(12 - 48\xi^2 + 16\xi^4) - 8(-12\xi + 8\xi^3) = \boxed{120\xi - 160\xi^3 + 32\xi^5.}$$

$$H_6 = 2\xi H_5 - 10H_4 = 2\xi(120\xi - 160\xi^3 + 32\xi^5) - 10(12 - 48\xi^2 + 16\xi^4) = \boxed{-120 + 720\xi^2 - 480\xi^4 + 64\xi^6.}$$

(c)

$$\frac{dH_5}{d\xi} = 120 - 480\xi^2 + 160\xi^4 = 10(12 - 48\xi^2 + 16\xi^4) = (2)(5)H_4. \checkmark$$

$$\frac{dH_6}{d\xi} = 1440\xi - 1920\xi^3 + 384\xi^5 = 12(120\xi - 160\xi^3 + 32\xi^5) = (2)(6)H_5. \checkmark$$

(d)

$$\frac{d}{dz}(e^{-z^2+2z\xi}) = (-2z + 2\xi)e^{-z^2+2z\xi}; \text{ setting } z = 0, \ \boxed{H_1(\xi) = 2\xi.}$$

$$\begin{aligned}\left(\frac{d}{dz}\right)^2 (e^{-z^2+2z\xi}) &= \frac{d}{dz}\left[(-2z + 2\xi)e^{-z^2+2z\xi}\right] \\ &= \left[-2 + (-2z + 2\xi)^2\right]e^{-z^2+2z\xi}; \text{ setting } z = 0, \ \boxed{H_2(\xi) = -2 + 4\xi^2.}\end{aligned}$$

$$\begin{aligned}\left(\frac{d}{dz}\right)^3 (e^{-z^2+2z\xi}) &= \frac{d}{dz}\left\{\left[-2 + (-2z + 2\xi)^2\right]e^{-z^2+2z\xi}\right\} \\ &= \left\{2(-2z + 2\xi)(-2) + \left[-2 + (-2z + 2\xi)^2\right](-2z + 2\xi)\right\}e^{-z^2+2z\xi};\end{aligned}$$

$$\text{setting } z = 0, \ H_3(\xi) = -8\xi + (-2 + 4\xi^2)(2\xi) = \boxed{-12\xi + 8\xi^3.}$$

Problem 2.17

$$\begin{aligned}Ae^{ikx} + Be^{-ikx} &= A(\cos kx + i\sin kx) + B(\cos kx - i\sin kx) = (A + B)\cos kx + i(A - B)\sin kx \\ &= C\cos kx + D\sin kx, \text{ with } \boxed{C = A + B; \ D = i(A - B).}\end{aligned}$$

$$\begin{aligned}C\cos kx + D\sin kx &= C\left(\frac{e^{ikx} + e^{-ikx}}{2}\right) + D\left(\frac{e^{ikx} - e^{-ikx}}{2i}\right) = \frac{1}{2}(C - iD)e^{ikx} + \frac{1}{2}(C + iD)e^{-ikx} \\ &= Ae^{ikx} + Be^{-ikx}, \text{ with } \boxed{A = \frac{1}{2}(C - iD); \ B = \frac{1}{2}(C + iD).}\end{aligned}$$

Problem 2.18

Equation 2.95 says $\Psi = Ae^{i(kx-\frac{\hbar k^2}{2m}t)}$, so

$$\begin{aligned}J &= \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right) = \frac{i\hbar}{2m}|A|^2\left[e^{i(kx-\frac{\hbar k^2}{2m}t)}(-ik)e^{-i(kx-\frac{\hbar k^2}{2m}t)} - e^{-i(kx-\frac{\hbar k^2}{2m}t)}(ik)e^{i(kx-\frac{\hbar k^2}{2m}t)}\right]\\ &= \frac{i\hbar}{2m}|A|^2(-2ik) = \boxed{\frac{\hbar k}{m}|A|^2.}\end{aligned}$$

It flows in the positive (x) direction (as you would expect).

Problem 2.19

(a)

$$\begin{aligned}f(x) &= b_0 + \sum_{n=1}^{\infty}\frac{a_n}{2i}\left(e^{in\pi x/a} - e^{-in\pi x/a}\right) + \sum_{n=1}^{\infty}\frac{b_n}{2}\left(e^{in\pi x/a} + e^{-in\pi x/a}\right)\\ &= b_0 + \sum_{n=1}^{\infty}\left(\frac{a_n}{2i} + \frac{b_n}{2}\right)e^{in\pi x/a} + \sum_{n=1}^{\infty}\left(-\frac{a_n}{2i} + \frac{b_n}{2}\right)e^{-in\pi x/a}.\end{aligned}$$

Let

$$\boxed{c_0 \equiv b_0;\ c_n = \tfrac{1}{2}\left(-ia_n + b_n\right),\ \text{for } n = 1,2,3,\dots;\ c_n \equiv \tfrac{1}{2}\left(ia_{-n} + b_{-n}\right),\ \text{for } n = -1,-2,-3,\dots.}$$

Then $f(x) = \sum\limits_{n=-\infty}^{\infty} c_n e^{in\pi x/a}$. QED

(b)

$$\int_{-a}^{a} f(x)e^{-im\pi x/a}dx = \sum_{n=-\infty}^{\infty} c_n\int_{-a}^{a} e^{i(n-m)\pi x/a}dx. \quad \text{But for } n \neq m,$$

$$\int_{-a}^{a} e^{i(n-m)\pi x/a}dx = \left.\frac{e^{i(n-m)\pi x/a}}{i(n-m)\pi/a}\right|_{-a}^{a} = \frac{e^{i(n-m)\pi} - e^{-i(n-m)\pi}}{i(n-m)\pi/a} = \frac{(-1)^{n-m} - (-1)^{n-m}}{i(n-m)\pi/a} = 0,$$

whereas for $n = m$,

$$\int_{-a}^{a} e^{i(n-m)\pi x/a}dx = \int_{-a}^{a} dx = 2a.$$

So all terms except $n = m$ are zero, and

$$\int_{-a}^{a} f(x)e^{-im\pi x/a} = 2ac_m, \text{ so } c_n = \frac{1}{2a}\int_{-a}^{a} f(x)e^{-in\pi x/a}dx. \quad \text{QED}$$

(c)

$$f(x) = \sum_{n=-\infty}^{\infty}\sqrt{\frac{\pi}{2}}\frac{1}{a}F(k)e^{ikx} = \frac{1}{\sqrt{2\pi}}\sum F(k)e^{ikx}\Delta k,$$

where $\boxed{\Delta k \equiv \frac{\pi}{a}}$ is the increment in k from n to $(n+1)$.

$$F(k) = \sqrt{\frac{2}{\pi}} a \frac{1}{2a} \int_{-a}^{a} f(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} f(x) e^{-ikx} dx.$$

(d) As $a \to \infty$, k becomes a continuous variable,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk; \; F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx.$$

Problem 2.20

(a)

$$1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 2|A|^2 \int_0^{\infty} e^{-2ax} dx = 2|A|^2 \left. \frac{e^{-2ax}}{-2a} \right|_0^{\infty} = \frac{|A|^2}{a} \Rightarrow A = \boxed{\sqrt{a}.}$$

(b)

$$\phi(k) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-a|x|} e^{-ikx}\, dx = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-a|x|} (\cos kx - i \sin kx) dx.$$

The cosine integrand is even, and the sine is odd, so the latter vanishes and

$$\begin{aligned}
\phi(k) &= 2\frac{A}{\sqrt{2\pi}} \int_0^{\infty} e^{-ax} \cos kx\, dx = \frac{A}{\sqrt{2\pi}} \int_0^{\infty} e^{-ax} \left(e^{ikx} + e^{-ikx} \right) dx \\
&= \frac{A}{\sqrt{2\pi}} \int_0^{\infty} \left(e^{(ik-a)x} + e^{-(ik+a)x} \right) dx = \frac{A}{\sqrt{2\pi}} \left[\frac{e^{(ik-a)x}}{ik-a} + \frac{e^{-(ik+a)x}}{-(ik+a)} \right] \Bigg|_0^{\infty} \\
&= \frac{A}{\sqrt{2\pi}} \left(\frac{-1}{ik-a} + \frac{1}{ik+a} \right) = \frac{A}{\sqrt{2\pi}} \frac{-ik-a+ik-a}{-k^2-a^2} = \boxed{\sqrt{\frac{a}{2\pi}} \frac{2a}{k^2+a^2}.}
\end{aligned}$$

(c)

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} 2 \sqrt{\frac{a^3}{2\pi}} \int_{-\infty}^{\infty} \frac{1}{k^2+a^2} e^{i(kx - \frac{\hbar k^2}{2m} t)} dk = \boxed{\frac{a^{3/2}}{\pi} \int_{-\infty}^{\infty} \frac{1}{k^2+a^2} e^{i(kx - \frac{\hbar k^2}{2m} t)} dk.}$$

(d) For *large* a, $\Psi(x,0)$ is a sharp narrow spike whereas $\phi(k) \cong \sqrt{2/\pi a}$ is broad and flat; position is well-defined but momentum is ill-defined. For *small* a, $\Psi(x,0)$ is a broad and flat whereas $\phi(k) \cong (\sqrt{2a^3/\pi})/k^2$ is a sharp narrow spike; position is ill-defined but momentum is well-defined.

Problem 2.21

(a)

$$1 = |A|^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = |A|^2 \sqrt{\frac{\pi}{2a}}; \quad \boxed{A = \left(\frac{2a}{\pi}\right)^{1/4}.}$$

(b)

$$\int_{-\infty}^{\infty} e^{-(ax^2+bx)} dx = \int_{-\infty}^{\infty} e^{-y^2+(b^2/4a)} \frac{1}{\sqrt{a}}\, dy = \frac{1}{\sqrt{a}} e^{b^2/4a} \int_{-\infty}^{\infty} e^{-y^2} dy = \sqrt{\frac{\pi}{a}} e^{b^2/4a}.$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} A \int_{-\infty}^{\infty} e^{-ax^2} e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{1/4} \sqrt{\frac{\pi}{a}} e^{-k^2/4a} = \frac{1}{(2\pi a)^{1/4}} e^{-k^2/4a}.$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a)^{1/4}} \int_{-\infty}^{\infty} \underbrace{e^{-k^2/4a} e^{i(kx - \hbar k^2 t/2m)}}_{e^{-[(\frac{1}{4a} + i\hbar t/2m)k^2 - ixk]}} dk$$

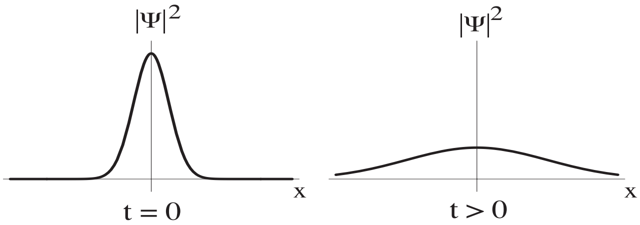
$$= \frac{1}{\sqrt{2\pi}(2\pi a)^{1/4}} \frac{\sqrt{\pi}}{\sqrt{\frac{1}{4a} + i\hbar t/2m}} e^{-x^2/4(\frac{1}{4a} + i\hbar t/2m)} = \boxed{\left(\frac{2a}{\pi}\right)^{1/4} \frac{e^{-ax^2/(1+2i\hbar at/m)}}{\sqrt{1 + 2i\hbar at/m}}.}$$

(c)

Let $\theta \equiv 2\hbar at/m$. Then $|\Psi|^2 = \sqrt{\frac{2a}{\pi}} \dfrac{e^{-ax^2/(1+i\theta)} e^{-ax^2/(1-i\theta)}}{\sqrt{(1+i\theta)(1-i\theta)}}$. The exponent is

$$-\frac{ax^2}{(1+i\theta)} - \frac{ax^2}{(1-i\theta)} = -ax^2 \frac{(1 - i\theta + 1 + i\theta)}{(1+i\theta)(1-i\theta)} = \frac{-2ax^2}{1+\theta^2}; \ |\Psi|^2 = \sqrt{\frac{2a}{\pi}} \frac{e^{-2ax^2/(1+\theta^2)}}{\sqrt{1+\theta^2}}.$$

Or, with $w \equiv \sqrt{\dfrac{a}{1+\theta^2}}$, $\boxed{|\Psi|^2 = \sqrt{\frac{2}{\pi}} w e^{-2w^2x^2}.}$ As t increases, the graph of $|\Psi|^2$ flattens out and broadens.



(d)

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi|^2 dx = \boxed{0} \text{ (odd integrand)}; \ \langle p \rangle = m\frac{d\langle x \rangle}{dt} = \boxed{0.}$$

$$\langle x^2 \rangle = \sqrt{\frac{2}{\pi}} w \int_{-\infty}^{\infty} x^2 e^{-2w^2x^2} dx = \sqrt{\frac{2}{\pi}} w \frac{1}{4w^2} \sqrt{\frac{\pi}{2w^2}} = \boxed{\frac{1}{4w^2}.} \ \langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx.$$

Write $\Psi = Be^{-bx^2}$, where $B \equiv \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{1+i\theta}}$ and $b \equiv \frac{a}{1+i\theta}$.

$$\frac{\partial^2\Psi}{\partial x^2} = B\frac{\partial}{\partial x}\left(-2bxe^{-bx^2}\right) = -2bB(1-2bx^2)e^{-bx^2}.$$

$$\Psi^*\frac{\partial^2\Psi}{d\partial x^2} = -2b|B|^2(1-2bx^2)e^{-(b+b^*)x^2};\ b+b^* = \frac{a}{1+i\theta} + \frac{a}{1-i\theta} = \frac{2a}{1+\theta^2} = 2w^2.$$

$$|B|^2 = \sqrt{\frac{2a}{\pi}}\frac{1}{\sqrt{1+\theta^2}} = \sqrt{\frac{2}{\pi}}w. \quad \text{So } \Psi^*\frac{\partial^2\Psi}{\partial x^2} = -2b\sqrt{\frac{2}{\pi}}w(1-2bx^2)e^{-2w^2x^2}.$$

$$\begin{aligned}\langle p^2\rangle &= 2b\hbar^2\sqrt{\frac{2}{\pi}}w\int_{-\infty}^{\infty}(1-2bx^2)e^{-2w^2x^2}\,dx \\ &= 2b\hbar^2\sqrt{\frac{2}{\pi}}w\left(\sqrt{\frac{\pi}{2w^2}} - 2b\frac{1}{4w^2}\sqrt{\frac{\pi}{2w^2}}\right) = 2b\hbar^2\left(1-\frac{b}{2w^2}\right).\end{aligned}$$

But $1-\frac{b}{2w^2} = 1-\left(\frac{a}{1+i\theta}\right)\left(\frac{1+\theta^2}{2a}\right) = 1-\frac{(1-i\theta)}{2} = \frac{1+i\theta}{2} = \frac{a}{2b}$, so

$$\langle p^2\rangle = 2b\hbar^2\frac{a}{2b} = \boxed{\hbar^2 a.} \qquad \boxed{\sigma_x = \frac{1}{2w};} \qquad \boxed{\sigma_p = \hbar\sqrt{a}.}$$

(e)

$$\sigma_x\sigma_p = \frac{1}{2w}\hbar\sqrt{a} = \frac{\hbar}{2}\sqrt{1+\theta^2} = \frac{\hbar}{2}\sqrt{1+(2\hbar at/m)^2} \geq \frac{\hbar}{2}. \checkmark$$

Closest at $\boxed{t=0,}$ at which time it is right *at* the uncertainty limit.

Problem 2.22

(a)

$$(-2)^3 - 3(-2)^2 + 2(-2) - 1 = -8 - 12 - 4 - 1 = \boxed{-25.}$$

(b)

$$\cos(3\pi) + 2 = -1 + 2 = \boxed{1.}$$

(c)

$\boxed{0}$ ($x = 2$ is outside the domain of integration).

Problem 2.23

(a) Let $y \equiv cx$, so $dx = \frac{1}{c}dy$. $\left\{\begin{array}{l}\text{If } c > 0,\ y : -\infty \to \infty. \\ \text{If } c < 0,\ y : \infty \to -\infty.\end{array}\right\}$

$$\int_{-\infty}^{\infty} f(x)\delta(cx)dx = \begin{cases} \frac{1}{c}\int_{-\infty}^{\infty} f(y/c)\delta(y)dy = \frac{1}{c}f(0) \quad (c>0);\ \text{or} \\ \\ \frac{1}{c}\int_{\infty}^{-\infty} f(y/c)\delta(y)dy = -\frac{1}{c}\int_{-\infty}^{\infty} f(y/c)\delta(y)dy = -\frac{1}{c}f(0)\ (c<0). \end{cases}$$

In either case, $\displaystyle\int_{-\infty}^{\infty} f(x)\delta(cx)dx = \frac{1}{|c|}f(0) = \int_{-\infty}^{\infty} f(x)\frac{1}{|c|}\delta(x)dx$. So $\delta(cx) = \frac{1}{|c|}\delta(x)$. ✓

(b)

$$\int_{-\infty}^{\infty} f(x)\frac{d\theta}{dx}dx = f\theta\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{df}{dx}\theta dx \quad \text{(integration by parts)}$$

$$= f(\infty) - \int_0^{\infty}\frac{df}{dx}dx = f(\infty) - f(\infty) + f(0) = f(0) = \int_{-\infty}^{\infty} f(x)\delta(x)dx.$$

So $d\theta/dx = \delta(x)$. ✓ [Makes sense: The θ function is constant (so derivative is zero) except at $x = 0$, where the derivative is infinite.]

Problem 2.24

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x|/\hbar^2} = \frac{\sqrt{m\alpha}}{\hbar}\begin{cases} e^{-m\alpha x/\hbar^2}, & (x \ge 0), \\ e^{m\alpha x/\hbar^2}, & (x \le 0). \end{cases}$$

$$\langle x\rangle = 0 \text{ (odd integrand).}$$

$$\langle x^2\rangle = \int_{-\infty}^{\infty} x^2|\psi|^2 dx = 2\frac{m\alpha}{\hbar^2}\int_0^{\infty} x^2 e^{-2m\alpha x/\hbar^2}dx = \frac{2m\alpha}{\hbar^2}2\left(\frac{\hbar^2}{2m\alpha}\right)^3 = \frac{\hbar^4}{2m^2\alpha^2}; \quad \sigma_x = \frac{\hbar^2}{\sqrt{2}m\alpha}.$$

$$\frac{d\psi}{dx} = \frac{\sqrt{m\alpha}}{\hbar}\left\{\begin{array}{ll} -\frac{m\alpha}{\hbar^2}e^{-m\alpha x/\hbar^2}, & (x \ge 0) \\ \\ \frac{m\alpha}{\hbar^2}e^{m\alpha x/\hbar^2}, & (x \le 0) \end{array}\right\} = \left(\frac{\sqrt{m\alpha}}{\hbar}\right)^3\left[-\theta(x)e^{-m\alpha x/\hbar^2} + \theta(-x)e^{m\alpha x/\hbar^2}\right].$$

$$\frac{d^2\psi}{dx^2} = \left(\frac{\sqrt{m\alpha}}{\hbar}\right)^3\left[-\delta(x)e^{-m\alpha x/\hbar^2} + \frac{m\alpha}{\hbar^2}\theta(x)e^{-m\alpha x/\hbar^2} - \delta(-x)e^{m\alpha x/\hbar^2} + \frac{m\alpha}{\hbar^2}\theta(-x)e^{m\alpha x/\hbar^2}\right]$$

$$= \left(\frac{\sqrt{m\alpha}}{\hbar}\right)^3\left[-2\delta(x) + \frac{m\alpha}{\hbar^2}e^{-m\alpha|x|/\hbar^2}\right].$$

In the last step I used the fact that $\delta(-x) = \delta(x)$ (Eq. 2.145), $f(x)\delta(x) = f(0)\delta(x)$ (Eq. 2.115), and $\theta(-x) + \theta(x) = 1$ (Eq. 2.146). Since $d\psi/dx$ is an odd function, $\langle p\rangle = 0$.

$$\langle p^2\rangle = -\hbar^2\int_{-\infty}^{\infty}\psi\frac{d^2\psi}{dx^2}dx = -\hbar^2\frac{\sqrt{m\alpha}}{\hbar}\left(\frac{\sqrt{m\alpha}}{\hbar}\right)^3\int_{-\infty}^{\infty} e^{-m\alpha|x|/\hbar^2}\left[-2\delta(x) + \frac{m\alpha}{\hbar^2}e^{-m\alpha|x|/\hbar^2}\right]dx$$

$$= \left(\frac{m\alpha}{\hbar}\right)^2\left[2 - 2\frac{m\alpha}{\hbar^2}\int_0^{\infty} e^{-2m\alpha x/\hbar^2}dx\right] = 2\left(\frac{m\alpha}{\hbar}\right)^2\left[1 - \frac{m\alpha}{\hbar^2}\frac{\hbar^2}{2m\alpha}\right] = \left(\frac{m\alpha}{\hbar}\right)^2.$$

Evidently

$$\sigma_p = \frac{m\alpha}{\hbar}, \quad \text{so} \quad \sigma_x\sigma_p = \frac{\hbar^2}{\sqrt{2}m\alpha}\frac{m\alpha}{\hbar} = \sqrt{2}\frac{\hbar}{2} > \frac{\hbar}{2}. \ ✓$$

Problem 2.25

$\langle\psi_{\text{bound}}|\psi_{\text{scattering}}\rangle$

$$= \frac{\sqrt{m\alpha}}{\hbar}\left[\int_{-\infty}^{0} e^{m\alpha x/\hbar^2}\left(Ae^{ikx}+Be^{-ikx}\right)dx + \int_{0}^{\infty} e^{-m\alpha x/\hbar^2}\left(Fe^{ikx}+Ge^{-ikx}\right)dx\right]$$
$$= \frac{\sqrt{m\alpha}}{\hbar}\left[A\int_{-\infty}^{0} e^{\left(\frac{m\alpha}{\hbar^2}+ik\right)x}dx + B\int_{-\infty}^{0} e^{\left(\frac{m\alpha}{\hbar^2}-ik\right)x}dx + F\int_{0}^{\infty} e^{\left(-\frac{m\alpha}{\hbar^2}+ik\right)x}dx + G\int_{0}^{\infty} e^{\left(-\frac{m\alpha}{\hbar^2}-ik\right)x}dx\right]$$
$$= \frac{\sqrt{m\alpha}}{\hbar}\left[A\left.\frac{e^{\left(\frac{m\alpha}{\hbar^2}+ik\right)x}}{\frac{m\alpha}{\hbar^2}+ik}\right|_{-\infty}^{0} + B\left.\frac{e^{\left(\frac{m\alpha}{\hbar^2}-ik\right)x}}{\frac{m\alpha}{\hbar^2}-ik}\right|_{-\infty}^{0} + F\left.\frac{e^{\left(-\frac{m\alpha}{\hbar^2}+ik\right)x}}{-\frac{m\alpha}{\hbar^2}+ik}\right|_{0}^{\infty} + G\left.\frac{e^{\left(-\frac{m\alpha}{\hbar^2}-ik\right)x}}{-\frac{m\alpha}{\hbar^2}-ik}\right|_{0}^{\infty}\right]$$
$$= \frac{\sqrt{m\alpha}}{\hbar}\left[\frac{A}{\frac{m\alpha}{\hbar^2}+ik} + \frac{B}{\frac{m\alpha}{\hbar^2}-ik} - \frac{F}{-\frac{m\alpha}{\hbar^2}+ik} - \frac{G}{-\frac{m\alpha}{\hbar^2}-ik}\right] = \frac{\sqrt{m\alpha}}{\hbar}\left[\frac{A+G}{\frac{m\alpha}{\hbar^2}+ik} + \frac{B+F}{\frac{m\alpha}{\hbar^2}-ik}\right]$$
$$= \frac{\sqrt{m\alpha}}{\hbar}\left[\frac{\left(\frac{m\alpha}{\hbar^2}-ik\right)(A+G)+\left(\frac{m\alpha}{\hbar^2}+ik\right)(B+F)}{\left(\frac{m\alpha}{\hbar^2}\right)^2+k^2}\right] = \frac{\sqrt{m\alpha}}{\hbar}\left[\frac{\frac{m\alpha}{\hbar^2}(A+G+B+F)+ik(B+F-A-G)}{\left(\frac{m\alpha}{\hbar^2}\right)^2+k^2}\right]$$

But Equation 2.136 says $(A+G+B+F) = 2(A+B)$, and Equation 2.137 says $ik(B+F-A-G) = -(2m\alpha/\hbar^2)(A+B)$, so

$$\langle\psi_{\text{bound}}|\psi_{\text{scattering}} =\rangle \frac{\sqrt{m\alpha}}{\hbar}\left[\frac{\frac{m\alpha}{\hbar^2}2(A+B)-\frac{2m\alpha}{\hbar^2}(A+B)}{\left(\frac{m\alpha}{\hbar^2}\right)^2+k^2}\right] = 0. \quad \checkmark$$

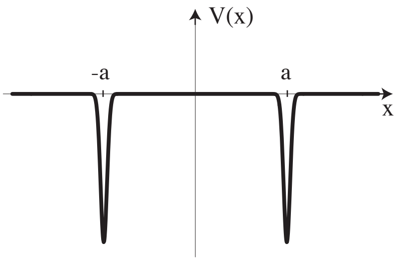
Problem 2.26

Put $f(x)=\delta(x)$ into Eq. 2.103: $F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\delta(x)e^{-ikx}dx = \boxed{\frac{1}{\sqrt{2\pi}}.}$

$\therefore f(x) = \delta(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}e^{ikx}dk = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ikx}dk.$ QED

Problem 2.27

(a)



(b) From Problem 2.1(c) the solutions are even or odd. Look first for *even solutions*:

$$\psi(x) = \begin{cases} Ae^{-\kappa x} & (x>a), \\ B(e^{\kappa x}+e^{-\kappa x}) & (-a<x<a), \\ Ae^{\kappa x} & (x<-a). \end{cases}$$

Continuity at a: $Ae^{-\kappa a} = B(e^{\kappa a}+e^{-\kappa a})$, or $A = B(e^{2\kappa a}+1)$.

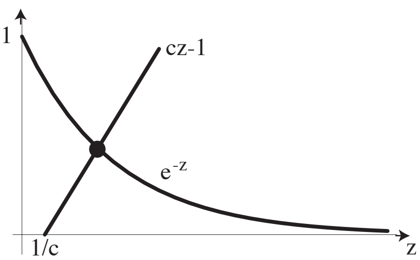
Discontinuous derivative at a, $\Delta\dfrac{d\psi}{dx} = -\dfrac{2m\alpha}{\hbar^2}\psi(a)$:

$$-\kappa A e^{-\kappa a} - B(\kappa e^{\kappa a} - \kappa e^{-\kappa a}) = -\frac{2m\alpha}{\hbar^2}Ae^{-\kappa a} \Rightarrow A + B(e^{2\kappa a} - 1) = \frac{2m\alpha}{\hbar^2\kappa}A; \text{ or}$$

$$B(e^{2\kappa a} - 1) = A\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right) = B(e^{2\kappa a} + 1)\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right) \Rightarrow e^{2\kappa a} - 1 = e^{2\kappa a}\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right) + \frac{2m\alpha}{\hbar^2\kappa} - 1.$$

$$1 = \frac{2m\alpha}{\hbar^2\kappa} - 1 + \frac{2m\alpha}{\hbar^2\kappa}e^{-2\kappa a}; \quad \frac{\hbar^2\kappa}{m\alpha} = 1 + e^{-2\kappa a}, \text{ or } \boxed{e^{-2\kappa a} = \frac{\hbar^2\kappa}{m\alpha} - 1.}$$

This is a transcendental equation for κ (and hence for E). I'll solve it graphically: Let $z \equiv 2\kappa a$, $c \equiv \frac{\hbar^2}{2am\alpha}$, so $e^{-z} = cz - 1$. Plot both sides and look for intersections:



From the graph, noting that c and z are both positive, we see that there is one (and only one) solution (for even ψ). If $\alpha = \frac{\hbar^2}{2ma}$, so $c = 1$, the calculator gives $z = 1.278$, so $\kappa^2 = -\frac{2mE}{\hbar^2} = \frac{z^2}{(2a)^2} \Rightarrow E = -\frac{(1.278)^2}{8}\left(\frac{\hbar^2}{ma^2}\right) = -0.204\left(\frac{\hbar^2}{ma^2}\right)$.

Now look for *odd solutions:*

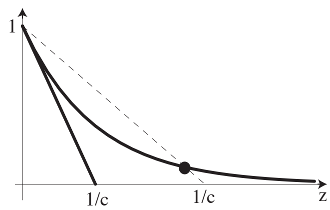
$$\psi(x) = \begin{cases} Ae^{-\kappa x} & (x > a), \\ B(e^{\kappa x} - e^{-\kappa x}) & (-a < x < a), \\ -Ae^{\kappa x} & (x < -a). \end{cases}$$

Continuity at a : $Ae^{-\kappa a} = B(e^{\kappa a} - e^{-\kappa a})$, or $A = B(e^{2\kappa a} - 1)$.

Discontinuity in ψ' : $-\kappa Ae^{-\kappa a} - B(\kappa e^{\kappa a} + \kappa e^{-\kappa a}) = -\dfrac{2m\alpha}{\hbar^2}Ae^{-\kappa a} \Rightarrow B(e^{2\kappa a} + 1) = A\left(\dfrac{2m\alpha}{\hbar^2\kappa} - 1\right)$,

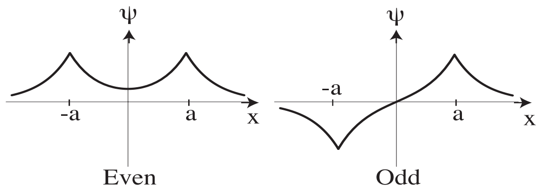
$$e^{2\kappa a} + 1 = (e^{2\kappa a} - 1)\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right) = e^{2\kappa a}\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right) - \frac{2m\alpha}{\hbar^2\kappa} + 1,$$

$$1 = \frac{2m\alpha}{\hbar^2\kappa} - 1 - \frac{2m\alpha}{\hbar^2\kappa}e^{-2\kappa a}; \quad \frac{\hbar^2\kappa}{m\alpha} = 1 - e^{-2\kappa a}, \quad \boxed{e^{-2\kappa a} = 1 - \frac{\hbar^2\kappa}{m\alpha},} \text{ or } e^{-z} = 1 - cz.$$



This time there may or may not be a solution. Both graphs have their y-intercepts at 1, but if c is too large (α too small), there may be no intersection (solid line), whereas if c is smaller (dashed line) there will be. (Note that $z = 0 \Rightarrow \kappa = 0$ is *not* a solution, since ψ is then non-normalizable.) The slope of e^{-z} (at $z = 0$) is -1; the slope of $(1 - cz)$ is $-c$. So there is an *odd* solution $\Leftrightarrow c < 1$, or $\alpha > \hbar^2/2ma$.

Conclusion: $\boxed{\textit{One}\text{ bound state if } \alpha \le \hbar^2/2ma;\ \textit{two}\text{ if } \alpha > \hbar^2/2ma.}$



$$\alpha = \frac{\hbar^2}{ma} \Rightarrow c = \frac{1}{2}. \begin{cases} \textit{Even: } e^{-z} = \frac{1}{2}z - 1 \Rightarrow z = 2.21772, \\ \textit{Odd: } \ e^{-z} = 1 - \frac{1}{2}z \Rightarrow z = 1.59362. \end{cases}$$

$$\boxed{E = -0.615(\hbar^2/ma^2);\ E = -0.317(\hbar^2/ma^2).}$$

$$\alpha = \frac{\hbar^2}{4ma} \Rightarrow c = 2. \ \textit{Only even: } \ e^{-z} = 2z - 1 \Rightarrow z = 0.738835; \ \boxed{E = -0.0682(\hbar^2/ma^2).}$$

(c) (i) There is *one* bound state (even); c is huge, so z is small, so $e^{-z} \approx 1 = cz - 1$, which means $z = 2/c$, or $2\kappa a = 2(2am\alpha/\hbar^2) \Rightarrow \kappa = (2m\alpha/\hbar^2)$.

$$E = -\frac{\hbar^2\kappa^2}{2m} = \boxed{-\frac{2m\alpha^2}{\hbar^2}.}$$

This makes sense: the two delta-functions coincide, so there is really just *one* delta-function, with "strength" 2α. Putting this into Equation 2.130 we recover the answer in the box.

(ii) There are two bound states, one even and one odd; c is small, so z is huge, and $e^{-z} \approx 0$. For the even case, $0 = cz - 1 \Rightarrow z = 1/c \Rightarrow \kappa = (m\alpha/\hbar^2)$. For the odd case, $0 = 1 - cz$, which leads to the same result: the two states are degenerate, each with energy $\boxed{-\frac{m\alpha^2}{2\hbar^2}.}$ Any linear combination of the two will be an eigenstate (with the same energy); the *sum* (properly normalized) would represent a particle in the delta-function out at large *positive* x, and the difference would be a particle in the delta-function at large *negative* x (the other—distant—delta-function becomes irrelevant), so it makes sense that we get two states, each with the energy of a particle in a single delta-function well.

Problem 2.28

$$\psi = \left\{ \begin{array}{ll} Ae^{ikx} + Be^{-ikx} & (x < -a) \\ Ce^{ikx} + De^{-ikx} & (-a < x < a) \\ Fe^{ikx} & (x > a) \end{array} \right\}. \quad \text{Impose boundary conditions:}$$

(1) Continuity at $-a$: $Ae^{-ika} + Be^{ika} = Ce^{-ika} + De^{ika} \Rightarrow \beta A + B = \beta C + D$, where $\beta \equiv e^{-2ika}$.

(2) Continuity at $+a$: $Ce^{ika} + De^{-ika} = Fe^{ika} \Rightarrow F = C + \beta D$.

(3) Discontinuity in ψ' at $-a$: $ik(Ce^{-ika} - De^{ika}) - ik(Ae^{-ika} - Be^{ika}) = -\frac{2m\alpha}{\hbar^2}(Ae^{-ika} + Be^{ika})$
$\Rightarrow \beta C - D = \beta(\gamma+1)A + B(\gamma-1)$, where $\gamma \equiv i2m\alpha/\hbar^2 k$.

(4) Discontinuity in ψ' at $+a$: $ikFe^{ika} - ik(Ce^{ika} - De^{-ika}) = -\frac{2m\alpha}{\hbar^2}(Fe^{ika})$
$\Rightarrow C - \beta D = (1-\gamma)F$.

To solve for C and D, $\begin{cases} \text{add (2) and (4)}: & 2C = F + (1-\gamma)F \quad \Rightarrow 2C = (2-\gamma)F. \\ \text{subtract (2) and (4)}: & 2\beta D = F - (1-\gamma)F \Rightarrow 2D = (\gamma/\beta)F. \end{cases}$

$$\begin{cases} \text{add (1) and (3)}: & 2\beta C = \beta A + B + \beta(\gamma+1)A + B(\gamma-1) \Rightarrow 2C = (\gamma+2)A + (\gamma/\beta)B. \\ \text{subtract (1) and (3)}: & 2D = \beta A + B - \beta(\gamma+1)A - B(\gamma-1) \quad \Rightarrow 2D = -\gamma\beta A + (2-\gamma)B. \end{cases}$$

$$\begin{cases} \text{Equate the two expressions for } 2C: \ (2-\gamma)F = (\gamma+2)A + (\gamma/\beta)B. \\ \text{Equate the two expressions for } 2D: \ (\gamma/\beta)F = -\gamma\beta A + (2-\gamma)B. \end{cases}$$

Solve these for F and B, in terms of A. Multiply the first by $\beta(2-\gamma)$, the second by γ, and subtract:

$$\left[\beta(2-\gamma)^2 F = \beta(4-\gamma^2)A + \gamma(2-\gamma)B\right]; \quad \left[(\gamma^2/\beta)F = -\beta\gamma^2 A + \gamma(2-\gamma)B\right].$$

$$\Rightarrow \left[\beta(2-\gamma)^2 - \gamma^2/\beta\right] F = \beta\left[4-\gamma^2+\gamma^2\right] A = 4\beta A \Rightarrow \frac{F}{A} = \frac{4}{(2-\gamma)^2 - \gamma^2/\beta^2}.$$

Let $g \equiv i/\gamma = \dfrac{\hbar^2 k}{2m\alpha}$; $\phi \equiv 4ka$, so $\gamma = \dfrac{i}{g}$, $\beta^2 = e^{-i\phi}$. Then: $\dfrac{F}{A} = \dfrac{4g^2}{(2g-i)^2 + e^{i\phi}}$.

Denominator: $4g^2 - 4ig - 1 + \cos\phi + i\sin\phi = (4g^2 - 1 + \cos\phi) + i(\sin\phi - 4g)$.

$$\begin{aligned} |\text{Denominator}|^2 &= (4g^2 - 1 + \cos\phi)^2 + (\sin\phi - 4g)^2 \\ &= 16g^4 + 1 + \cos^2\phi - 8g^2 - 2\cos\phi + 8g^2\cos\phi + \sin^2\phi - 8g\sin\phi + 16g^2 \\ &= 16g^4 + 8g^2 + 2 + (8g^2 - 2)\cos\phi - 8g\sin\phi. \end{aligned}$$

$$T = \left|\frac{F}{A}\right|^2 = \boxed{\frac{8g^4}{(8g^4 + 4g^2 + 1) + (4g^2 - 1)\cos\phi - 4g\sin\phi}, \text{ where } g \equiv \frac{\hbar^2 k}{2m\alpha} \text{ and } \phi \equiv 4ka.}$$

Problem 2.29

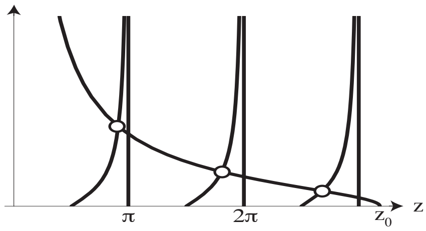
In place of Eq. 2.154, we have: $\psi(x) = \left\{ \begin{array}{ll} Fe^{-\kappa x} & (x > a) \\ D\sin(lx) & (0 < x < a) \\ -\psi(-x) & (x < 0) \end{array} \right\}$.

Continuity of ψ : $Fe^{-\kappa a} = D\sin(la)$; continuity of ψ' : $-F\kappa e^{-\kappa a} = Dl\cos(la)$.

Divide: $-\kappa = l\cot(la)$, or $-\kappa a = la\cot(la) \Rightarrow \sqrt{z_0^2 - z^2} = -z\cot z$, or $\boxed{-\cot z = \sqrt{(z_0/z)^2 - 1}.}$

Wide, deep well: Intersections are at $\pi, 2\pi, 3\pi$, etc. Same as Eq. 2.160, but now for n *even*. This fills in the rest of the states for the infinite square well.

Shallow, narrow well: If $z_0 < \pi/2$, there is *no* odd bound state. The corresponding condition on V_0 is $\boxed{V_0 < \dfrac{\pi^2\hbar^2}{8ma^2} \Rightarrow \textit{no} \text{ odd bound state.}}$



Problem 2.30

$$1 = 2\int_0^\infty |\psi|^2 dx = 2\left(|D|^2 \int_0^a \cos^2 lx\, dx + |F|^2 \int_a^\infty e^{-2\kappa x} dx\right)$$
$$= 2\left[|D|^2 \left(\frac{x}{2} + \frac{1}{4l}\sin 2lx\right)\Big|_0^a + |F|^2\left(-\frac{1}{2\kappa}e^{-2\kappa x}\right)\Big|_a^\infty\right] = 2\left[|D|^2\left(\frac{a}{2} + \frac{\sin 2la}{4l}\right) + |F|^2 \frac{e^{-2\kappa a}}{2\kappa}\right].$$

But $F = De^{\kappa a}\cos la$ (Eq. 2.152), so $1 = |D|^2\left(a + \dfrac{\sin(2la)}{2l} + \dfrac{\cos^2(la)}{\kappa}\right)$.

Furthermore $\kappa = l\tan(la)$ (Eq. 2.157), so

$$1 = |D|^2\left(a + \frac{2\sin la\cos la}{2l} + \frac{\cos^3 la}{l\sin la}\right) = |D|^2\left[a + \frac{\cos la}{l\sin la}(\sin^2 la + \cos^2 la)\right]$$
$$= |D|^2\left(a + \frac{1}{l\tan la}\right) = |D|^2\left(a + \frac{1}{\kappa}\right). \quad \boxed{D = \frac{1}{\sqrt{a+1/\kappa}},} \quad \boxed{F = \frac{e^{\kappa a}\cos la}{\sqrt{a+1/\kappa}}.}$$

Problem 2.31

Equation 2.158 $\Rightarrow z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$. We want $\alpha =$ *area of potential* $= 2aV_0$ held constant as $a \to 0$. Therefore $V_0 = \frac{\alpha}{2a}$; $z_0 = \frac{a}{\hbar}\sqrt{2m\frac{\alpha}{2a}} = \frac{1}{\hbar}\sqrt{m\alpha a} \to 0$. So z_0 is *small*, and the intersection in Fig. 2.17 occurs at very small z. Solve Eq. 2.159 for very small z, by expanding $\tan z$:

$$\tan z \cong z = \sqrt{(z_0/z)^2 - 1} = (1/z)\sqrt{z_0^2 - z^2}.$$

Now (from Eqs. 2.149, 2.151 and 2.158) $z_0^2 - z^2 = \kappa^2 a^2$, so $z^2 = \kappa a$. But $z_0^2 - z^2 = z^4 \ll 1 \Rightarrow z \cong z_0$, so $\kappa a \cong z_0^2$. But we found that $z_0 \cong \frac{1}{\hbar}\sqrt{m\alpha a}$ here, so $\kappa a = \frac{1}{\hbar^2}m\alpha a$, or $\kappa = \frac{m\alpha}{\hbar^2}$. (At this point the a's have canceled, and we can go to the limit $a \to 0$.)

$$\frac{\sqrt{-2mE}}{\hbar} = \frac{m\alpha}{\hbar^2} \Rightarrow -2mE = \frac{m^2\alpha^2}{\hbar^2}. \quad \boxed{E = -\frac{m\alpha^2}{2\hbar^2}} \text{ (which agrees with Eq. 2.132).}$$

In Eq. 2.172, $V_0 \gg E \Rightarrow T^{-1} \cong 1 + \frac{V_0^2}{4EV_0}\sin^2\left(\frac{2a}{\hbar}\sqrt{2mV_0}\right)$. But $V_0 = \frac{\alpha}{2a}$, so the argument of the sine is small, and we can replace $\sin\epsilon$ by ϵ: $T^{-1} \cong 1 + \frac{V_0}{4E}\left(\frac{2a}{\hbar}\right)^2 2mV_0 = 1 + (2aV_0)^2\frac{m}{2\hbar^2 E}$. But $2aV_0 = \alpha$, so $T^{-1} = 1 + \frac{m\alpha^2}{2\hbar^2 E}$, in agreement with Eq. 2.144.

Problem 2.32

Multiply Eq. 2.168 by $\sin la$, Eq. 2.169 by $\frac{1}{l}\cos la$, and add:

$$\left.\begin{aligned} C\sin^2 la + D\sin la\cos la &= Fe^{ika}\sin la \\ C\cos^2 la - D\sin la\cos la &= \tfrac{ik}{l}Fe^{ika}\cos la \end{aligned}\right\} \quad C = Fe^{ika}\left[\sin la + \frac{ik}{l}\cos la\right].$$

Multiply Eq. 2.168 by $\cos la$, Eq. 2.169 by $\frac{1}{l}\sin la$, and subtract:

$$\left.\begin{aligned} C\sin la\cos la + D\cos^2 la &= Fe^{ika}\cos la \\ C\sin la\cos la - D\sin^2 la &= \tfrac{ik}{l}Fe^{ika}\sin la \end{aligned}\right\} \quad D = Fe^{ika}\left[\cos la - \frac{ik}{l}\sin la\right].$$

Put these into Eq. 2.166:

$$\begin{aligned} (\mathbf{1})\ Ae^{-ika} + Be^{ika} &= -Fe^{ika}\left[\sin la + \frac{ik}{l}\cos la\right]\sin la + Fe^{ika}\left[\cos la - \frac{ik}{l}\sin la\right]\cos la \\ &= Fe^{ika}\left[\cos^2 la - \frac{ik}{l}\sin la\cos la - \sin^2 la - \frac{ik}{l}\sin la\cos la\right] \\ &= Fe^{ika}\left[\cos(2la) - \frac{ik}{l}\sin(2la)\right]. \end{aligned}$$

Likewise, from Eq. 2.167:

$$\begin{aligned} (\mathbf{2})\ Ae^{-ika} - Be^{ika} &= -\frac{il}{k}Fe^{ika}\left[\left(\sin la + \frac{ik}{l}\cos la\right)\cos la + \left(\cos la - \frac{ik}{l}\sin la\right)\sin la\right] \\ &= -\frac{il}{k}Fe^{ika}\left[\sin la\cos la + \frac{ik}{l}\cos^2 la + \sin la\cos la - \frac{ik}{l}\sin^2 la\right] \\ &= -\frac{il}{k}Fe^{ika}\left[\sin(2la) + \frac{ik}{l}\cos(2la)\right] = Fe^{ika}\left[\cos(2la) - \frac{il}{k}\sin(2la)\right]. \end{aligned}$$

Add **(1)** and **(2)**: $2Ae^{-ika} = Fe^{ika}\left[2\cos(2la) - i\left(\frac{k}{l} + \frac{l}{k}\right)\sin(2la)\right]$, or:

$F = \dfrac{e^{-2ika}A}{\cos(2la) - i\frac{\sin(2la)}{2kl}(k^2+l^2)}$ (confirming Eq. 2.171). Now subtract **(2)** from **(1)**:

$2Be^{ika} = Fe^{ika}\left[i\left(\frac{l}{k} - \frac{k}{l}\right)\sin(2la)\right] \Rightarrow B = i\dfrac{\sin(2la)}{2kl}(l^2 - k^2)F$ (confirming Eq. 2.170).

$$T^{-1} = \left|\frac{A}{F}\right|^2 = \left|\cos(2la) - i\frac{\sin(2la)}{2kl}(k^2+l^2)\right|^2 = \cos^2(2la) + \frac{\sin^2(2la)}{(2lk)^2}(k^2+l^2)^2.$$

But $\cos^2(2la) = 1 - \sin^2(2la)$, so

$$T^{-1} = 1 + \sin^2(2la)\Bigg[\underbrace{\frac{(k^2+l^2)^2}{(2lk)^2} - 1}_{\frac{1}{(2kl)^2}[k^4+2k^2l^2+l^4-4k^2l^2]=\frac{1}{(2kl)^2}[k^4-2k^2l^2+l^4]=\frac{(k^2-l^2)^2}{(2kl)^2}.}\Bigg] = 1 + \frac{(k^2-l^2)^2}{(2kl)^2}\sin^2(2la).$$

But $k = \dfrac{\sqrt{2mE}}{\hbar}$, $l = \dfrac{\sqrt{2m(E+V_0)}}{\hbar}$; so $(2la) = \dfrac{2a}{\hbar}\sqrt{2m(E+V_0)}$; $k^2 - l^2 = -\dfrac{2mV_0}{\hbar^2}$, and

$$\frac{(k^2-l^2)^2}{(2kl)^2} = \frac{\left(\frac{2m}{\hbar^2}\right)^2 V_0^2}{4\left(\frac{2m}{\hbar^2}\right)^2 E(E+V_0)} = \frac{V_0^2}{4E(E+V_0)}.$$

$$\therefore T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right),$$ confirming Eq. 2.172.

Problem 2.33

$\underline{\mathbf{E < V_0}}$. $\quad \psi = \begin{Bmatrix} Ae^{ikx} + Be^{-ikx} & (x < -a) \\ Ce^{\kappa x} + De^{-\kappa x} & (-a < x < a) \\ Fe^{ikx} & (x > a) \end{Bmatrix} \quad k = \dfrac{\sqrt{2mE}}{\hbar};\ \kappa = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar}.$

(1) Continuity of ψ at $-a$: $Ae^{-ika} + Be^{ika} = Ce^{-\kappa a} + De^{\kappa a}$.

(2) Continuity of ψ' at $-a$: $ik(Ae^{-ika} - Be^{ika}) = \kappa(Ce^{-\kappa a} - De^{\kappa a})$.

$$\Rightarrow 2Ae^{-ika} = \left(1 - i\frac{\kappa}{k}\right) Ce^{-\kappa a} + \left(1 + i\frac{\kappa}{k}\right) De^{\kappa a}.$$

(3) Continuity of ψ at $+a$: $Ce^{\kappa a} + De^{-\kappa a} = Fe^{ika}$.

(4) Continuity of ψ' at $+a$: $\kappa(Ce^{\kappa a} - De^{-\kappa a}) = ikFe^{ika}$.

$$\Rightarrow 2Ce^{\kappa a} = \left(1 + \frac{ik}{\kappa}\right) Fe^{ika}; \quad 2De^{-\kappa a} = \left(1 - \frac{ik}{\kappa}\right) Fe^{ika}.$$

$$\begin{aligned}
2Ae^{-ika} &= \left(1 - \frac{i\kappa}{k}\right)\left(1 + \frac{ik}{\kappa}\right) Fe^{ika}\frac{e^{-2\kappa a}}{2} + \left(1 + \frac{i\kappa}{k}\right)\left(1 - \frac{ik}{\kappa}\right) Fe^{ika}\frac{e^{2\kappa a}}{2} \\
&= \frac{Fe^{ika}}{2}\left\{\left[1 + i\left(\frac{k}{\kappa} - \frac{\kappa}{k}\right) + 1\right] e^{-2\kappa a} + \left[1 + i\left(\frac{\kappa}{k} - \frac{k}{\kappa}\right) + 1\right] e^{2\kappa a}\right\} \\
&= \frac{Fe^{ika}}{2}\left[2\left(e^{-2\kappa a} + e^{2\kappa a}\right) + i\frac{(\kappa^2 - k^2)}{k\kappa}\left(e^{2\kappa a} - e^{-2\kappa a}\right)\right].
\end{aligned}$$

But $\sinh x \equiv \dfrac{e^x - e^{-x}}{2}$, $\cosh x \equiv \dfrac{e^x + e^{-x}}{2}$, so

$$\begin{aligned}
&= \frac{Fe^{ika}}{2}\left[4\cosh(2\kappa a) + i\frac{(\kappa^2 - k^2)}{k\kappa}2\sinh(2\kappa a)\right] \\
&= 2Fe^{ika}\left[\cosh(2\kappa a) + i\frac{(\kappa^2 - k^2)}{2k\kappa}\sinh(2\kappa a)\right].
\end{aligned}$$

$$T^{-1} = \left|\frac{A}{F}\right|^2 = \cosh^2(2\kappa a) + \frac{(\kappa^2 - k^2)^2}{(2\kappa k)^2}\sinh^2(2\kappa a). \quad \text{But } \cosh^2 = 1 + \sinh^2, \text{ so}$$

$$T^{-1} = 1 + \underbrace{\left[1 + \frac{(\kappa^2 - k^2)^2}{(2\kappa k)^2}\right]}_{\bigstar}\sinh^2(2\kappa a) = \boxed{1 + \frac{V_0^2}{4E(V_0 - E)}\sinh^2\left(\frac{2a}{\hbar}\sqrt{2m(V_0 - E)}\right)},$$

$$\text{where } \bigstar = \frac{4\kappa^2k^2 + k^4 + \kappa^4 - 2\kappa^2k^2}{(2\kappa k)^2} = \frac{(\kappa^2 + k^2)^2}{(2\kappa k)^2} = \frac{\left(\frac{2mE}{\hbar^2} + \frac{2m(V_0-E)}{\hbar^2}\right)^2}{4\frac{2mE}{\hbar^2}\frac{2m(V_0-E)}{\hbar^2}} = \frac{V_0^2}{4E(V_0 - E)}.$$

(You can also get this from Eq. 2.172 by switching the sign of V_0 and using $\sin(i\theta) = i\sinh\theta$.)

$\underline{\mathbf{E = V_0}}$. $\quad \psi = \begin{Bmatrix} Ae^{ikx} + Be^{-ikx} & (x < -a) \\ C + Dx & (-a < x < a) \\ Fe^{ikx} & (x > a) \end{Bmatrix}$

(In central region $-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi}{dx^2} + V_0\psi = E\psi \Rightarrow \dfrac{d^2\psi}{dx^2} = 0$, so $\psi = C + Dx$.)

(1) Continuous ψ at $-a$: $Ae^{-ika} + Be^{ika} = C - Da.$

(2) Continuous ψ at $+a$: $Fe^{ika} = C + Da.$

$$\Rightarrow \ \textbf{(2.5)}\ 2Da = Fe^{ika} - Ae^{-ika} - Be^{ika}.$$

(3) Continuous ψ' at $-a$: $ik\left(Ae^{-ika} - Be^{ika}\right) = D.$

(4) Continuous ψ' at $+a$: $ikFe^{ika} = D.$

$$\Rightarrow \ \textbf{(4.5)}\ Ae^{-2ika} - B = F.$$

Use **(4)** to eliminate D in **(2.5)**: $Ae^{-2ika} + B = F - 2aikF = (1 - 2iak)F$, and add to **(4.5)**:

$$2Ae^{-2ika} = 2F(1 - ika), \ \text{so} \ T^{-1} = \left|\frac{A}{F}\right|^2 = 1 + (ka)^2 = \boxed{1 + \frac{2mE}{\hbar^2}a^2.}$$

(You can also get this from Eq. 2.172 by changing the sign of V_0 and taking the limit $E \to V_0$, using $\sin\epsilon \cong \epsilon$.)

$\underline{\mathbf{E > V_0}}$. This case is identical to the one in the book, only with $V_0 \to -V_0$. So

$$\boxed{T^{-1} = 1 + \frac{V_0^2}{4E(E - V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E - V_0)}\right).}$$

Problem 2.34

(a)

$$\psi = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x < 0) \\ Fe^{-\kappa x} & (x > 0) \end{cases} \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}; \ \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}.$$

(1) Continuity of ψ : $A + B = F.$

(2) Continuity of ψ' : $ik(A - B) = -\kappa F.$

$$\Rightarrow A + B = -\frac{ik}{\kappa}(A - B) \Rightarrow A\left(1 + \frac{ik}{\kappa}\right) = -B\left(1 - \frac{ik}{\kappa}\right).$$

$$R = \left|\frac{B}{A}\right|^2 = \frac{|(1 + ik/\kappa)|^2}{|(1 - ik/\kappa)|^2} = \frac{1 + (k/\kappa)^2}{1 + (k/\kappa)^2} = \boxed{1.}$$

Although the wave function penetrates into the barrier, it is eventually all reflected.

(b)

$$\psi = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x < 0) \\ Fe^{ilx} & (x > 0) \end{cases} \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}; \ l = \frac{\sqrt{2m(E - V_0)}}{\hbar}.$$

(1) Continuity of ψ : $A + B = F.$

(2) Continuity of ψ' : $ik(A - B) = ilF.$

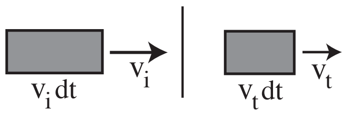
$$\Rightarrow A+B=\frac{k}{l}(A-B);\; A\left(1-\frac{k}{l}\right)=-B\left(1+\frac{k}{l}\right).$$

$$R=\left|\frac{B}{A}\right|^2=\frac{(1-k/l)^2}{(1+k/l)^2}=\frac{(k-l)^2}{(k+l)^2}=\frac{(k-l)^4}{(k^2-l^2)^2}.$$

Now $k^2-l^2=\frac{2m}{\hbar^2}(E-E+V_0)=\left(\frac{2m}{\hbar^2}\right)V_0;\; k-l=\frac{\sqrt{2m}}{\hbar}[\sqrt{E}-\sqrt{E-V_0}]$, so

$$\boxed{R=\frac{(\sqrt{E}-\sqrt{E-V_0})^4}{V_0^2}.}$$

(c)



From the diagram, $T=P_t/P_i=|F|^2v_t/|A|^2v_i$, where P_i is the probability of finding the incident particle in the box corresponding to the time interval dt, and P_t is the probability of finding the transmitted particle in the associated box to the *right* of the barrier.
But $\frac{v_t}{v_i}=\frac{\sqrt{E-V_0}}{\sqrt{E}}$ (from Eq. 2.98). So $T=\sqrt{\frac{E-V_0}{E}}\left|\frac{F}{A}\right|^2$. Alternatively, from Problem 2.18:

$$J_i=\frac{\hbar k}{m}|A|^2;\quad J_t=\frac{\hbar l}{m}|F|^2;\quad T=\frac{J_t}{J_i}=\left|\frac{F}{A}\right|^2\frac{l}{k}=\left|\frac{F}{A}\right|^2\sqrt{\frac{E-V_0}{E}}.$$

For $E<V_0$, of course, $\boxed{T=0.}$

(d)

$$\text{For } E>V_0,\; F=A+B=A+A\frac{\left(\frac{k}{l}-1\right)}{\left(\frac{k}{l}+1\right)}=A\frac{2k/l}{\left(\frac{k}{l}+1\right)}=\frac{2k}{k+l}A.$$

$$T=\left|\frac{F}{A}\right|^2\frac{l}{k}=\left(\frac{2k}{k+l}\right)^2\frac{l}{k}=\frac{4kl}{(k+l)^2}=\frac{4kl(k-l)^2}{(k^2-l^2)^2}=\boxed{\frac{4\sqrt{E}\sqrt{E-V_0}(\sqrt{E}-\sqrt{E-V_0})^2}{V_0^2}.}$$

$$T+R=\frac{4kl}{(k+l)^2}+\frac{(k-l)^2}{(k+l)^2}=\frac{4kl+k^2-2kl+l^2}{(k+l)^2}=\frac{k^2+2kl+l^2}{(k+l)^2}=\frac{(k+l)^2}{(k+l)^2}=1.\ \checkmark$$

Problem 2.35

(a)

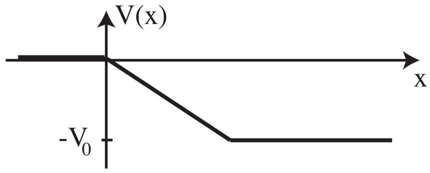
$$\psi(x)=\begin{cases}Ae^{ikx}+Be^{-ikx} & (x<0)\\ Fe^{ilx} & (x>0)\end{cases}\quad\text{where } k\equiv\frac{\sqrt{2mE}}{\hbar},\; l\equiv\frac{\sqrt{2m(E+V_0)}}{\hbar}.$$

$$\left.\begin{array}{l}\text{Continuity of } \psi \;\Rightarrow A+B=F\\ \text{Continuity of } \psi' \Rightarrow ik(A-B)=ilF\end{array}\right\}\Longrightarrow$$

$$A+B=\frac{k}{l}(A-B);\quad A\left(1-\frac{k}{l}\right)=-B\left(1+\frac{k}{l}\right);\quad \frac{B}{A}=-\left(\frac{1-k/l}{1+k/l}\right).$$

$$R = \left|\frac{B}{A}\right|^2 = \left(\frac{l-k}{l+k}\right)^2 = \left(\frac{\sqrt{E+V_0}-\sqrt{E}}{\sqrt{E+V_0}+\sqrt{E}}\right)^2$$
$$= \left(\frac{\sqrt{1+V_0/E}-1}{\sqrt{1+V_0/E}+1}\right)^2 = \left(\frac{\sqrt{1+3}-1}{\sqrt{1+3}+1}\right)^2 = \left(\frac{2-1}{2+1}\right)^2 = \boxed{\frac{1}{9}.}$$

(b) The cliff is *two*-dimensional, and even if we pretend the car drops straight down, the potential *as a function of distance along the* (crooked, but now one-dimensional) *path* is $-mgx$ (with x the vertical coordinate), as shown.



(c) Here $V_0/E = 12/4 = 3$, the same as in part (a), so $R = 1/9$, and hence $T = \boxed{8/9 = 0.8889.}$

Problem 2.36

Start with Eq. 2.25: $\psi(x) = A\sin kx + B\cos kx$. This time the boundary conditions are $\psi(a) = \psi(-a) = 0$:

$$A\sin ka + B\cos ka = 0; \quad -A\sin ka + B\cos ka = 0.$$

$$\begin{cases} \textit{Subtract}: & A\sin ka = 0 \Rightarrow ka = j\pi \text{ or } A = 0, \\ \textit{Add}: & B\cos ka = 0 \Rightarrow ka = (j-\frac{1}{2})\pi \text{ or } B = 0, \end{cases}$$

(where $j = 1, 2, 3, \ldots$).

If $B = 0$ (so $A \neq 0$), $k = j\pi/a$. In this case let $n \equiv 2j$ (so n is an *even* integer); then $k = n\pi/2a$, $\psi = A\sin(n\pi x/2a)$. Normalizing: $1 = |A|^2 \int_{-a}^{a} \sin^2(n\pi x/2a)\,dx = |A|^2 a \Rightarrow A = 1/\sqrt{a}$.

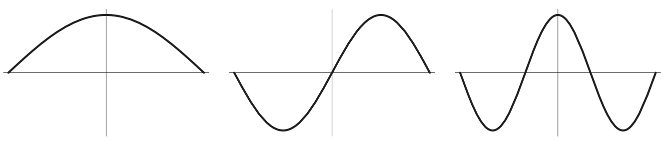
If $A = 0$ (so $B \neq 0$), $k = (j-\frac{1}{2})\pi/a$. In this case let $n \equiv 2j-1$ (n is an *odd* integer); again $k = n\pi/2a$, $\psi = B\cos(n\pi x/2a)$. Normalizing: $1 = |B|^2 \int_{-a}^{a} \cos^2(n\pi x/2a)dx = |B|^2 a \Rightarrow B = 1/\sqrt{a}$.

In either case Eq. 2.24 yields $E = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$ (in agreement with Eq. 2.30 for a well of width $2a$).

The substitution $x \to (x+a)/2$ takes Eq. 2.31 to

$$\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}\frac{(x+a)}{2}\right) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{2a} + \frac{n\pi}{2}\right) = \begin{cases} (-1)^{n/2}\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{2a}\right) & (n \text{ even}), \\ (-1)^{(n-1)/2}\sqrt{\frac{2}{a}}\cos\left(\frac{n\pi x}{2a}\right) & (n \text{ odd}). \end{cases}$$

So (apart from normalization) we recover the results above. The graphs are the same as Figure 2.2, except that some are upside down (different normalization).



cos(πx/2a) sin(2πx/2a) cos(3πx/2a)

Problem 2.37

Use the trig identity $\sin 3\theta = 3\sin\theta - 4\sin^3\theta$ to write

$$\sin^3\left(\frac{\pi x}{a}\right) = \frac{3}{4}\sin\left(\frac{\pi x}{a}\right) - \frac{1}{4}\sin\left(\frac{3\pi x}{a}\right). \quad \text{So (Eq. 2.31): } \Psi(x,0) = A\sqrt{\frac{a}{2}}\left[\frac{3}{4}\psi_1(x) - \frac{1}{4}\psi_3(x)\right].$$

Normalize using Eq. 2.20: $|A|^2\frac{a}{2}\left(\frac{9}{16}+\frac{1}{16}\right) = \frac{5}{16}a|A|^2 = 1 \Rightarrow \boxed{A = \frac{4}{\sqrt{5a}}.}$

So $\Psi(x,0) = \frac{1}{\sqrt{10}}\left[3\psi_1(x) - \psi_3(x)\right]$, and hence (Eq. 2.17)

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{10}}\left[3\psi_1(x)e^{-iE_1t/\hbar} - \psi_3(x)e^{-iE_3t/\hbar}\right].}$$

$$|\Psi(x,t)|^2 = \frac{1}{10}\left[9\psi_1^2 + \psi_3^2 - 6\psi_1\psi_3\cos\left(\frac{E_3-E_1}{\hbar}t\right)\right]; \text{ so}$$

$$\langle x\rangle = \int_0^a x|\Psi(x,t)|^2dx = \frac{9}{10}\langle x\rangle_1 + \frac{1}{10}\langle x\rangle_3 - \frac{3}{5}\cos\left(\frac{E_3-E_1}{\hbar}t\right)\int_0^a x\psi_1(x)\psi_3(x)dx,$$

where $\langle x\rangle_n = a/2$ is the expectation value of x in the nth stationary state. The remaining integral is

$$\frac{2}{a}\int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{3\pi x}{a}\right)dx = \frac{1}{a}\int_0^a x\left[\cos\left(\frac{2\pi x}{a}\right) - \cos\left(\frac{4\pi x}{a}\right)\right]dx$$
$$= \frac{1}{a}\left[\left(\frac{a}{2\pi}\right)^2\cos\left(\frac{2\pi x}{a}\right) + \left(\frac{xa}{2\pi}\right)\sin\left(\frac{2\pi x}{a}\right) - \left(\frac{a}{4\pi}\right)^2\cos\left(\frac{4\pi x}{a}\right) - \left(\frac{xa}{4\pi}\right)\sin\left(\frac{4\pi x}{a}\right)\right|_0^a = 0.$$

Evidently then,

$$\langle x\rangle = \frac{9}{10}\left(\frac{a}{2}\right) + \frac{1}{10}\left(\frac{a}{2}\right) = \boxed{\frac{a}{2}.}$$

Using Eq. 2.21,

$$\langle H\rangle = |c_1|^2E_1 + |c_3|^2E_3 = \left(\frac{9}{10}\right)\frac{\pi^2\hbar^2}{2ma^2} + \left(\frac{1}{10}\right)\frac{9\pi^2\hbar^2}{2ma^2} = \boxed{\frac{9\pi^2\hbar^2}{10ma^2}.}$$

Problem 2.38

(a) According to Eq. 2.39, the most general solution to the time-dependent Schrödinger equation for the infinite square well is

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)e^{-i(n^2\pi^2\hbar/2ma^2)t}.$$

Now $\frac{n^2\pi^2\hbar}{2ma^2}T = \frac{n^2\pi^2\hbar}{2ma^2}\frac{4ma^2}{\pi\hbar} = 2\pi n^2$, so $e^{-i(n^2\pi^2\hbar/2ma^2)(t+T)} = e^{-i(n^2\pi^2\hbar/2ma^2)t}e^{-i2\pi n^2}$, and since n^2 is an integer, $e^{-i2\pi n^2} = 1$. Therefore $\Psi(x,t+T) = \Psi(x,t)$. QED

(b) The classical revival time is the time it takes the particle to go down and back: $T_c = 2a/v$, with the velocity given by

$$E = \frac{1}{2}mv^2 \Rightarrow v = \sqrt{\frac{2E}{m}} \Rightarrow \boxed{T_c = a\sqrt{\frac{2m}{E}}.}$$

(c) The two revival times are equal if

$$\frac{4ma^2}{\pi\hbar} = a\sqrt{\frac{2m}{E}}, \quad \text{or} \quad \boxed{E = \frac{\pi^2\hbar^2}{8ma^2} = \frac{E_1}{4}.}$$

Problem 2.39

(a)

$$\frac{d\Psi}{dx} = \frac{2\sqrt{3}}{a\sqrt{a}} \cdot \left\{ \begin{array}{ll} 1, & (0 < x < a/2) \\ -1, & (a/2 < x < a) \end{array} \right\} = \boxed{\frac{2\sqrt{3}}{a\sqrt{a}}\left[1 - 2\theta\left(x - \frac{a}{2}\right)\right].}$$

(b)

$$\frac{d^2\Psi}{dx^2} = \frac{2\sqrt{3}}{a\sqrt{a}}\left[-2\delta\left(x - \frac{a}{2}\right)\right] = \boxed{-\frac{4\sqrt{3}}{a\sqrt{a}}\delta\left(x - \frac{a}{2}\right).}$$

(c)

$$\langle H\rangle = -\frac{\hbar^2}{2m}\left(-\frac{4\sqrt{3}}{a\sqrt{a}}\right)\int \Psi^*\delta\left(x - \frac{a}{2}\right)dx = \frac{2\sqrt{3}\hbar^2}{ma\sqrt{a}}\underbrace{\Psi^*\left(\frac{a}{2}\right)}_{\sqrt{3/a}} = \frac{2\cdot 3\cdot \hbar^2}{m\cdot a\cdot a} = \boxed{\frac{6\hbar^2}{ma^2}.}\ \checkmark$$

Problem 2.40

(a) In the standard notation $\xi \equiv \sqrt{m\omega/\hbar}\,x,\ \alpha \equiv (m\omega/\pi\hbar)^{1/4}$,

$$\Psi(x,0) = A(1-2\xi)^2 e^{-\xi^2/2} = A(1 - 4\xi + 4\xi^2)e^{-\xi^2/2}.$$

It can be expressed as a linear combination of the first three stationary states (Eq. 2.60 and 2.63, and Problem 2.10):

$$\psi_0(x) = \alpha e^{-\xi^2/2}, \qquad \psi_1(x) = \sqrt{2}\,\alpha\xi e^{-\xi^2/2}, \qquad \psi_2(x) = \frac{\alpha}{\sqrt{2}}(2\xi^2 - 1)e^{-\xi^2/2}.$$

So $\Psi(x,0) = c_0\psi_0 + c_1\psi_1 + c_2\psi_2 = \alpha(c_0 + \sqrt{2}\xi c_1 + \sqrt{2}\xi^2 c_2 - \frac{1}{\sqrt{2}}c_2)e^{-\xi^2/2}$ with (equating like powers)

$$\begin{cases} \alpha\sqrt{2}c_2 = 4A & \Rightarrow c_2 = 2\sqrt{2}A/\alpha, \\ \alpha\sqrt{2}c_1 = -4A & \Rightarrow c_1 = -2\sqrt{2}A/\alpha, \\ \alpha(c_0 - c_2/\sqrt{2}) = A & \Rightarrow c_0 = (A/\alpha) + c_2/\sqrt{2} = (1+2)A/\alpha = 3A/\alpha. \end{cases}$$

Normalizing: $1 = |c_0|^2 + |c_1|^2 + |c_2|^2 = (8+8+9)(A/\alpha)^2 = 25(A/\alpha)^2 \;\Rightarrow A = \alpha/5 = \boxed{\frac{1}{5}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}.}$

$$\boxed{c_0 = \frac{3}{5}, \quad c_1 = -\frac{2\sqrt{2}}{5}, \quad c_2 = \frac{2\sqrt{2}}{5}.}$$

(b) You could get $\boxed{\frac{1}{2}\hbar\omega,\text{ probability }\frac{9}{25};\,\frac{3}{2}\hbar\omega,\text{ probability }\frac{8}{25};\,\frac{5}{2}\hbar\omega,\text{ probability }\frac{8}{25}.}$

$$\langle H\rangle = \frac{9}{25}\left(\frac{1}{2}\hbar\omega\right) + \frac{8}{25}\left(\frac{3}{2}\hbar\omega\right) + \frac{8}{25}\left(\frac{5}{2}\hbar\omega\right) = \frac{\hbar\omega}{50}(9+24+40) = \boxed{\frac{73}{50}\hbar\omega.}$$

(c)

$$\Psi(x,t) = \frac{3}{5}\psi_0 e^{-i\omega t/2} - \frac{2\sqrt{2}}{5}\psi_1 e^{-3i\omega t/2} + \frac{2\sqrt{2}}{5}\psi_2 e^{-5i\omega t/2} = e^{-i\omega t/2}\left[\frac{3}{5}\psi_0 - \frac{2\sqrt{2}}{5}\psi_1 e^{-i\omega t} + \frac{2\sqrt{2}}{5}\psi_2 e^{-2i\omega t}\right].$$

To change the sign of the middle term we need $e^{-i\omega T} = -1$ (then $e^{-2i\omega T} = 1$); evidently $\omega T = \pi$, or $\boxed{T = \pi/\omega.}$

Problem 2.41

Everything in Section 2.3.2 still applies, except that there is an additional boundary condition: $\psi(0) = 0$. This eliminates all the *even* solutions ($n = 0, 2, 4, \ldots$), leaving only the odd solutions. So

$$\boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega,\; n = 1, 3, 5, \ldots.}$$

Problem 2.42

(a) Normalization is the same as before: $A = \left(\frac{2a}{\pi}\right)^{1/4}$.

(b) Equation 2.104 says

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\left(\frac{2a}{\pi}\right)^{1/4}\int_{-\infty}^{\infty} e^{-ax^2}e^{ilx}e^{-ikx}dx \quad [\text{same as before, only } k \to k-l] = \frac{1}{(2\pi a)^{1/4}}e^{-(k-l)^2/4a}.$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\frac{1}{(2\pi a)^{1/4}}\int_{-\infty}^{\infty} e^{-(k-l)^2/4a}e^{i(kx-\hbar k^2 t/2m)}\,dk$$

Let $u \equiv k - l$, so $k = u + l$ and $dk = du$:

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\sqrt{2\pi}}\frac{1}{(2\pi a)^{1/4}}\int_{-\infty}^{\infty} e^{-u^2/4a}e^{i[ux+lx-(\hbar t/2m)(u^2+2ul+l^2)]}\,du \\ &= \frac{1}{\sqrt{2\pi}}\frac{1}{(2\pi a)^{1/4}}e^{il\left(x-\frac{\hbar l t}{2m}\right)}\int_{-\infty}^{\infty} e^{-u^2\left(\frac{1}{4a}+i\frac{\hbar t}{2m}\right)+iu\left(x-\frac{\hbar l t}{m}\right)}\,du.\end{aligned}$$

Using the hint in Problem 2.21, the integral becomes

$$\frac{1}{\sqrt{\frac{1}{4a}+i\frac{\hbar t}{2m}}} e^{\left(x-\frac{\hbar l t}{m}\right)^2/4\left(\frac{1}{4a}+i\frac{\hbar t}{2m}\right)} \int_{-\infty}^{\infty} e^{-y^2}\,dy = \frac{2\sqrt{a}}{\gamma} e^{-a\left(x-\frac{\hbar l t}{m}\right)^2/\gamma^2}\sqrt{\pi},$$

so

$$\Psi(x,t) = \boxed{\left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\gamma} e^{-a\left(x-\frac{\hbar l t}{m}\right)^2/\gamma^2} e^{il\left(x-\frac{\hbar l t}{2m}\right)}.}$$

The gaussian envelope (the first exponential) travels at speed $\boxed{\hbar l/m;}$ the sinusoidal wave (the second exponential) travels at speed $\boxed{\hbar l/2m}$.

(c)

$$|\Psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}}\frac{1}{|\gamma|^2} e^{a\left(x-\frac{\hbar l t}{m}\right)^2\left[\frac{1}{\gamma^2}+\frac{1}{(\gamma^*)^2}\right]}.$$

The term in square brackets simplifies:

$$\left[\frac{1}{\gamma^2}+\frac{1}{(\gamma^*)^2}\right] = \frac{1}{|\gamma|^4}[(\gamma^*)^2+\gamma^2] = \frac{1}{|\gamma|^4}\left(1-\frac{2i\hbar t}{m}+1+\frac{2i\hbar t}{m}\right) = \frac{2}{|\gamma|^4}.$$

$$|\gamma|^2 = \sqrt{\left(1+\frac{2ia\hbar t}{m}\right)\left(1-\frac{2ia\hbar t}{m}\right)} = \sqrt{1+\theta^2},$$

where (as before) $\theta \equiv 2\hbar a t/m$. So

$$|\Psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}}\frac{1}{\sqrt{1+\theta^2}} e^{2a\left(x-\frac{\hbar l t}{m}\right)^2/(1+\theta^2)} = \boxed{\sqrt{\frac{2}{\pi}} w e^{-2w^2\left(x-\frac{\hbar l t}{m}\right)^2}.}$$

where (as before) $w \equiv \sqrt{a/(1+\theta^2)}$. The result is the same as in Problem 2.21, except that $x \to \left(x-\frac{\hbar l}{m}t\right)$, so $|\Psi|^2$ has the same (flattening gaussian) shape – only this time the center moves at constant speed $v = \hbar l/m$.

(d)

$$\langle x\rangle = \int_{-\infty}^{\infty} x|\Psi(x,t)|^2 dx. \qquad \text{Let } y \equiv x - vt, \text{ so } x = y + vt.$$

$$= \int_{-\infty}^{\infty}(y+vt)\sqrt{\frac{2}{\pi}} w e^{-2w^2y^2} dy = vt = \boxed{\frac{\hbar l}{m}t.}$$

(The first integral is trivially zero; the second is 1 by normalization.)

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = \boxed{\hbar l.}$$

$$\langle x^2\rangle = \int_{-\infty}^{\infty}(y+vt)^2\sqrt{\frac{2}{\pi}} w e^{-2w^2y^2} dy = \frac{1}{4w^2}+0+(vt)^2 = \boxed{\frac{1}{4w^2}+\left(\frac{\hbar l t}{m}\right)^2.}$$

(The first integral is same as in Problem 2.21).

$$\langle p^2\rangle = -\hbar^2\int_{-\infty}^{\infty}\Psi^*\frac{\partial^2\Psi}{\partial x^2}dx; \quad \frac{\partial\Psi}{\partial x} = \left[-\frac{2a}{\gamma^2}\left(x-\frac{\hbar l t}{m}\right)+il\right]\Psi,$$

$$\frac{\partial^2\Psi}{\partial x^2} = -\frac{2a}{\gamma^2}\Psi + \left[-\frac{2a}{\gamma^2}\left(x-\frac{\hbar l t}{m}\right)+il\right]^2\Psi = \left[Ax^2+Bx+C\right]\Psi,$$

where

$$A \equiv \left(\frac{2a}{\gamma^2}\right)^2, \quad B \equiv -\left(\frac{2a}{\gamma^2}\right)^2 \frac{2\hbar lt}{m} - \frac{4ial}{\gamma^2} = -\frac{4ial}{\gamma^4},$$

$$C \equiv -\frac{2a}{\gamma^2} + \left(\frac{2a}{\gamma^2}\right)^2\left(\frac{\hbar lt}{m}\right)^2 + \left(\frac{4ial}{\gamma^2}\right)\left(\frac{\hbar lt}{m}\right) - l^2 = -\frac{1}{\gamma^4}(2a\gamma^2 + l^2).$$

$$\begin{aligned}
\langle p^2\rangle &= -\hbar^2\int_{-\infty}^{\infty}\Psi^*[Ax^2 + Bx + C]\Psi\,dx = -\hbar^2[A\langle x^2\rangle + B\langle x\rangle + C] \\
&= -\frac{\hbar^2}{\gamma^4}\left[4a^2\left(\frac{1}{4w^2} + \left(\frac{\hbar lt}{m}\right)^2\right) - 4ial\left(\frac{\hbar lt}{m}\right) - (2a\gamma^2 + l^2)\right] \\
&= -\frac{\hbar^2}{\gamma^4}\left\{\left[a + a\left(\frac{2\hbar at}{m}\right)^2 - 2a - \frac{4ia^2\hbar t}{m}\right] + l^2\left[-1 - \frac{4ia\hbar t}{m} + 4\left(\frac{\hbar at}{m}\right)^2\right]\right\} \\
&= -\frac{\hbar^2}{\gamma^4}(-a\gamma^4 - l^2\gamma^4) = \boxed{\hbar^2(a + l^2).}
\end{aligned}$$

$$\sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{1}{4w^2} + \left(\frac{\hbar lt}{m}\right)^2 - \left(\frac{\hbar lt}{m}\right)^2 = \frac{1}{4w^2} \Rightarrow \boxed{\sigma_x = \frac{1}{2w};}$$

$$\sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2 = \hbar^2 a + \hbar^2 l^2 - \hbar^2 l^2 = \hbar^2 a, \text{ so } \boxed{\sigma_p = \hbar\sqrt{a}.}$$

(e) σ_x and σ_p are same as before, so the uncertainty principle still holds.

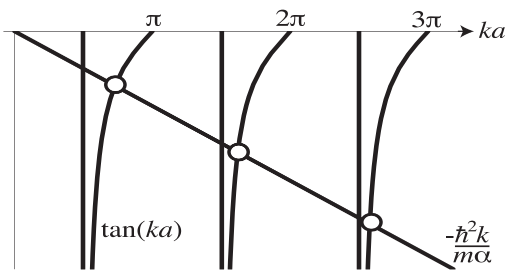
Problem 2.43

Equation 2.25 $\Rightarrow \psi(x) = A\sin kx + B\cos kx,\ 0 \le x \le a,$ with $k = \sqrt{2mE}/\hbar^2$.

Even solutions: $\psi(x) = \psi(-x) = A\sin(-kx) + B\cos(-kx) = -A\sin kx + B\cos kx \quad (-a \le x \le 0)$.

Boundary conditions $\begin{cases} \psi \text{ continuous at } 0: B = B \text{ (no new condition).} \\ \psi' \text{ discontinuous (Eq. 2.128 with sign of } \alpha \text{ switched): } Ak + Ak = \frac{2m\alpha}{\hbar^2}B \Rightarrow B = \frac{\hbar^2 k}{m\alpha}A. \\ \psi \to 0 \text{ at } x = a: \ A\sin(ka) + \frac{\hbar^2 k}{m\alpha}A\cos(ka) = 0 \Rightarrow \tan(ka) = -\frac{\hbar^2 k}{m\alpha}. \end{cases}$

$$\boxed{\psi(x) = A\left(\sin kx + \frac{\hbar^2 k}{m\alpha}\cos kx\right) \ (0 \le x \le a);\ \psi(-x) = \psi(x).}$$



From the graph, the allowed energies are slightly above

$$ka = \frac{n\pi}{2}\ (n = 1, 3, 5, \ldots) \text{ so } \boxed{E_n \gtrsim \frac{n^2\pi^2\hbar^2}{2m(2a)^2}\ (n = 1, 3, 5, \ldots).}$$

These energies are somewhat higher than the corresponding energies for the infinite square well (Eq. 2.30, with $a \to 2a$). As $\alpha \to 0$, the straight line $(-\hbar^2 k/m\alpha)$ gets steeper and steeper, and the intersections get closer to $n\pi/2$; the energies then reduce to those of the ordinary infinite well. As $\alpha \to \infty$, the straight line approaches horizontal, and the intersections are at $n\pi$ $(n = 1, 2, 3, \ldots)$, so $E_n \to \frac{n^2\pi^2\hbar^2}{2ma^2}$ – these are the allowed energies for the infinite square well *of width* a. At this point the barrier is impenetrable, and we have two isolated infinite square wells.

Odd solutions: $\psi(x) = -\psi(-x) = -A\sin(-kx) - B\cos(-kx) = A\sin(kx) - B\cos(kx) \quad (-a \le x \le 0)$.

$$\text{Boundary conditions } \begin{cases} \psi \text{ continuous at } 0: \ B = -B \Rightarrow B = 0. \\ \psi' \text{ discontinuous: } Ak - Ak = \frac{2m\alpha}{\hbar^2}(0) \text{ (no new condition).} \\ \psi(a) = 0 \Rightarrow A\sin(ka) = 0 \Rightarrow ka = \frac{n\pi}{2}\ (n = 2, 4, 6, \ldots). \end{cases}$$

$$\boxed{\psi(x) = A\sin(kx),\ (-a < x < a); \quad E_n = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}\ (n = 2, 4, 6, \ldots).}$$

These are the *exact* (even n) energies (and wave functions) for the infinite square well (of width $2a$). The point is that the *odd* solutions (even n) are *zero* at the origin, so they never "feel" the delta function at all.

Problem 2.44

$$\left.\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + V\psi_1 = E\psi_1 &\Rightarrow -\frac{\hbar^2}{2m}\psi_2\frac{d^2\psi_1}{dx^2} + V\psi_1\psi_2 = E\psi_1\psi_2 \\ -\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2 = E\psi_2 &\Rightarrow -\frac{\hbar^2}{2m}\psi_1\frac{d^2\psi_2}{dx^2} + V\psi_1\psi_2 = E\psi_1\psi_2 \end{aligned}\right\} \Rightarrow -\frac{\hbar^2}{2m}\left[\psi_2\frac{d^2\psi_1}{dx^2} - \psi_1\frac{d^2\psi_2}{dx^2}\right] = 0.$$

But $\frac{d}{dx}\left[\psi_2\frac{d\psi_1}{dx} - \psi_1\frac{d\psi_2}{dx}\right] = \frac{d\psi_2}{dx}\frac{d\psi_1}{dx} + \psi_2\frac{d^2\psi_1}{dx^2} - \frac{d\psi_1}{dx}\frac{d\psi_2}{dx} - \psi_1\frac{d^2\psi_2}{dx^2} = \psi_2\frac{d^2\psi_1}{dx^2} - \psi_1\frac{d^2\psi_2}{dx^2}$. Since this is zero, it follows that $\psi_2\frac{d\psi_1}{dx} - \psi_1\frac{d\psi_2}{dx} = K$ (a constant). But $\psi \to 0$ at ∞ so the constant must be zero. Thus $\psi_2\frac{d\psi_1}{dx} = \psi_1\frac{d\psi_2}{dx}$, or $\frac{1}{\psi_1}\frac{d\psi_1}{dx} = \frac{1}{\psi_2}\frac{d\psi_2}{dx}$, so $\ln\psi_1 = \ln\psi_2 +$ constant, or $\psi_1 = (\text{constant})\psi_2$. QED

Problem 2.45

(a)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} + V\psi_n = E_n\psi_n \Rightarrow \frac{d^2\psi_n}{dx^2} = -\frac{2m}{\hbar^2}(E_n - V)\psi_n; \quad \frac{d^2\psi_m}{dx^2} = -\frac{2m}{\hbar^2}(E_m - V)\psi_m.$$

$$\frac{d}{dx}\left(\frac{d\psi_m}{dx}\psi_n - \psi_m\frac{d\psi_n}{dx}\right) = \frac{d^2\psi_m}{dx^2}\psi_n + \cancel{\frac{d\psi_m}{dx}\frac{d\psi_n}{dx}} - \cancel{\frac{d\psi_m}{dx}\frac{d\psi_n}{dx}} - \psi_m\frac{d^2\psi_n}{dx^2}$$
$$= -\frac{2m}{\hbar^2}\left[(E_m - V)\psi_m\psi_n - \psi_m(E_n - V)\psi_n\right] = -\frac{2m}{\hbar^2}(E_m - E_n)\psi_m\psi_n. \quad \checkmark$$

(b) Integrate both sides:

$$\int_{x_1}^{x_2} \frac{d}{dx}\left(\frac{d\psi_m}{dx}\psi_n - \psi_m\frac{d\psi_n}{dx}\right)dx = [\psi_m'(x_2)\psi_n(x_2) - \cancel{\psi_m(x_2)}\psi_n'(x_2) - \psi_m'(x_1)\psi_n(x_1) + \cancel{\psi_m(x_1)}\psi_n'(x_1)]$$

$$= \psi_m'(x_2)\psi_n(x_2) - \psi_m'(x_1)\psi_n(x_1) = \frac{2m}{\hbar^2}(E_n - E_m)\int_{x_1}^{x_2}\psi_m\psi_n\,dx. \quad [\bigstar]$$

(c) Because x_1 and x_2 are *adjacent* nodes of ψ_m, $\psi_m(x)$ must either be posiitive or negative throughout the interval. We might as well make it positive (if it's not, multiply ψ_m by -1). Then

$$\psi_m(x) \geq 0 \text{ for } x_1 \leq x \leq x_2; \quad \psi'(x_1) \geq 0 \text{ and } \psi'(x_2) \leq 0.$$

If $\psi_n(x)$ has no nodes between x_1 and x_2 then it *too* must have the same sign throughout the interval (and we may as well choose it to be positive):

$$\psi_n(x) \geq 0 \text{ for } x_1 \leq x \leq x_2.$$

In that case $\psi_m'(x_2)\psi_n(x_2) - \psi_m'(x_1)\psi_n(x_1) \leq 0$, but $(E_n - E_m)\int_{x_1}^{x_2}\psi_m\psi_n\,dx > 0$, in contradiction to Equation [★]. *Conclusion:* $\psi_n(x)$ must have at least one node between x_1 and x_2.

Problem 2.46

$-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi}{dx^2} = E\psi$ (where x is measured around the circumference), or $\dfrac{d^2\psi}{dx^2} = -k^2\psi$, with $k \equiv \dfrac{\sqrt{2mE}}{\hbar}$, so

$$\psi(x) = Ae^{ikx} + Be^{-ikx}.$$

But $\psi(x+L) = \psi(x)$, since $x+L$ is the same point as x, so

$$Ae^{ikx}e^{ikL} + Be^{-ikx}e^{-ikL} = Ae^{ikx} + Be^{-ikx},$$

and this is true for *all* x. In particular, for $x = 0$:

(1) $\quad Ae^{ikL} + Be^{-ikL} = A + B.$ And for $x = \dfrac{\pi}{2k}$:

$Ae^{i\pi/2}e^{ikL} + Be^{-i\pi/2}e^{-ikL} = Ae^{i\pi/2} + Be^{-i\pi/2}$, or $iAe^{ikL} - iBe^{-ikL} = iA - iB$, so

(2) $\quad Ae^{ikL} - Be^{-ikL} = A - B.$ Add (1) and (2): $2Ae^{ikL} = 2A.$

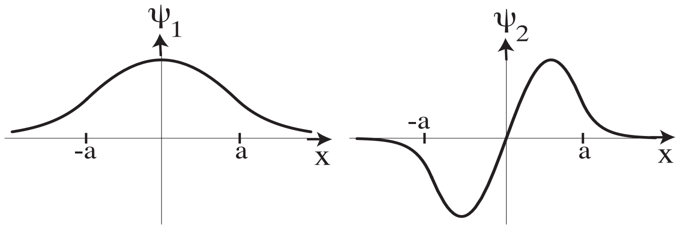
Either $A = 0$, or else $e^{ikL} = 1$, in which case $kL = 2n\pi$ $(n = 0, \pm1, \pm2, \ldots)$. But if $A = 0$, then $Be^{-ikL} = B$, leading to the same conclusion. So for every positive n there are *two* solutions: $\psi_n^+(x) = Ae^{i(2n\pi x/L)}$ and $\psi_n^-(x) = Be^{-i(2n\pi x/L)}$ ($n = 0$ is ok too, but in that case there is just *one* solution). Normalizing: $\int_0^L |\psi_\pm|^2 dx = 1 \Rightarrow A = B = 1/\sqrt{L}$. Any *other* solution (with the same energy) is a linear combination of these.

$$\boxed{\psi_n^\pm(x) = \frac{1}{\sqrt{L}}e^{\pm i(2n\pi x/L)}; \; E_n = \frac{2n^2\pi^2\hbar^2}{mL^2} \; (n = 0, 1, 2, 3, \ldots).}$$

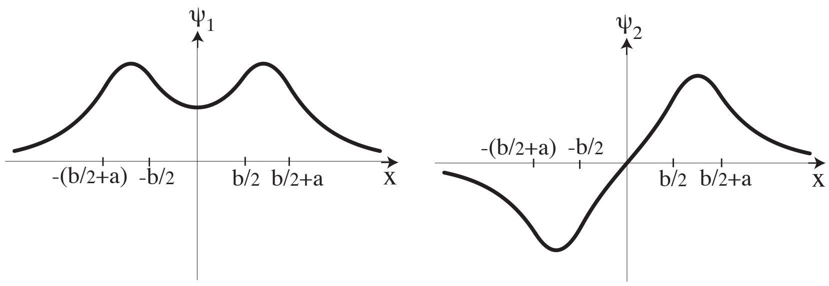
The theorem fails because here ψ does *not* go to zero at ∞; x is restricted to a finite range, and we are unable to determine the constant K (in Problem 2.44).

Problem 2.47

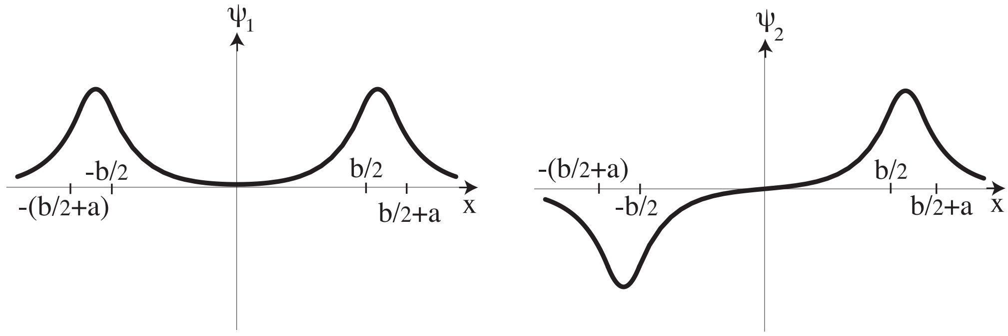
(a) **(i)** $b = 0 \Rightarrow$ ordinary finite square well. Exponential decay outside; sinusoidal inside (cos for ψ_1, sin for ψ_2). No nodes for ψ_1, one node for ψ_2.



(ii) Ground state is *even*. Exponential decay outside, sinusoidal inside the wells, hyperbolic cosine in barrier. First excited state is *odd* – hyperbolic sine in barrier. No nodes for ψ_1, one node for ψ_2.



(iii) For $b \gg a$, same as (ii), but wave function very small in barrier region. Essentially two isolated finite square wells; ψ_1 and ψ_2 are degenerate (in energy); they are even and odd linear combinations of the ground states of the two separate wells.

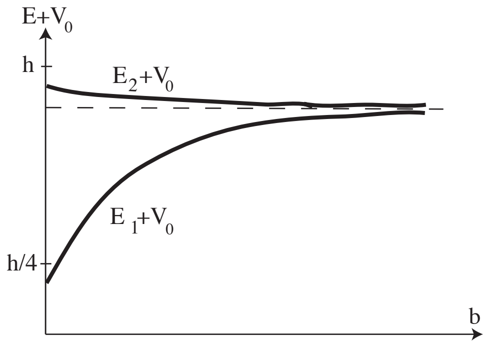


(b) From Eq. 2.160 we know that for $b = 0$ the energies fall slightly below

$$\left.\begin{array}{l} E_1 + V_0 \approx \frac{\pi^2\hbar^2}{2m(2a)^2} = \frac{h}{4} \\ E_2 + V_0 \approx \frac{4\pi^2\hbar^2}{2m(2a)^2} = h \end{array}\right\} \text{ where } h \equiv \frac{\pi^2\hbar^2}{2ma^2}.$$

For $b \gg a$, the width of each (isolated) well is a, so

$$E_1 + V_0 \approx E_2 + V_0 \approx \frac{\pi^2\hbar^2}{2ma^2} = h \text{ (again, slightly } below \text{ this).}$$



[Within each well, $\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(V_0 + E)\psi$, so the more *curved* the wave function, the higher the energy.]

(c) In the (even) ground state the energy is *lowest* in configuration (i), with $b \to 0$, so the electron tends to draw the nuclei $\boxed{\text{together,}}$ promoting *bonding* of the atoms. In the (odd) first excited state, by contrast, the electron drives the nuclei $\boxed{\text{apart.}}$

Problem 2.48

(a) Let $V_0 \equiv 32\hbar^2/ma^2$. This is just like the *odd* bound states for the finite square well, since they are the ones that go to zero at the origin. Referring to the solution to Problem 2.29, the wave function is

$$\psi(x) = \begin{cases} D \sin lx, & l \equiv \sqrt{2m(E+V_0)}/\hbar \quad (0 < x < a), \\ Fe^{-\kappa x}, & \kappa \equiv \sqrt{-2mE}/\hbar \quad (x > a), \end{cases}$$

and the boundary conditions at $x = a$ yield

$$-\cot z = \sqrt{(z_0/z)^2 - 1}$$

with

$$z_0 = \frac{\sqrt{2mV_0}}{\hbar}a = \frac{\sqrt{2m(32\hbar^2/ma^2)}}{\hbar}a = 8.$$

Referring to the figure (Problem 2.29), and noting that $(5/2)\pi = 7.85 < z_0 < 3\pi = 9.42$, we see that there are $\boxed{\text{three bound states.}}$

(b) Let

$$I_1 \equiv \int_0^a |\psi|^2 dx = |D|^2 \int_0^a \sin^2 lx\, dx = |D|^2 \left[\frac{x}{2} - \frac{1}{2l}\sin lx \cos lx\right]\Bigg|_0^a = |D|^2 \left[\frac{a}{2} - \frac{1}{2l}\sin la \cos la\right];$$

$$I_2 \equiv \int_a^\infty |\psi|^2 dx = |F|^2 \int_a^\infty e^{-2\kappa x}\, dx = |F|^2 \left[-\frac{e^{-2\kappa x}}{2\kappa}\right]\Bigg|_a^\infty = |F|^2 \frac{e^{-2\kappa a}}{2\kappa}.$$

But continuity at $x = a \Rightarrow Fe^{-\kappa a} = D \sin la$, so $I_2 = |D|^2 \frac{\sin^2 la}{2\kappa}$.
Normalizing:

$$1 = I_1 + I_2 = |D|^2 \left[\frac{a}{2} - \frac{1}{2l}\sin la \cos la + \frac{\sin^2 la}{2\kappa}\right] = \frac{1}{2\kappa}|D|^2 \left[\kappa a - \frac{\kappa}{l}\sin la \cos la + \sin^2 la\right]$$

But (referring again to Problem 2.29) $\kappa/l = -\cot la$, so

$$= \frac{1}{2\kappa}|D|^2 \left[\kappa a + \cot la \sin la \cos la + \sin^2 la\right] = |D|^2 \frac{(1+\kappa a)}{2\kappa}.$$

So $|D|^2 = 2\kappa/(1+\kappa a)$, and the probability of finding the particle outside the well is

$$P = I_2 = \frac{2\kappa}{1+\kappa a}\frac{\sin^2 la}{2\kappa} = \frac{\sin^2 la}{1+\kappa a}.$$

We can express this in terms of $z \equiv la$ and z_0: $\kappa a = \sqrt{z_0^2 - z^2}$ (page 80),

$$\sin^2 la = \sin^2 z = \frac{1}{1+\cot^2 z} = \frac{1}{1+(z_0/z)^2 - 1} = \left(\frac{z}{z_0}\right)^2 \Rightarrow P = \frac{z^2}{z_0^2(1+\sqrt{z_0^2 - z^2})}.$$

So far, this is correct for *any* bound state. In the present case $z_0 = 8$ and z is the third solution to $-\cot z = \sqrt{(8/z)^2 - 1}$, which occurs somewhere in the interval $7.85 < z < 8$. Mathematica gives $z = 7.9573$ and $\boxed{P = 0.54204.}$

```
FindRoot[Cot[z] == -√((8/z)^2 - 1), {z, 7.9}]
{z → 7.95732}
z^2/(64 (1 + √(64 - z^2)))
      z²
─────────────────
64 (1 + √(64 - z²))
% /. z -> 7.957321523328964`
0.542041
```

Problem 2.49

(a)

$$\frac{\partial\Psi}{\partial t} = \left(-\frac{m\omega}{2\hbar}\right)\left[\frac{x_0^2}{2}\left(-2i\omega e^{-2i\omega t}\right) + \frac{i\hbar}{m} - 2x_0 x(-i\omega)e^{-i\omega t}\right]\Psi, \text{ so}$$

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[-\frac{1}{2}m x_0^2\omega^2 e^{-2i\omega t} + \frac{1}{2}\hbar\omega + m x_0 x\omega^2 e^{-i\omega t}\right]\Psi.$$

$$\frac{\partial\Psi}{\partial x} = \left[\left(-\frac{m\omega}{2\hbar}\right)\left(2x - 2x_0 e^{-i\omega t}\right)\right]\Psi = -\frac{m\omega}{\hbar}\left(x - x_0 e^{-i\omega t}\right)\Psi;$$

$$\frac{\partial^2\Psi}{\partial x^2} = -\frac{m\omega}{\hbar}\Psi - \frac{m\omega}{\hbar}\left(x - x_0 e^{-i\omega t}\right)\frac{\partial\Psi}{\partial x} = \left[-\frac{m\omega}{\hbar} + \left(\frac{m\omega}{\hbar}\right)^2\left(x - x_0 e^{-i\omega t}\right)^2\right]\Psi.$$

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+\frac{1}{2}m\omega^2x^2\Psi &= -\frac{\hbar^2}{2m}\left[-\frac{m\omega}{\hbar}+\left(\frac{m\omega}{\hbar}\right)^2\left(x-x_0e^{-i\omega t}\right)^2\right]\Psi+\frac{1}{2}m\omega^2x^2\Psi \\
&= \left[\frac{1}{2}\hbar\omega-\frac{1}{2}m\omega^2\left(x^2-2x_0xe^{-i\omega t}+x_0^2e^{-2i\omega t}\right)+\frac{1}{2}m\omega^2x^2\right]\Psi \\
&= \left[\frac{1}{2}\hbar\omega+mx_0x\omega^2e^{-i\omega t}-\frac{1}{2}m\omega^2x_0^2e^{-2i\omega t}\right]\Psi \\
&= i\hbar\frac{\partial\Psi}{\partial t}\ \text{(comparing second line above).}\quad\checkmark
\end{aligned}
$$

(b)

$$
\begin{aligned}
|\Psi|^2 &= \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{m\omega}{2\hbar}\left[\left(x^2+\frac{x_0^2}{2}\left(1+e^{2i\omega t}\right)-\frac{i\hbar t}{m}-2x_0xe^{i\omega t}\right)+\left(x^2+\frac{x_0^2}{2}\left(1+e^{-2i\omega t}\right)+\frac{i\hbar t}{m}-2x_0xe^{-i\omega t}\right)\right]} \\
&= \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{m\omega}{2\hbar}\left[2x^2+x_0^2+x_0^2\cos(2\omega t)-4x_0x\cos(\omega t)\right]}.\quad\text{But } x_0^2[1+\cos(2\omega t)]=2x_0^2\cos^2\omega t,\ \text{so} \\
&= \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{m\omega}{\hbar}\left[x^2-2x_0x\cos(\omega t)+x_0^2\cos^2(\omega t)\right]} = \boxed{\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{m\omega}{\hbar}(x-x_0\cos\omega t)^2}.}
\end{aligned}
$$

The wave packet is a *Gaussian* of fixed shape, whose *center* oscillates back and forth sinusoidally, with amplitude x_0 and angular frequency ω.

(c) Note that this wave function *is* correctly normalized (compare Eq. 2.60). Let $y\equiv x-x_0\cos\omega t$:

$$
\langle x\rangle=\int x|\Psi|^2dx=\int(y+x_0\cos\omega t)|\Psi|^2dy=0+x_0a\cos\omega t\int|\Psi|^2dy=\boxed{x_0\cos\omega t.}
$$

$$
\langle p\rangle=m\frac{d\langle x\rangle}{dt}=\boxed{-mx_0\omega\sin\omega t.}\quad \frac{d\langle p\rangle}{dt}=-mx_0\omega^2\cos\omega t.\quad V=\frac{1}{2}m\omega^2x^2\Longrightarrow\frac{dV}{dx}=m\omega^2x.
$$

$$
\langle-\frac{dV}{dx}\rangle=-m\omega^2\langle x\rangle=-m\omega^2x_0\cos\omega t=\frac{d\langle p\rangle}{dt},\ \text{so Ehrenfest's theorem } \textit{is} \text{ satisfied.}
$$

Problem 2.50

(a)

$$
\frac{\partial\Psi}{\partial t}=\left[-\frac{m\alpha}{\hbar^2}\frac{\partial}{\partial t}|x-vt|-i\frac{(E+\frac{1}{2}mv^2)}{\hbar}\right]\Psi;\quad \frac{\partial}{\partial t}|x-vt|=\left\{\begin{array}{ll}-v, & \text{if } x-vt>0\\ v, & \text{if } x-vt<0\end{array}\right\}.
$$

We can write this in terms of the θ-function (Eq. 2.146):

$$
2\theta(z)-1=\left\{\begin{array}{ll}1, & \text{if } z>0\\ -1, & \text{if } z<0\end{array}\right\},\ \text{so}\ \frac{\partial}{\partial t}|x-vt|=-v[2\theta(x-vt)-1].
$$

$$
i\hbar\frac{\partial\Psi}{\partial t}=\left\{i\frac{m\alpha v}{\hbar}[2\theta(x-vt)-1]+E+\frac{1}{2}mv^2\right\}\Psi.\qquad[\bigstar]
$$

$$\frac{\partial\Psi}{\partial x} = \left[-\frac{m\alpha}{\hbar^2}\frac{\partial}{\partial x}|x-vt| + \frac{imv}{\hbar}\right]\Psi$$

$$\frac{\partial}{\partial x}|x-vt| = \{1, \text{if } x > vt;\ -1, \text{if } x < vt\} = 2\theta(x-vt) - 1.$$

$$= \left\{-\frac{m\alpha}{\hbar^2}[2\theta(x-vt)-1] + \frac{imv}{\hbar}\right\}\Psi.$$

$$\frac{\partial^2\Psi}{\partial x^2} = \left\{-\frac{m\alpha}{\hbar^2}[2\theta(x-vt)-1] + \frac{imv}{\hbar}\right\}^2\Psi - \frac{2m\alpha}{\hbar^2}\left[\frac{\partial}{\partial x}\theta(x-vt)\right]\Psi.$$

But (from Problem 2.23(b)) $\frac{\partial}{\partial x}\theta(x-vt) = \delta(x-vt)$, so

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - \alpha\delta(x-vt)\Psi$$
$$= \left(-\frac{\hbar^2}{2m}\left\{-\frac{m\alpha}{\hbar^2}[2\theta(x-vt)-1] + \frac{imv}{\hbar}\right\}^2 + \alpha\delta(x-vt) - \alpha\delta(x-vt)\right)\Psi$$
$$= -\frac{\hbar^2}{2m}\left\{\frac{m^2\alpha^2}{\hbar^4}\underbrace{[2\theta(x-vt)-1]^2}_{1} - \frac{m^2v^2}{\hbar^2} - 2i\frac{mv}{\hbar}\frac{m\alpha}{\hbar^2}[2\theta(x-vt)-1]\right\}\Psi$$
$$= \left\{-\frac{m\alpha^2}{2\hbar^2} + \frac{1}{2}mv^2 + i\frac{mv\alpha}{\hbar}[2\theta(x-vt)-1]\right\}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \text{ (compare [}\bigstar\text{]).} \quad \checkmark$$

(b)

$$|\Psi|^2 = \frac{m\alpha}{\hbar^2}e^{-2m\alpha|y|/\hbar^2} \quad (y \equiv x - vt).$$

Check normalization: $2\frac{m\alpha}{\hbar^2}\int_0^\infty e^{-2m\alpha y/\hbar^2}dy = \frac{2m\alpha}{\hbar^2}\frac{\hbar^2}{2m\alpha} = 1.$ ✓

$$\langle H\rangle = \int_{-\infty}^{\infty}\Psi^* H\Psi dx. \quad \text{But } H\Psi = i\hbar\frac{\partial\Psi}{\partial t}, \text{ which we calculated above [}\bigstar\text{].}$$
$$= \int\left\{\frac{im\alpha v}{\hbar}[2\theta(y)-1] + E + \frac{1}{2}mv^2\right\}|\Psi|^2 dy = \boxed{E + \frac{1}{2}mv^2.}$$

(Note that $[2\theta(y)-1]$ is an *odd* function of y.) *Interpretation:* The wave packet is dragged along (at speed v) with the delta-function. The total energy is the energy it *would* have in a stationary delta-function (E), plus *kinetic* energy due to the motion ($\frac{1}{2}mv^2$).

Problem 2.51

$$\Psi_0 = \left(\frac{2a}{\pi}\right)^{1/4}\frac{1}{\gamma}e^{-a(x+\frac{1}{2}gt^2)^2/\gamma^2}; \quad \gamma = \sqrt{1 + 2ia\hbar t/m}.$$

$$\frac{\partial\Psi}{\partial t} = \left[\frac{\partial\Psi_0}{\partial t} + \Psi_0\left(-\frac{img}{\hbar}\right)\left(x + \frac{1}{2}gt^2\right)\right]\exp\left[-i\frac{mgt}{\hbar}\left(x + \frac{1}{6}gt^2\right)\right],$$

$$
\begin{aligned}
\frac{\partial \Psi_0}{\partial t} &= \left(\frac{2a}{\pi}\right)^{1/4}\left\{-\frac{1}{\gamma^2}\left(\frac{d\gamma}{dt}\right)+\frac{1}{\gamma}\left[-\frac{2a}{\gamma^2}\left(x+\frac{1}{2}gt^2\right)gt - a\left(x+\frac{1}{2}gt^2\right)^2\left(-\frac{2}{\gamma^3}\frac{d\gamma}{dt}\right)\right]\right\}e^{-a(x+\frac{1}{2}gt^2)^2/\gamma^2} \\
&= \left[-\frac{1}{\gamma}\frac{d\gamma}{dt}-\frac{2agt}{\gamma^2}\left(x+\frac{1}{2}gt^2\right)+\frac{2a}{\gamma^3}\left(x+\frac{1}{2}gt^2\right)^2\frac{d\gamma}{dt}\right]\Psi_0.
\end{aligned}
$$

But $\quad \dfrac{d\gamma}{dt}=\dfrac{1}{2\gamma}\left(\dfrac{2ia\hbar}{m}\right)=\dfrac{ia\hbar}{\gamma m}, \quad$ so

$$
\begin{aligned}
\frac{\partial \Psi_0}{\partial t} &= \left[\frac{-ia\hbar}{\gamma^2 m}-\frac{2agt}{\gamma^2}\left(x+\frac{1}{2}gt^2\right)+\frac{2ia^2\hbar}{\gamma^4 m}\left(x+\frac{1}{2}gt^2\right)^2\right]\Psi_0, \quad \text{and hence} \\
\frac{\partial \Psi}{\partial t} &= \left[-\frac{ia\hbar}{\gamma^2 m}-\frac{2agt}{\gamma^2}\left(x+\frac{1}{2}gt^2\right)+\frac{2ia^2\hbar}{\gamma^4 m}\left(x+\frac{1}{2}gt^2\right)^2-\frac{img}{\hbar}\left(x+\frac{1}{2}gt^2\right)\right]\Psi. \qquad [\bigstar]
\end{aligned}
$$

Meanwhile

$$
\begin{aligned}
\frac{\partial \Psi}{\partial x} &= \left[\frac{\partial \Psi_0}{\partial x}-\Psi_0\frac{imgt}{\hbar}\right]\exp\left[-\frac{imgt}{\hbar}\left(x+\frac{1}{6}gt^2\right)\right] \\
\frac{\partial \Psi_0}{\partial x} &= -2a\left[\left(x+\frac{1}{2}gt^2\right)/\gamma^2\right]\Psi_0, \quad \text{so} \\
\frac{\partial \Psi}{\partial x} &= \left[-2a\left(x+\frac{1}{2}gt^2\right)/\gamma^2-\frac{imgt}{\hbar}\right]\Psi, \quad \text{and hence} \\
\frac{\partial^2 \Psi}{\partial x^2} &= \left\{-\frac{2a}{\gamma^2}\Psi+\left[-2a\left(x+\frac{1}{2}gt^2\right)/\gamma^2-\frac{imgt}{\hbar}\right]\frac{\partial \Psi}{\partial x}\right\} = \left\{-\frac{2a}{\gamma^2}+\left[-2a\left(x+\frac{1}{2}gt^2\right)/\gamma^2-\frac{imgt}{\hbar}\right]^2\right\}\Psi.
\end{aligned}
$$

$$
-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi = \left\{\frac{\hbar^2 a}{m\gamma^2}-\frac{\hbar^2}{2m}\left[-2a\left(x+\frac{1}{2}gt^2\right)/\gamma^2-\frac{imgt}{\hbar}\right]^2+mgx\right\}\Psi. \qquad [\bigstar\bigstar]
$$

So the time-dependent Schrödinger equation is satisfied if $i\hbar$ times the square bracket in Equation $[\bigstar]$ is equal to the curly bracket in Equation $[\bigstar\bigstar]$:

$$
\begin{aligned}
&\cancel{\frac{a\hbar^2}{\gamma^2 m}}-\frac{2ia\hbar gt}{\gamma^2}\left(x+\frac{1}{2}gt^2\right)-\frac{2a^2\hbar^2}{\gamma^4 m}\left(x+\frac{1}{2}gt^2\right)^2+mg\left(\cancel{x}+\frac{1}{2}gt^2\right) \\
&\qquad \stackrel{?}{=} \cancel{\frac{\hbar^2 a}{m\gamma^2}}-\frac{\hbar^2}{2m}\left[-2a\left(x+\frac{1}{2}gt^2\right)/\gamma^2-\frac{imgt}{\hbar}\right]^2+\cancel{mgx}.
\end{aligned}
$$

I have cancelled the first terms on either side, and also the mgx terms. This leaves

$$
\begin{aligned}
&-\frac{2ia\hbar gt}{\gamma^2}\left(x+\frac{1}{2}gt^2\right)-\frac{2a^2\hbar^2}{\gamma^4 m}\left(x+\frac{1}{2}gt^2\right)^2+\frac{mg^2t^2}{2} \\
&\qquad \stackrel{?}{=} -\frac{\hbar^2}{2m}\left[\frac{4a^2}{\gamma^4}\left(x+\frac{1}{2}gt^2\right)^2+\frac{4iamgt}{\hbar\gamma^2}\left(x+\frac{1}{2}gt^2\right)-\frac{m^2g^2t^2}{\hbar^2}\right].
\end{aligned}
$$

The terms quadratic in $\left(x+\frac{1}{2}gt^2\right)$ cancel, as do the linear terms, and so do those of zeroth order. This confirms that Ψ satisfies the Schrödinger equation.

To calculate the expectation value of x, first note that

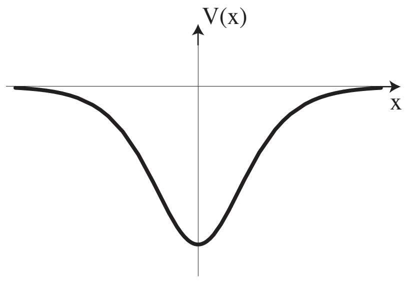
$|\Psi|^2 = \Psi_0|^2 = \sqrt{\frac{2a}{\pi}}\frac{1}{|\gamma|^2}e^{-\left(x+\frac{1}{2}gt^2\right)^2\left(\frac{1}{\gamma^2}+\frac{1}{(\gamma^*)^2}\right)}$. But $\frac{1}{\gamma^2}+\frac{1}{(\gamma^*)^2} = \frac{(\gamma^*)+\gamma^2}{|\gamma|^4} = \frac{2}{|\gamma|^4}$, so (letting $y \equiv x+\frac{1}{2}gt^2$)

$$\begin{aligned}
\langle x\rangle &= \sqrt{\frac{2a}{\pi}}\frac{1}{|\gamma|^2}\int_{-\infty}^{\infty} xe^{-2a\left(x+\frac{1}{2}gt^2\right)^2/|\gamma|^4}\,dx = \sqrt{\frac{2a}{\pi}}\frac{1}{|\gamma|^2}\int_{-\infty}^{\infty}\left(y-\frac{1}{2}gt^2\right)e^{-2ay^2/|\gamma|^4}\,dy \\
&= \sqrt{\frac{2a}{\pi}}\frac{1}{|\gamma|^2}\left(-\frac{1}{2}gt^2\right)\int_{-\infty}^{\infty}e^{-2ay^2/|\gamma|^4}\,dy.
\end{aligned}$$

The integral is $\sqrt{\pi/2a}\,|\gamma|^2$, so $\boxed{\langle x\rangle = -\frac{1}{2}gt^2.}$ This is precisely the *classical* motion under free fall—as we should have anticipated from Ehrenfest's theorem.

Problem 2.52

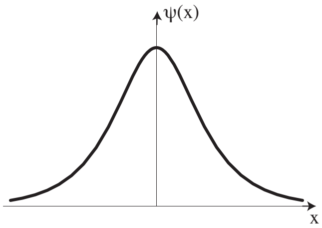
(a)



(b) $\frac{d\psi_0}{dx} = -Aa\,\text{sech}(ax)\tanh(ax)$; $\quad \frac{d^2\psi_0}{dx^2} = -Aa^2\left[-\text{sech}(ax)\tanh^2(ax) + \text{sech}(ax)\,\text{sech}^2(ax)\right].$

$$\begin{aligned}
H\psi_0 &= -\frac{\hbar^2}{2m}\frac{d^2\psi_0}{dx^2} - \frac{\hbar^2a^2}{m}\text{sech}^2(ax)\psi_0 \\
&= \frac{\hbar^2}{2m}Aa^2\left[-\text{sech}(ax)\tanh^2(ax) + \text{sech}^3(ax)\right] - \frac{\hbar^2a^2}{m}A\,\text{sech}^3(ax) \\
&= \frac{\hbar^2a^2A}{2m}\left[-\text{sech}(ax)\tanh^2(ax) + \text{sech}^3(ax) - 2\,\text{sech}^3(ax)\right] \\
&= -\frac{\hbar^2a^2}{2m}A\,\text{sech}(ax)\left[\tanh^2(ax) + \text{sech}^2(ax)\right]. \\
&\quad \text{But } (\tanh^2\theta + \text{sech}^2\theta) = \frac{\sinh^2\theta}{\cosh^2\theta} + \frac{1}{\cosh^2\theta} = \frac{\sinh^2\theta + 1}{\cosh^2\theta} = 1, \text{ so} \\
&= -\frac{\hbar^2a^2}{2m}\psi_0. \quad \text{QED} \quad \text{Evidently } \boxed{E = -\frac{\hbar^2a^2}{2m}.}
\end{aligned}$$

$$1 = |A|^2\int_{-\infty}^{\infty}\text{sech}^2(ax)dx = |A|^2\,\frac{1}{a}\tanh(ax)\Big|_{-\infty}^{\infty} = \frac{2}{a}|A|^2 \Longrightarrow \boxed{A = \sqrt{\frac{a}{2}}.}$$



(c)

$$\frac{d\psi_k}{dx} = \frac{A}{ik+a}\left[(ik - a\tanh ax)ik - a^2\operatorname{sech}^2 ax\right]e^{ikx}.$$

$$\frac{d^2\psi_k}{dx^2} = \frac{A}{ik+a}\left\{ik\left[(ik - a\tanh ax)ik - a^2\operatorname{sech}^2 ax\right] - a^2 ik\operatorname{sech}^2 ax + 2a^3\operatorname{sech}^2 ax\tanh ax\right\}e^{ikx}.$$

$$\begin{aligned}-\frac{\hbar^2}{2m}\frac{d^2\psi_k}{dx^2} + V\psi_k &= \frac{A}{ik+a}\left\{\frac{-\hbar^2 ik}{2m}\left[-k^2 - iak\tanh ax - a^2\operatorname{sech}^2 ax\right] + \frac{\hbar^2 a^2}{2m}ik\operatorname{sech}^2 ax\right.\\ &\quad\left.-\frac{\hbar^2 a^3}{m}\operatorname{sech}^2 ax\tanh ax - \frac{\hbar^2 a^2}{m}\operatorname{sech}^2 ax(ik - a\tanh ax)\right\}e^{ikx}\\ &= \frac{Ae^{ikx}}{ik+a}\frac{\hbar^2}{2m}\left(ik^3 - ak^2\tanh ax + ia^2k\operatorname{sech}^2 ax + ia^2k\operatorname{sech}^2 ax\right.\\ &\quad\left.-2a^3\operatorname{sech}^2 ax\tanh ax - 2ia^2k\operatorname{sech}^2 ax + 2a^3\operatorname{sech}^2 ax\tanh ax\right)\\ &= \frac{Ae^{ikx}}{ik+a}\frac{\hbar^2}{2m}k^2(ik - a\tanh ax) = \frac{\hbar^2k^2}{2m}\psi_k = E\psi_k.\quad \text{QED}\end{aligned}$$

As $x \to +\infty$, $\tanh ax \to +1$, so $\boxed{\psi_k(x) \to A\left(\frac{ik-a}{ik+a}\right)e^{ikx},}$ which represents a transmitted wave.

$$\boxed{R = 0.}\qquad T = \left|\frac{ik-a}{ik+a}\right|^2 = \left(\frac{-ik-a}{-ik+a}\right)\left(\frac{ik-a}{ik+a}\right) = \boxed{1.}$$

Problem 2.53

(a) (1) From Eq. 2.136: $F + G = A + B$.
(2) From Eq. 2.138: $F - G = (1+2i\beta)A - (1-2i\beta)B$, where $\beta = m\alpha/\hbar^2 k$.
Subtract: $2G = -2i\beta A + 2(1-i\beta)B \Rightarrow B = \frac{1}{1-i\beta}(i\beta A + G)$. Multiply (1) by $(1-2i\beta)$ and add:
$2(1-i\beta)F - 2i\beta G = 2A \Rightarrow F = \frac{1}{1-i\beta}(A + i\beta G)$. $\boxed{\mathsf{S} = \frac{1}{1-i\beta}\begin{pmatrix} i\beta & 1 \\ 1 & i\beta\end{pmatrix}.}$

(b) For an *even* potential, $V(-x) = V(x)$, scattering from the right is the same as scattering from the left, with $x \leftrightarrow -x$, $A \leftrightarrow G$, $B \leftrightarrow F$ (see Fig. 2.21): $F = S_{11}G + S_{12}A$, $B = S_{21}G + S_{22}A$. So $S_{11} = S_{22}$, $S_{21} = S_{12}$. (Note that the delta-well S matrix in (a) has this property.) In the case of the finite square well, Eqs. 2.170 and 2.171 give

$$S_{21} = \frac{e^{-2ika}}{\cos 2la - i\frac{(k^2+l^2)}{2kl}\sin 2la};\qquad S_{11} = \frac{i\frac{(l^2-k^2)}{2kl}\sin 2la\, e^{-2ika}}{\cos 2la - i\frac{(k^2+l^2)}{2kl}\sin 2la}.\quad \text{So}$$

$$\boxed{\mathsf{S} = \frac{e^{-2ika}}{\cos 2la - i\frac{(k^2+l^2)}{2kl}\sin 2la}\begin{pmatrix} i\frac{(l^2-k^2)}{2kl}\sin 2la & 1 \\ 1 & i\frac{(l^2-k^2)}{2kl}\sin 2la \end{pmatrix}.}$$

Problem 2.54

(a)

$$B = S_{11}A + S_{12}G \Rightarrow G = \frac{1}{S_{12}}(B - S_{11}A) = M_{21}A + M_{22}B \Rightarrow M_{21} = -\frac{S_{11}}{S_{12}},\ M_{22} = \frac{1}{S_{12}}.$$

$$F = S_{21}A + S_{22}G = S_{21}A + \frac{S_{22}}{S_{12}}(B - S_{11}A) = -\frac{(S_{11}S_{22} - S_{12}S_{21})}{S_{12}}A + \frac{S_{22}}{S_{12}}B = M_{11}A + M_{12}B.$$

$$\Rightarrow M_{11} = -\frac{\det S}{S_{12}},\ M_{12} = \frac{S_{22}}{S_{12}}.\quad \boxed{\mathsf{M} = \frac{1}{S_{12}}\begin{pmatrix} -\det(\mathsf{S}) & S_{22} \\ -S_{11} & 1 \end{pmatrix}.}\quad \text{Conversely:}$$

$$G = M_{21}A + M_{22}B \Rightarrow B = \frac{1}{M_{22}}(G - M_{21}A) = S_{11}A + S_{12}G \Rightarrow S_{11} = -\frac{M_{21}}{M_{22}};\ S_{12} = \frac{1}{M_{22}}.$$

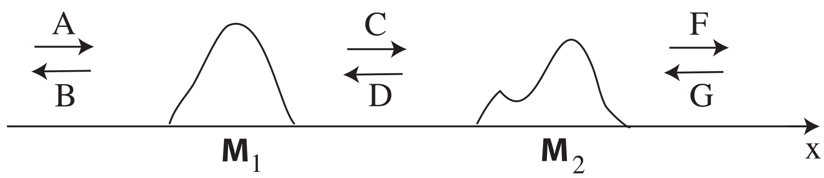
$$F = M_{11}A + M_{12}B = M_{11}A + \frac{M_{12}}{M_{22}}(G - M_{21}A) = \frac{(M_{11}M_{22} - M_{12}M_{21})}{M_{22}}A + \frac{M_{12}}{M_{22}}G = S_{21}A + S_{22}G.$$

$$\Rightarrow S_{21} = \frac{\det M}{M_{22}};\ S_{22} = \frac{M_{12}}{M_{22}}.\quad \boxed{\mathsf{S} = \frac{1}{M_{22}}\begin{pmatrix} -M_{21} & 1 \\ \det(\mathsf{M}) & M_{12} \end{pmatrix}.}$$

[It happens that the time-reversal invariance of the Schrödinger equation, plus conservation of probability, requires $M_{22} = M_{11}^*,\ M_{21} = M_{12}^*$, and $\det(\mathsf{M}) = 1$, but I won't use this here. See Merzbacher's *Quantum Mechanics*. Similarly, for *even* potentials $S_{11} = S_{22},\ S_{12} = S_{21}$ (Problem 2.53).]

$$R_l = |S_{11}|^2 = \boxed{\left|\frac{M_{21}}{M_{22}}\right|^2},\ T_l = |S_{21}|^2 = \boxed{\left|\frac{\det(\mathsf{M})}{M_{22}}\right|^2},\ R_r = |S_{22}|^2 = \boxed{\left|\frac{M_{12}}{M_{22}}\right|^2},\ T_r = |S_{12}|^2 = \boxed{\frac{1}{|M_{22}|^2}}.$$

(b)



$$\begin{pmatrix} F \\ G \end{pmatrix} = \mathsf{M}_2\begin{pmatrix} C \\ D \end{pmatrix},\ \begin{pmatrix} C \\ D \end{pmatrix} = \mathsf{M}_1\begin{pmatrix} A \\ B \end{pmatrix},\ \text{so}\ \begin{pmatrix} F \\ G \end{pmatrix} = \mathsf{M}_2\mathsf{M}_1\begin{pmatrix} A \\ B \end{pmatrix} = \mathsf{M}\begin{pmatrix} A \\ B \end{pmatrix},\ \text{with } \mathsf{M} = \mathsf{M}_2\mathsf{M}_1.\quad \text{QED}$$

(c)

$$\psi(x) = \left\{ \begin{array}{ll} Ae^{ikx} + Be^{-ikx} & (x < a) \\ Fe^{ikx} + Ge^{-ikx} & (x > a) \end{array} \right\}.$$

$$\left\{ \begin{array}{ll} \text{Continuity of } \psi: & Ae^{ika} + Be^{-ika} = Fe^{ika} + Ge^{-ika} \\ \text{Discontinuity of } \psi': & ik\left(Fe^{ika} - Ge^{-ika}\right) - ik\left(Ae^{ika} - Be^{-ika}\right) = -\frac{2m\alpha}{\hbar^2}\psi(a) = -\frac{2m\alpha}{\hbar^2}\left(Ae^{ika} + Be^{-ika}\right). \end{array} \right.$$

(1) $Fe^{2ika} + G = Ae^{2ika} + B.$

(2) $Fe^{2ika} - G = Ae^{2ika} - B + i\frac{2m\alpha}{\hbar^2 k}\left(Ae^{2ika} + B\right).$

Add (1) and (2):

$$2Fe^{2ika} = 2Ae^{2ika} + i\frac{2m\alpha}{\hbar^2 k}\left(Ae^{2ika} + B\right) \Rightarrow F = \left(1 + i\frac{m\alpha}{\hbar^2 k}\right)A + i\frac{m\alpha}{\hbar^2 k}e^{-2ika}B = M_{11}A + M_{12}B.$$

$$\text{So } M_{11} = (1 + i\beta);\ M_{12} = i\beta e^{-2ika};\ \beta \equiv \frac{m\alpha}{\hbar^2 k}.$$

Subtract (2) from (1):

$$2G = 2B - 2i\beta e^{2ika}A - 2i\beta B \Rightarrow G = (1 - i\beta)B - i\beta e^{2ika}A = M_{21}A + M_{22}B.$$

$$\text{So } M_{21} = -i\beta e^{2ika};\ M_{22} = (1 - i\beta). \qquad \boxed{\mathsf{M} = \begin{pmatrix} (1+i\beta) & i\beta e^{-2ika} \\ -i\beta e^{2ika} & (1-i\beta) \end{pmatrix}.}$$

(d)

$$\mathsf{M}_2 = \begin{pmatrix} (1+i\beta) & i\beta e^{-2ika} \\ -i\beta e^{2ika} & (1-i\beta) \end{pmatrix};\ \text{to get } \mathsf{M}_1,\ \text{just switch the sign of } a\text{: } \mathsf{M}_1 = \begin{pmatrix} (1+i\beta) & i\beta e^{2ika} \\ -i\beta e^{-2ika} & (1-i\beta) \end{pmatrix}.$$

$$\mathsf{M} = \mathsf{M}_2\mathsf{M}_1 = \boxed{\begin{pmatrix} [1 + 2i\beta + \beta^2(e^{-4ika} - 1)] & 2i\beta[\cos 2ka - \beta\sin 2ka] \\ -2i\beta[\cos 2ka - \beta\sin 2ka] & [1 - 2i\beta + \beta^2(e^{4ika} - 1)] \end{pmatrix}.}$$

$$T = T_l = T_r = \frac{1}{|M_{22}|^2} \Rightarrow$$

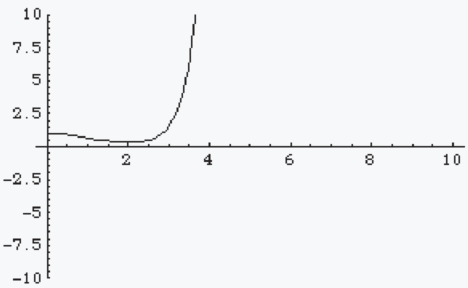
$$\begin{aligned} T^{-1} &= [1 + 2i\beta + \beta^2(e^{-4ika} - 1)][1 - 2i\beta + \beta^2(e^{4ika} - 1)] \\ &= 1 - 2i\beta + \beta^2 e^{4ika} - \beta^2 + 2i\beta + 4\beta^2 + 2i\beta^3 e^{4ika} - 2i\beta^3 + \beta^2 e^{-4ika} \\ &\quad - \beta^2 - 2i\beta^3 e^{-4ika} + 2i\beta^3 + \beta^4(1 - e^{-4ika} - e^{4ika} + 1) \\ &= 1 + 2\beta^2 + \beta^2(e^{-4ika} + e^{4ika}) - 2i\beta^3(e^{-4ika} - e^{4ika}) + 2\beta^4 - \beta^4(e^{-4ika} + e^{4ika}) \\ &= 1 + 2\beta^2 + 2\beta^2\cos 4ka + 2i\beta^3 2i\sin 4ka + 2\beta^4 - 2\beta^4\cos 4ka \\ &= 1 + 2\beta^2(1 + \cos 4ka) - 4\beta^3\sin 4ka + 2\beta^4(1 - \cos 4ka) \\ &= 1 + 4\beta^2\cos^2 2ka - 8\beta^3\sin 2ka\cos 2ka - 4\beta^4\sin^2 2ka \end{aligned}$$

$$\boxed{T = \frac{1}{1 + 4\beta^2(\cos 2ka - \beta\sin 2ka)^2}}$$

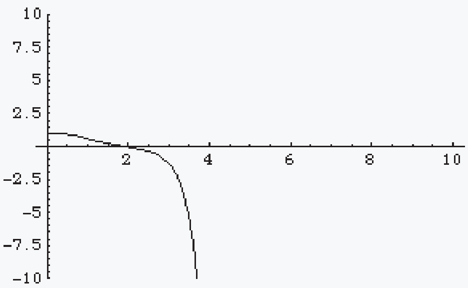
Problem 2.55

I'll just show the first two graphs, and the last two. Evidently K lies between 0.9999 and 1.0001

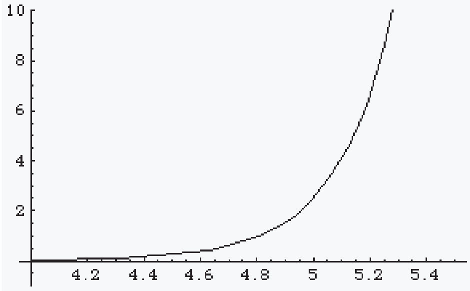
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 0.9) * u[x] == 0, u[0] == 1,
      u'[0] == 0}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 10},
  PlotRange -> {-10, 10}];
```



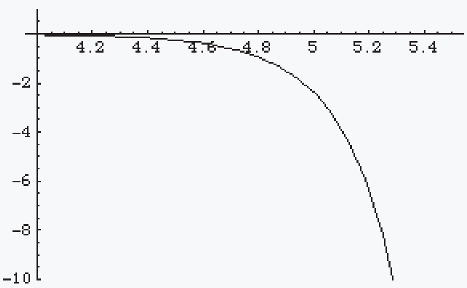

```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 1.1) * u[x] == 0, u[0] == 1,
      u'[0] == 0}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 10},
  PlotRange -> {-10, 10}];
```




```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 0.9999) * u[x] == 0, u[0] == 1,
      u'[0] == 0}, u[x], {x, 10^-8, 10}, MaxSteps -> 10000]],
  {x, 4, 5.5}, PlotRange -> {-1, 10}];
```



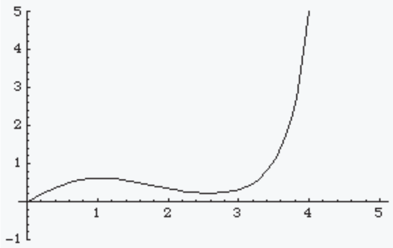

```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 1.0001) * u[x] == 0, u[0] == 1,
      u'[0] == 0}, u[x], {x, 10^-8, 10}, MaxSteps -> 10000]],
  {x, 4, 5.5}, PlotRange -> {-10, 1}];
```



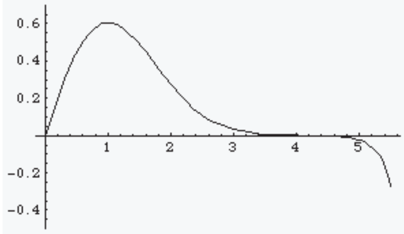
Problem 2.56

The *correct* values (in Eq. 2.73) are $K = 2n + 1$ (corresponding to $E_n = (n + \frac{1}{2})\hbar\omega$). I'll start by "guessing" 2.9, 4.9, and 6.9, and tweaking the number until I've got 5 reliable significant digits. The results (see below) are $\boxed{3.0000,\ 5.0000,\ 7.0000.}$ (The actual *energies* are these numbers multiplied by $\frac{1}{2}\hbar\omega$.)

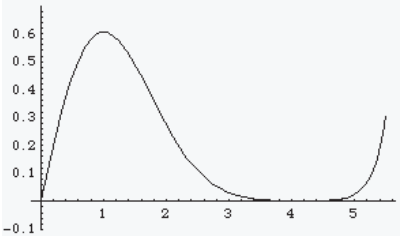
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 2.9)*u[x] == 0, u[0] == 0,
      u'[0] == 1}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 5},
  PlotRange -> {-1, 5}];
```



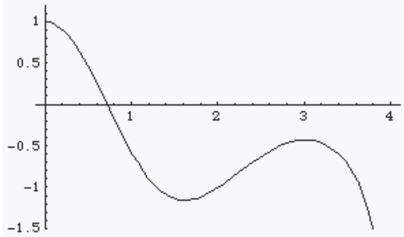
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 3.00001)*u[x] == 0,
      u[0] == 0, u'[0] == 1}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 5.5},
  PlotRange -> {-.5, .7}];
```



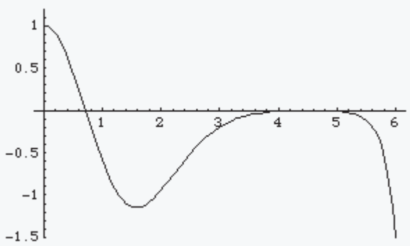
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 2.99999)*u[x] == 0,
      u[0] == 0, u'[0] == 1}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 5.5},
  PlotRange -> {-.1, .7}];
```



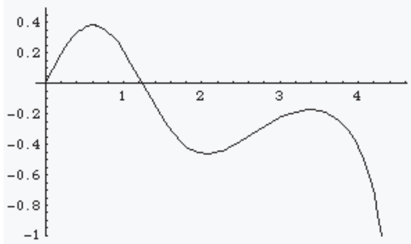
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 4.9)*u[x] == 0, u[0] == 1,
      u'[0] == 0}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 4},
  PlotRange -> {-1.5, 1.2}];
```



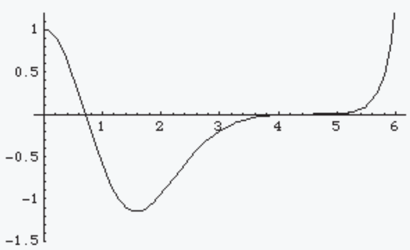
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 4.99999)*u[x] == 0,
      u[0] == 1, u'[0] == 0}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 6},
  PlotRange -> {-1.5, 1.2}];
```



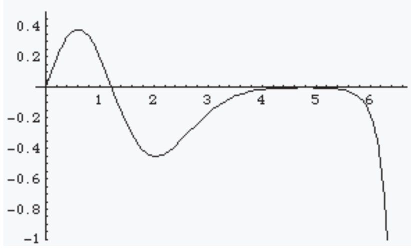
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 6.9)*u[x] == 0, u[0] == 0,
      u'[0] == 1}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 4.5},
  PlotRange -> {-1, .5}];
```



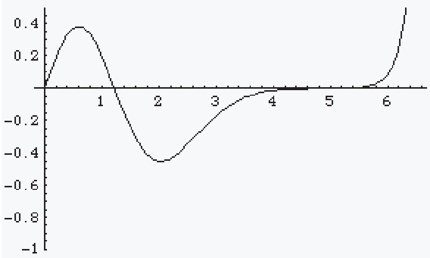
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 5.00001)*u[x] == 0,
      u[0] == 1, u'[0] == 0}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 6},
  PlotRange -> {-1.5, 1.2}];
```



```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 6.99999)*u[x] == 0,
      u[0] == 0, u'[0] == 1}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 6.5},
  PlotRange -> {-1, .5}];
```



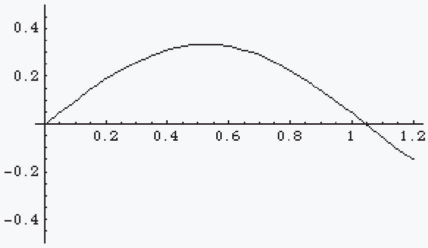
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] - (x^2 - 7.00001) * u[x] == 0,
      u[0] == 0, u'[0] == 1}, u[x], {x, 10^-8, 10},
     MaxSteps -> 10000]], {x, 0, 6.5},
  PlotRange -> {-1, .5}];
```



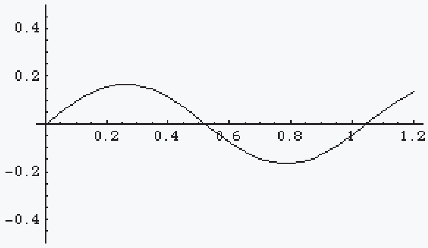
Problem 2.57

The Schrödinger equation says $-\frac{\hbar^2}{2m}\psi'' = E\psi$, or, with the *correct* energies (Eq. 2.30) and $a = 1$, $\psi'' + (n\pi)^2\psi = 0$. I'll start with a "guess" using 9 in place of π^2 (that is, I'll use 9 for the ground state, 36 for the first excited state, 81 for the next, and finally 144). Then I'll tweak the parameter until the graph crosses the axis right at $x = 1$. The results (see below) are, to five significant digits: $\boxed{9.8696,\ 39.478,\ 88.826,\ 157.91.}$ (The actual *energies* are these numbers multiplied by $\hbar^2/2ma^2$.)

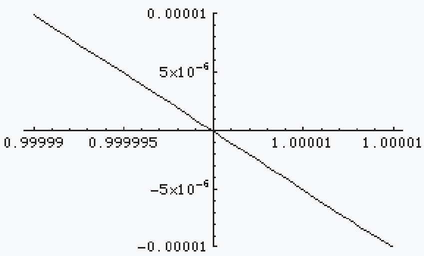
```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] + (9) * u[x] == 0, u[0] == 0, u'[0] == 1},
     u[x], {x, 10^-8, 1.5}, MaxSteps -> 10000]],
  {x, 0, 1.2}, PlotRange -> {-.5, .5}];
```



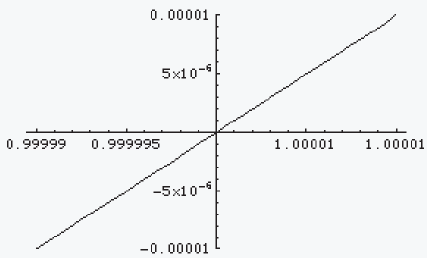

```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] + (36) * u[x] == 0, u[0] == 0, u'[0] == 1},
     u[x], {x, 10^-8, 1.5}, MaxSteps -> 10000]],
  {x, 0, 1.2}, PlotRange -> {-.5, .5}];
```



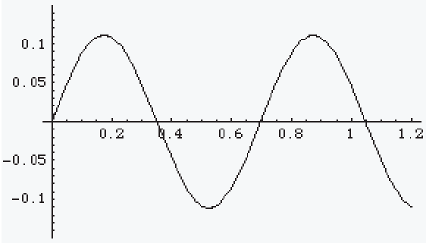

```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] + (9.86959) * u[x] == 0, u[0] == 0,
      u'[0] == 1}, u[x], {x, 10^-8, 1.005},
     MaxSteps -> 10000]], {x, 0.99999, 1.00001},
  PlotRange -> {-.00001, .00001}];
```



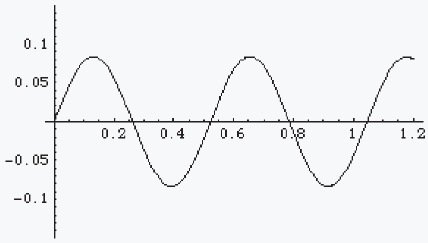

```
Plot[Evaluate[u[x] /.
    NDSolve[{u''[x] + (39.47803) * u[x] == 0, u[0] == 0,
      u'[0] == 1}, u[x], {x, 10^-8, 1.005},
     MaxSteps -> 10000]], {x, 0.99999, 1.00001},
  PlotRange -> {-.00001, .00001}];
```



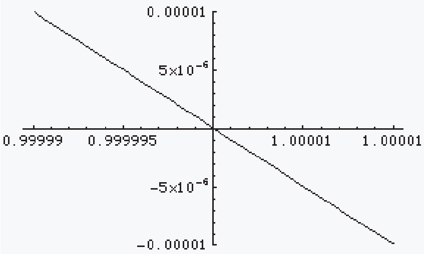
```
Plot[Evaluate[u[x] /.
   NDSolve[{u''[x] + (81) *u[x] == 0, u[0] == 0, u'[0] == 1},
    u[x], {x, 10^-8, 1.5}, MaxSteps -> 10000]],
  {x, 0, 1.2}, PlotRange -> {-.15, .15}];
```



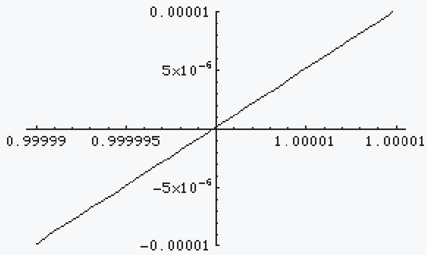

```
Plot[Evaluate[u[x] /.
   NDSolve[{u''[x] + (144) *u[x] == 0, u[0] == 0, u'[0] == 1},
    u[x], {x, 10^-8, 1.5}, MaxSteps -> 10000]],
  {x, 0, 1.2}, PlotRange -> {-.1, .1}];
```




```
Plot[Evaluate[u[x] /.
   NDSolve[{u''[x] + (88.82630) *u[x] == 0, u[0] == 0,
     u'[0] == 1}, u[x], {x, 10^-8, 1.005},
    MaxSteps -> 10000]], {x, 0.99999, 1.00001},
  PlotRange -> {-.00001, .00001}];
```




```
Plot[Evaluate[u[x] /.
   NDSolve[{u''[x] + (157.9129) *u[x] == 0, u[0] == 0,
     u'[0] == 1}, u[x], {x, 10^-8, 1.005},
    MaxSteps -> 10000]], {x, 0.99999, 1.00001},
  PlotRange -> {-.00001, .00001}];
```



Problem 2.58

(a) The total energy is simply N times the ground state energy of the infinite square well:

$$\boxed{E_a = N\frac{\pi^2\hbar^2}{2ma^2}.}$$

(b) Filling the lowest N energy levels of the infinite square well (with width Na) gives

$$E_b = \sum_{n=1} N\frac{n^2\pi^2\hbar^2}{2m(NA)^2} = \frac{\pi^2\hbar^2}{2mN^2a^2}\sum_{n=1}^{N} n^2.$$

The sum is $N(N+1)(2N+1)/6$, so

$$\boxed{E_b = \left(\frac{N}{3}+\frac{1}{2}+\frac{1}{6N}\right)\frac{\pi^2\hbar^2}{2ma^2}.}$$

(c)

$$\frac{\Delta E}{N} = \frac{E_a - E_b}{N} \approx \left(\frac{N-(N/3)}{N}\right)\frac{\pi^2\hbar^2}{2ma^2} = \boxed{\frac{\pi^2\hbar^2}{3ma^2}.}$$

(d) The binding energy of hydrogen (13.6 eV) is $\hbar^2/2ma_B^2$, where $a_B = 0.529$ Å is the Bohr radius, so

$$\frac{\Delta E}{N} = \frac{2}{3}\pi^2\left(\frac{a_B}{a}\right)^2 E_{\text{binding}} = \frac{2}{3}\left(\frac{0.529\,\pi}{4}\right)^2 (13.6)\,\text{eV} = \boxed{1.6\,\text{eV.}}$$

Problem 2.59

(a)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + mgx\,\psi = E\,\psi \qquad (x \geq 0; \quad \psi = 0 \text{ for } x \leq 0).$$

$$\frac{d\psi}{dx} = \frac{d\psi}{dz}\frac{dz}{dx} = a\frac{d\psi}{dz}; \quad \frac{d^2\psi}{dx^2} = a\frac{d^2\psi}{dz^2}\frac{dz}{dx} = a^2\frac{d^2\psi}{dz^2}.$$

$$-\frac{\hbar^2}{2m}a^2\frac{d^2\psi}{dz^2} + mg\frac{z}{a}\psi = E\psi \;\Rightarrow\; -\frac{\hbar^2}{2m}a^2\sqrt{a}\,y'' + mg\frac{z}{a}\sqrt{a}\,y = E\sqrt{a}\,y \;\Rightarrow\; -y'' + \frac{2m}{\hbar^2a^2}mg\frac{z}{a}\,y = \frac{2m}{\hbar^2a^2}E\,y.$$

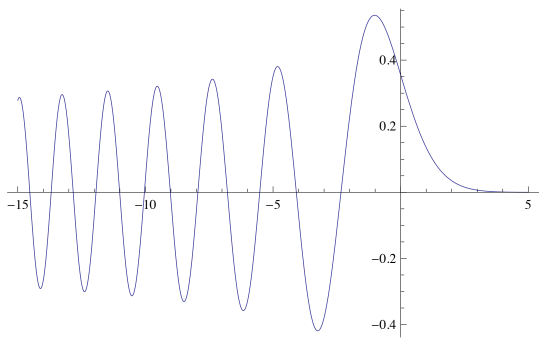
Let

$$\frac{2m}{\hbar^2a^2}mg\frac{1}{a} = 1, \text{ or } \boxed{a \equiv \left(\frac{2m^2g}{\hbar^2}\right)^{1/3}} \quad \text{and} \quad \epsilon \equiv \frac{2m}{\hbar^2a^2}E = \frac{2m}{\hbar^2}\left(\frac{\hbar^2}{2m^2g}\right)^{2/3}E = \boxed{\left(\frac{2}{m\hbar^2g^2}\right)^{1/3}E.}$$

Then $-y'' + zy = \epsilon y$. ✓

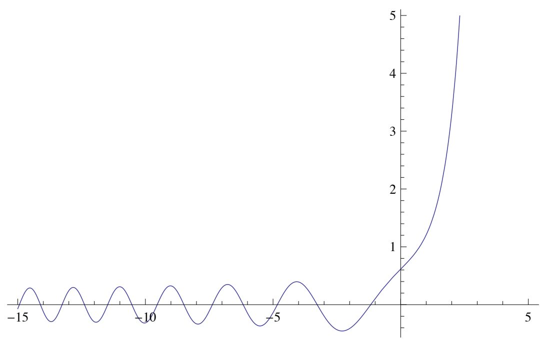
```
In[1]:= DSolve[-y''[x] + x y[x] == s y[x], y[x], x]
Out[1]= {{y[x] → AiryAi[-s + x] C[1] + AiryBi[-s + x] C[2]}}
In[2]:= Plot[AiryAi[x], {x, -15, 5}]
```

Out[2]=




```
In[3]:= Plot[AiryBi[x], {x, -15, 5}]
```

Out[3]=



```
In[12]:= FindRoot[AiryAi[x] == 0, {x, -2}]

Out[12]= {x → -2.33811}

In[13]:= FindRoot[AiryAi[x] == 0, {x, -12.8}]

Out[13]= {x → -12.8288}

In[14]:= NIntegrate[(AiryAi[x])^2, {x, -2.338107410459767`, ∞}]

Out[14]= 0.491697

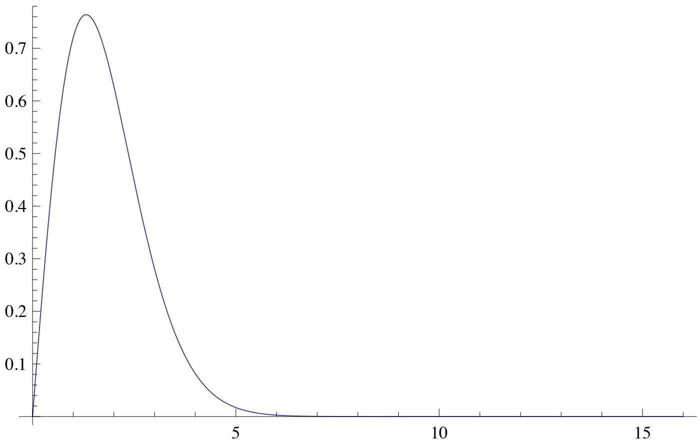
In[15]:= NIntegrate[(AiryAi[x])^2, {x, -12.828776752865757`, ∞}]

Out[15]= 1.14018

In[16]:= Pone[x_] := (0.4916966179009774`)^(-1 / 2) * AiryAi[x - 2.338107410459767`]

In[17]:= Plot[Pone[x], {x, 0, 16}]
```

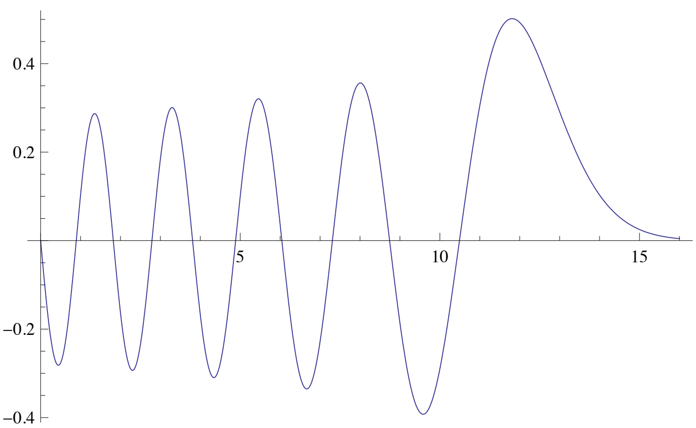
Out[17]=




```
In[18]:= Pten[x_] := (1.1401837256117164`)^(-1 / 2) * AiryAi[x - 12.828776752865757`]

In[19]:= Plot[Pten[x], {x, 0, 16}]
```

Out[19]=



```
In[20]:= NIntegrate[Pone[x] * Pten[x], {x, 0, ∞}]

NIntegrate::ncvb :
  NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in x near {x} = {1.72352}. NIntegrate
    obtained -9.19403×10^-17 and 1.5861121045064646`*^-16 for the integral and error estimates. ≫

Out[20]= -9.19403 × 10^-17
```

(b)

$$\text{For } \psi_1: \quad \sigma_x = 0.697089, \quad \sigma_p = 0.882819\,\hbar, \quad \sigma_x\sigma_p = 0.615403\,\hbar > 0.5\hbar \checkmark.$$
$$\text{For } \psi_{10}: \quad \sigma_x = 3.8248, \quad \sigma_p = 2.06791\,\hbar, \quad \sigma_x\sigma_p = 7.90935\,\hbar > 0.5\hbar \checkmark.$$

(See print-out.)

```
NIntegrate[x (Pone[x])^2, {x, 0, ∞}]
1.55874

NIntegrate[x^2 (Pone[x])^2, {x, 0, ∞}]
2.9156

√(2.9155980068599967` - (1.558738273638599`)^2)
0.697089

NIntegrate[x (Pten[x])^2, {x, 0, ∞}]
8.55252

NIntegrate[x^2 (Pten[x])^2, {x, 0, ∞}]
87.7747

√(87.77467357595424` - (8.552517834822023`)^2)
3.8248

NIntegrate[-i Pone[x] (Pone'[x]), {x, 0, ∞}]
NIntegrate::ncvb :
  NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in x near {x} = {1.2858}. NIntegrate
    obtained 0. + 6.07153×10^-18 i and 7.766131095614155`*^-17 for the integral and error estimates. ≫
0. + 6.07153 × 10^-18 i

NIntegrate[- Pone[x] (Pone''[x]), {x, 0, ∞}]
0.779369

NIntegrate[- Pten[x] (Pten''[x]), {x, 0, ∞}]
4.27626

√(0.7793691368188985`)
0.882819

√(4.276258918045443`)
2.06791

0.6970889478066314` * 0.8828188584409027`
0.615403

3.8248022512288737` * 2.067911728784728`
7.90935
```

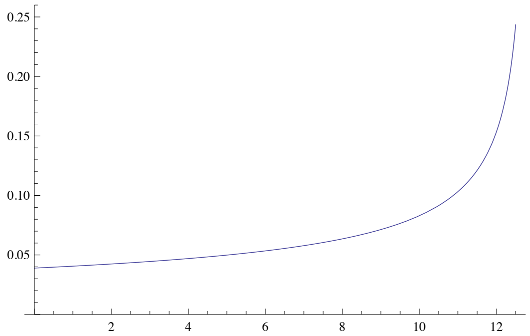
(c) $\rho_C(x) = \dfrac{1}{Tv(x)}$ (Equation 1.43). Here

$$E = \frac{1}{2}mv^2 + mgx \Rightarrow v = \sqrt{\frac{2}{m}(E - mgx)} \quad \text{and} \quad \frac{1}{2}gT^2 = h = \frac{E}{mg} \Rightarrow T = \sqrt{\frac{2E}{mg^2}}, \quad \text{so}$$

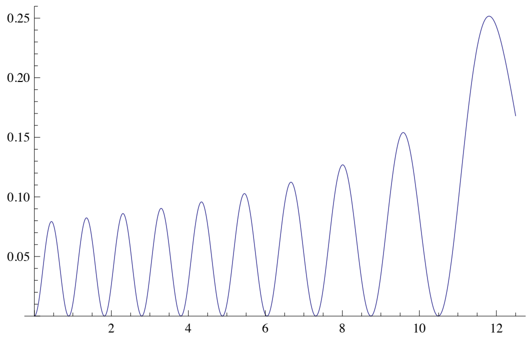
$$\rho_C(x) = \frac{mg}{2\sqrt{E(E-mgx)}} = \frac{mg}{2\sqrt{\frac{\hbar^2 a^2}{2m}\epsilon\left(\frac{\hbar^2 a^2}{2m}\epsilon - mgx\right)}} = \frac{1}{2}\frac{(2m^2 g/\hbar^2 a^2)}{\sqrt{\epsilon(\epsilon - (2m^2 g/\hbar^2 a^2)}} = \frac{1}{2}\frac{a}{\sqrt{\epsilon(\epsilon - a)}} \to \frac{1}{2\sqrt{\epsilon(\epsilon-1)}}.$$

For ψ_{10}, $\epsilon = 12.82877$ (Out[13] on page 64). The graphs are

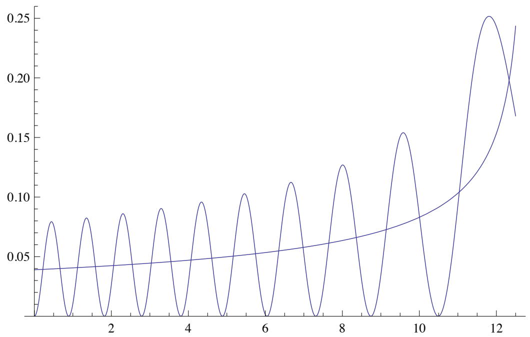
```
Plot[(4 * 12.828776752865757` (12.828776752865757` - x))^(-1/2),
 {x, 0, 12.5}, PlotRange → {0, .26}]
```




```
Plot[(Pten[x])^2, {x, 0, 12.5}, PlotRange → {0, .26}]
```




```
Show[%74, %75]
```



Comment: Well, they agree, in a kind of averaged sense.

Problem 2.60

(a)

$$E_0 = (\hbar)^n (m)^p (\alpha)^q = \left(\frac{\text{kg m}^2}{\text{s}}\right)^n (\text{kg})^p \left(\frac{\text{kg m}^4}{\text{s}^2}\right)^q = (\text{kg})^{n+p+q}\,(\text{m}^2)^{n+2q}\,(\text{s})^{-(n+2q)} = \frac{\text{kg m}^2}{\text{s}^2}.$$

So $n+p+q=1, \quad n+2q=1, \quad n+2q=2$. The last two are incompatible. Evidently there is, on purely dimensional grounds, no possible formula for E_0.

(b) Let $\psi_\lambda(x) \equiv \psi(y)$, where $y \equiv \lambda x$. Then

$$\frac{d^2\psi_\lambda(x)}{dx^2} = \frac{d^2\psi(y)}{d}y^2\left(\frac{dy}{dx}\right)^2 = \lambda^2\frac{d^2\psi(y)}{dy^2} = \lambda^2\left(-\frac{\beta}{y^2}\psi(y) + \kappa^2\psi(y)\right) = -\lambda^2\frac{\beta}{\lambda^2 x^2}\psi_\lambda(x) + \lambda^2\kappa^2\psi_\lambda(x),$$

or $\dfrac{d^2\psi_\lambda(x)}{dx^2} + \dfrac{\beta}{x^2}\psi_\lambda(x) = (\lambda\kappa)^2\psi_\lambda(x) = (\kappa')^2\psi_\lambda(x)$. So $\psi_\lambda(x)$ is a solution to Equation 2.190, with $\kappa' \equiv \lambda\kappa$. The corresponding energy is given by $\left(\dfrac{-2mE'}{\hbar^2}\right) = (\kappa')^2 = \lambda^2\kappa^2 = \lambda^2\left(\dfrac{-2mE}{\hbar^2}\right) \Rightarrow E' = \lambda^2 E$.

(c)

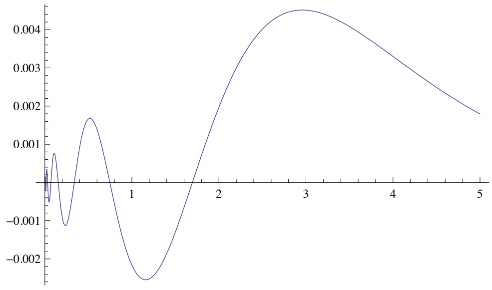
```
f[x_] := A √x BesselK[ⅈ √(b - (1/4)), k x]

FullSimplify[f''[x] + b/x^2 f[x] - k^2 f[x] == 0]

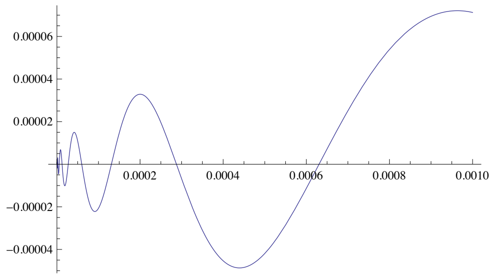
True

h[x_] := √x BesselK[4 ⅈ, x]

Plot[h[x], {x, 0, 5}]
```




```
Plot[h[x], {x, 0, .001}]
```




```
∫_0^∞ (f[x])^2 ⅆx

ConditionalExpression[
 A^2 √(-1 + 4 b) π Csch[√(-1/4 + b) π]
 ─────────────────────────────────────, Re[k] > 0 && -2 < Im[√(-1 + 4 b)] < 2]
                 4 k^2
```

So $\boxed{A = \kappa\sqrt{\dfrac{2\sinh(\pi g)}{\pi g}}.}$

(d) From the first plot on page 67 we see that the highest zero crossing occurs at $\kappa x \approx 1.7$; to find the exact value, use **FindRoot** (see print-out below). We want this to occur at $x = \epsilon = 1$, so $\kappa = 1.69541$.

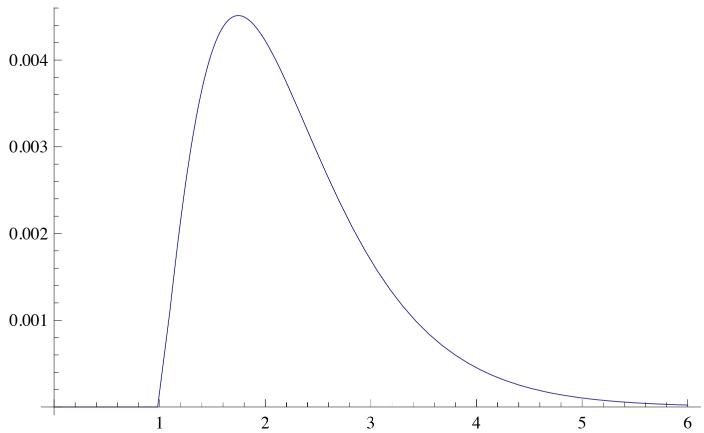
```
h[x_] := √x BesselK[4 i, x]

FindRoot[h[x] == 0, {x, 1.7}]

{x → 1.69541 + 0. i}

j[x_] := If[x >= 1, h[1.6954066933505485` x], 0]

Plot[j[x], {x, 0, 6}]
```



The parameter $\beta \equiv 2m\alpha/\hbar^2$ is dimensionless, so we may as well eliminate $\hbar$ (in favor of β, m, and α) in the dimensional analysis. This leaves $E_0 = m^p\,\alpha^q\,\epsilon^r = (\mathrm{kg})^p\left(\frac{\mathrm{kg\,m}^4}{\mathrm{s}^2}\right)^q(\mathrm{m})^r = (\mathrm{kg})^{p+q}(\mathrm{m})^{4q+r}(\mathrm{s})^{-2q} = \frac{\mathrm{kg\,m}^2}{\mathrm{s}^2}$, so $p+q = 1, 4q+r = 2,\ q = 1, \Rightarrow p = 0, r = -2$. On dimensional grounds, therefore, the expression for E_0 has to be of the form $E_0 = -\alpha/\epsilon^2$ times some function of β. As $\epsilon \to 0$ (for fixed values of m and α), $E_0 \to -\infty$, indicating once again that there is no ground state for this system.

Problem 2.61

(a) From Equation 2.197:

$$N=1:\ j=1:\ -\lambda\cancel{\psi_2}+(2\lambda)\psi_1-\lambda\cancel{\psi_0}=E\psi_1 \quad\Rightarrow\quad \boxed{\mathsf{H}=(2\lambda).}$$

$$N=2:\ \begin{cases} j=1:\ -\lambda\psi_2+(2\lambda)\psi_1-\lambda\cancel{\psi_0}=E\psi_1 \\ j=2:\ -\lambda\cancel{\psi_3}+(2\lambda)\psi_2-\lambda\psi_1=E\psi_2 \end{cases} \quad\Rightarrow\quad \boxed{\mathsf{H}=\begin{pmatrix} 2\lambda & -\lambda \\ -\lambda & 2\lambda \end{pmatrix}.}$$

$$N=3:\ \begin{cases} j=1:\ -\lambda\psi_2+(2\lambda)\psi_1-\lambda\cancel{\psi_0}=E\psi_1 \\ j=2:\ -\lambda\psi_3+(2\lambda)\psi_2-\lambda\psi_1=E\psi_2 \\ j=3:\ -\lambda\cancel{\psi_4}+(2\lambda)\psi_3-\lambda\psi_2=E\psi_2 \end{cases} \quad\Rightarrow\quad \boxed{\mathsf{H}=\begin{pmatrix} 2\lambda & -\lambda & 0 \\ -\lambda & 2\lambda & -\lambda \\ 0 & -\lambda & 2\lambda \end{pmatrix}.}$$

(b) Denote the eigenvalues by $\tilde{E}_n$:

$N=1:$ $\boxed{\tilde{E}_1 = 2\lambda} = \dfrac{2\hbar^2}{2m(a/2)^2} = \dfrac{8\hbar^2}{2ma^2}$. The exact energies are $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$, so $E_1 = \dfrac{\pi^2\hbar^2}{2ma^2}$; the agreement is not too bad: $8 \approx \pi^2 = 9.87$.

$N=2:$

$$\det\begin{pmatrix} 2\lambda - \tilde{E} & -\lambda \\ -\lambda & 2\lambda - \tilde{E}\end{pmatrix} = 0 \Rightarrow (2\lambda - \tilde{E})^2 - \lambda^2 = 0 \Rightarrow 2\lambda - \tilde{E} = \pm\lambda.$$

$\tilde{E}_1 = 2\lambda - \lambda = \boxed{\lambda} = \dfrac{\hbar^2}{2m(a/3)^2} = \dfrac{9\hbar^2}{2ma^2}$. This is better: 9 is closer to π^2 than 8 was.

$\tilde{E}_2 = 2\lambda + \lambda = \boxed{3\lambda} = \dfrac{3\hbar^2}{2m(a/3)^2} = \dfrac{27\hbar^2}{2ma^2}$. The exact answer has $4\pi^2 = 39.5$ instead of 27.

$N=3:$

$$\det\begin{pmatrix} 2\lambda - \tilde{E} & -\lambda & 0 \\ -\lambda & 2\lambda - \tilde{E} & -\lambda \\ 0 & -\lambda & 2\lambda - \tilde{E}\end{pmatrix} = 0 \Rightarrow (2\lambda - \tilde{E})^3 - 2\lambda^2(2\lambda - \tilde{E}) = 0 \Rightarrow 2\lambda - \tilde{E} = 0 \text{ or } 2\lambda - \tilde{E} = \pm\sqrt{2}\,\lambda.$$

$\tilde{E}_1 = 2\lambda - \sqrt{2}\,\lambda = \boxed{\lambda(2-\sqrt{2})} = \dfrac{(2-\sqrt{2})\hbar^2}{2m(a/4)^2} = \dfrac{16(2-\sqrt{2})\hbar^2}{2ma^2}$. This is better yet: $16(2-\sqrt{2}) = 9.37$.

$\tilde{E}_2 = \boxed{2\lambda} = \dfrac{2\hbar^2}{2m(a/4)^2} = \dfrac{32\hbar^2}{2ma^2}$. Improving: the exact answer is $4\pi^2 = 39.5$ instead of 32.

$\tilde{E}_3 = 2\lambda + \sqrt{2}\,\lambda = \boxed{\lambda(2+\sqrt{2})} = \dfrac{(2+\sqrt{2})\hbar^2}{2m(a/4)^2} = \dfrac{16(2+\sqrt{2})\hbar^2}{2ma^2}$; $16(2+\sqrt{2}) = 54.6 \approx 9\pi^2 = 88.8$.

(c)

```
h = Table[If[i == j, 2 λ, 0], {i, 10}, {j, 10}]

k = Table[If[i == j + 1, -λ, 0], {i, 10}, {j, 10}]

m = Table[If[i == j - 1, -λ, 0], {i, 10}, {j, 10}]

p = Table[h[[i, j]] + k[[i, j]] + m[[i, j]], {i, 10}, {j, 10}]

P = MatrixForm[%]
```

$$\begin{pmatrix}
2\lambda & -\lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\lambda & 2\lambda & -\lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\lambda & 2\lambda & -\lambda & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\lambda & 2\lambda & -\lambda & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\lambda & 2\lambda & -\lambda & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\lambda & 2\lambda & -\lambda & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\lambda & 2\lambda & -\lambda & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 2\lambda & -\lambda & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 2\lambda & -\lambda \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 2\lambda
\end{pmatrix}$$

```
λ = 1

1

EIG = Eigenvalues[N[p]]

{3.91899, 3.68251, 3.30972, 2.83083, 2.28463,
 1.71537, 1.16917, 0.690279, 0.317493, 0.0810141}
```

To get the eigenvalues, multiply by $\lambda = \dfrac{\hbar^2}{2m(a/11)^2} = \left(\dfrac{121}{\pi^2}\right) E_1$:

```
121 * EIG / (π^2)
{48.0462, 45.147, 40.5767, 34.7056,
 28.0092, 21.0302, 14.3339, 8.46272, 3.89242, 0.993221}
```

Thus the lowest five eigenvalues, in units of E_1, are $\boxed{0.9932, 3.8924, 8.4627, 14.3339, 21.0302,}$ as compared to the exact values $1, 4, 9, 16, 25$. Doing the same for $N = 100$:

```
h = Table[If[i == j, 2 λ, 0], {i, 100}, {j, 100}]

k = Table[If[i == j + 1, -λ, 0], {i, 100}, {j, 100}]

m = Table[If[i == j - 1, -λ, 0], {i, 100}, {j, 100}]

p = Table[h[[i, j]] + k[[i, j]] + m[[i, j]], {i, 100}, {j, 100}]

λ = 1
1

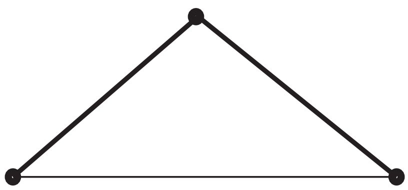
EIG = Eigenvalues[N[p]]

10 201 * EIG / (π^2)
{4133.31, 4130.31, 4125.32, 4118.33, 4109.36, 4098.41, 4085.5, 4070.64, 4053.84,
 4035.11, 4014.49, 3991.97, 3967.6, 3941.39, 3913.36, 3883.55, 3851.98,
 3818.69, 3783.7, 3747.04, 3708.77, 3668.9, 3627.49, 3584.57, 3540.18, 3494.36,
 3447.16, 3398.63, 3348.81, 3297.75, 3245.5, 3192.11, 3137.63, 3082.12,
 3025.62, 2968.2, 2909.9, 2850.79, 2790.92, 2730.35, 2669.14, 2607.35, 2545.03,
 2482.25, 2419.07, 2355.55, 2291.76, 2227.74, 2163.57, 2099.3, 2035.01,
 1970.74, 1906.57, 1842.55, 1778.75, 1715.24, 1652.06, 1589.28, 1526.96,
 1465.17, 1403.96, 1343.39, 1283.52, 1224.41, 1166.11, 1108.69, 1052.19,
 996.679, 942.201, 888.81, 836.559, 785.499, 735.679, 687.147, 639.95, 594.133,
 549.742, 506.819, 465.405, 425.541, 387.265, 350.614, 315.624, 282.328,
 250.76, 220.948, 192.922, 166.71, 142.336, 119.824, 99.1963, 80.4724,
 63.6704, 48.8067, 35.8956, 24.9496, 15.9794, 8.99347, 3.99871, 0.999919}
```

This time the lowest five eigenvalues are $\boxed{0.9999, 3.9987, 8.9934, 15.9794, 24.9496.}$

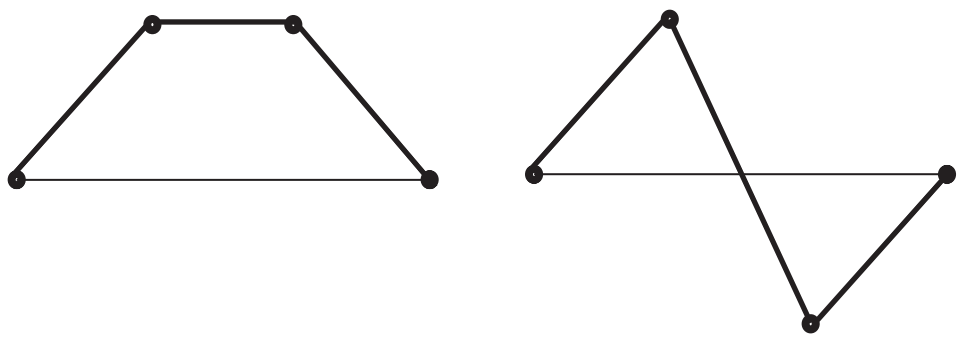
(d) Always, $\psi_0 = \psi_{N+1} = 0$; might as well set $\lambda = 1$ for this part.

$N = 1:\ 2\psi_1 = \tilde{E}\psi_1,\ \tilde{E}_1 = 2.$ Up to normalization:



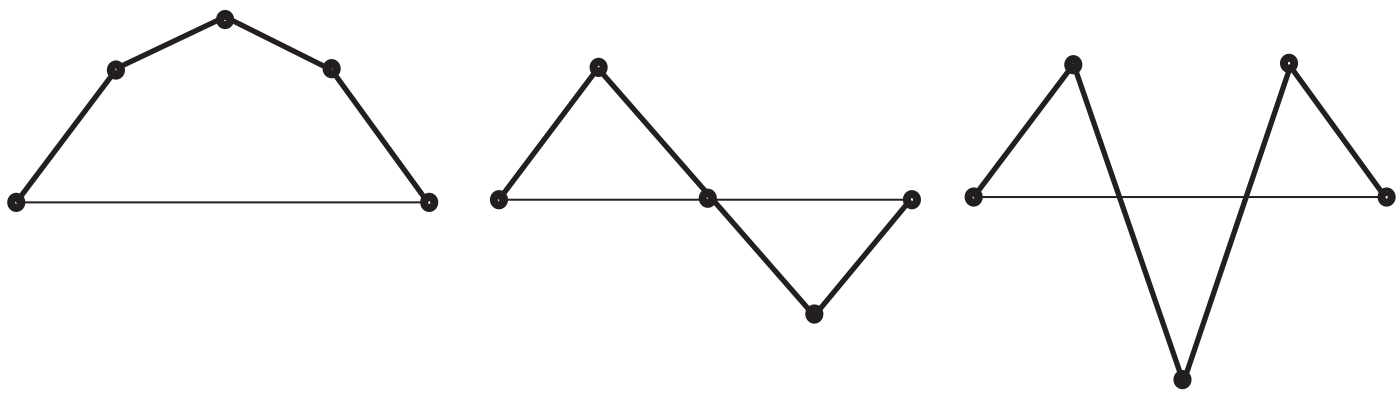
$N = 2: \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \tilde{E} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \Rightarrow 2\psi_1 - \psi_2 = \tilde{E}\psi_1$ and $-\psi_1 + 2\psi_2 = \tilde{E}\psi_2.$

$$n = 1: \ \tilde{E}_1 = 1 \Rightarrow 2\psi_1 - \psi_2 = \psi_1 \Rightarrow \psi_2 = \psi_1$$
$$n = 2: \ \tilde{E}_2 = 3 \Rightarrow 2\psi_1 - \psi_2 = 3\psi_1 \Rightarrow \psi_2 = -\psi_1$$



$$N = 3: \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = \tilde{E} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} \Rightarrow 2\psi_1 - \psi_2 = \tilde{E}\psi_1, \ -\psi_1 + 2\psi_2 - \psi_3 = \tilde{E}\psi_2, \ -\psi_2 + 2\psi_3 = \tilde{E}\psi_3.$$

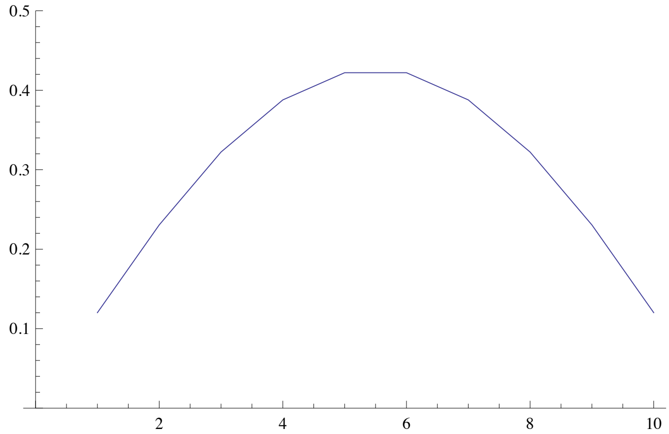
$$n = 1: \ \tilde{E}_1 = 2 - \sqrt{2} \Rightarrow 2\psi_1 - \psi_2 = (2 - \sqrt{2})\psi_1 \Rightarrow \psi_2 = \sqrt{2}\psi_1;$$
$$-\psi_1 + 2\psi_2 - \psi_3 = (2 - \sqrt{2})\psi_2 \Rightarrow \psi_1 + \psi_3 = \sqrt{2}\psi_2 = 2\psi_1 \Rightarrow \psi_3 = \psi_1$$
$$n = 2: \ \tilde{E}_2 = 2 \Rightarrow 2\psi_1 - \psi_2 = 2\psi_1 \Rightarrow \psi_2 = 0; \ -\psi_1 + 2\psi_2 - \psi_3 = 2\psi_2 \Rightarrow \psi_3 = -\psi_1$$
$$n = 3: \ \tilde{E}_3 = 2 + \sqrt{2} \Rightarrow 2\psi_1 - \psi_2 = (2 + \sqrt{2})\psi_1 \Rightarrow \psi_2 = -\sqrt{2}\psi_1;$$
$$-\psi_1 + 2\psi_2 - \psi_3 = (2 + \sqrt{2})\psi_2 \Rightarrow \psi_1 + \psi_3 = -\sqrt{2}\psi_2 = 2\psi_1 \Rightarrow \psi_3 = \psi_1$$



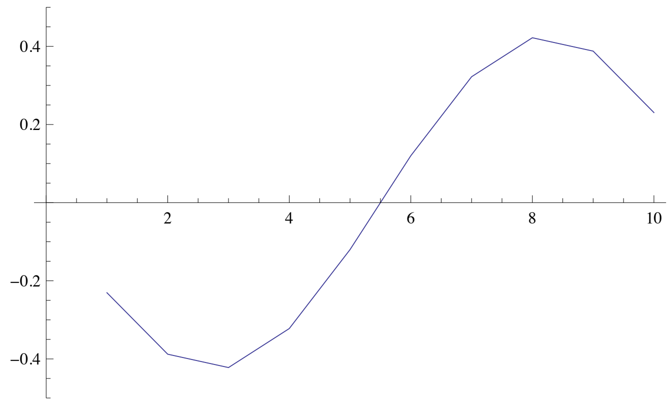
For $N = 10$ we get

```
EVE = Eigenvectors[N[p]]

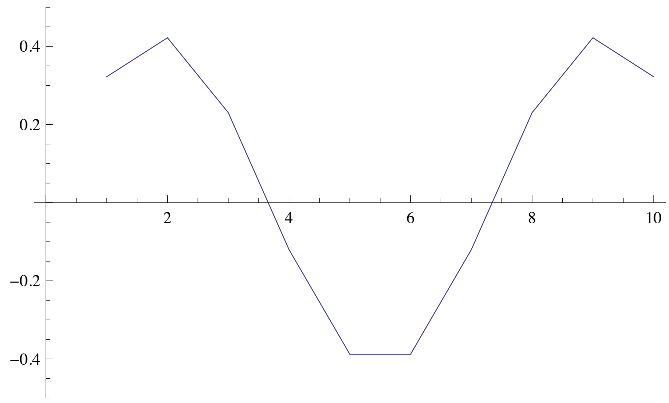
ListLinePlot[EVE[[10]], PlotRange → {0, 0.5}]
```




```
ListLinePlot[EVE[[9]], PlotRange → {-0.5, 0.5}]
```



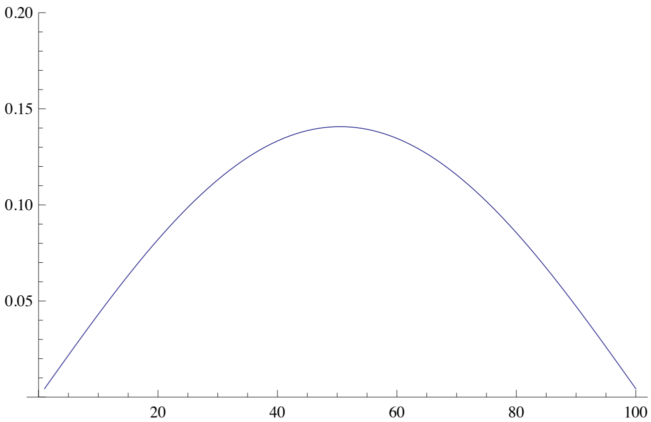

```
ListLinePlot[EVE[[8]], PlotRange → {-0.5, 0.5}]
```



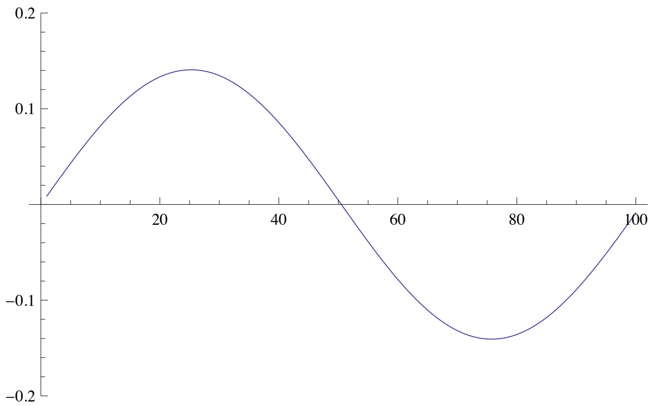
and for $N = 100$

```
EVE = Eigenvectors[N[p]]
```

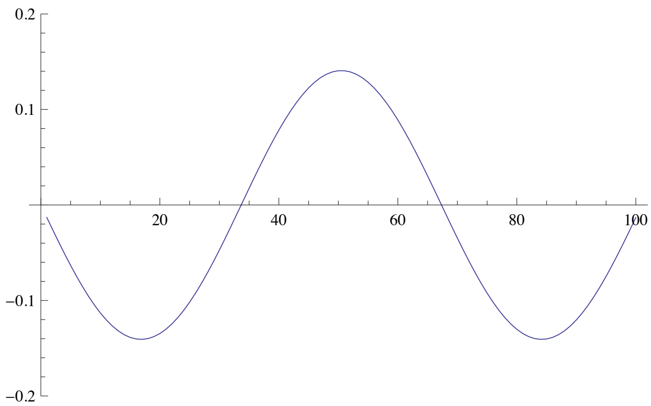
```
ListLinePlot[EVE[[100]], PlotRange -> {0, 0.2}]
```




```
ListLinePlot[EVE[[99]], PlotRange -> {-0.2, 0.2}]
```




```
ListLinePlot[EVE[[98]], PlotRange -> {-0.2, 0.2}]
```



Problem 2.62

$$\lambda = \frac{\hbar^2}{2ma^2}(N+1)^2 = (N+1)^2 V_0 \quad \text{(here } N = 100\text{);}$$
$$V_j = bV_0 \sin\left(\frac{\pi x_j}{a}\right) = bV_0 \sin\left(\frac{\pi j \Delta x}{a}\right) = bV_0 \sin\left(\frac{\pi j}{N+1}\right) \quad \text{(here } b = 500\text{);}$$
$$v_j = \frac{V_j}{\lambda} = \frac{b}{(N+1)^2}\sin\left(\frac{\pi j}{N+1}\right).$$

Factoring out λ, the diagonal elements of H are

$$2 + v_j = 2 + \frac{b}{(N+1)^2}\sin\left(\frac{\pi j}{N+1}\right) = 2 + \frac{500}{10201}\sin\left(\frac{\pi j}{101}\right).$$

```
h = Table[If[i == j, 2 + (500 / 10201) Sin[π j / 101], 0], {i, 100}, {j, 100}]

k = Table[If[i == j + 1, -1, 0], {i, 100}, {j, 100}]
m = Table[If[i == j - 1, -1, 0], {i, 100}, {j, 100}]

p = Table[h[[i, j]] + k[[i, j]] + m[[i, j]], {i, 100}, {j, 100}]

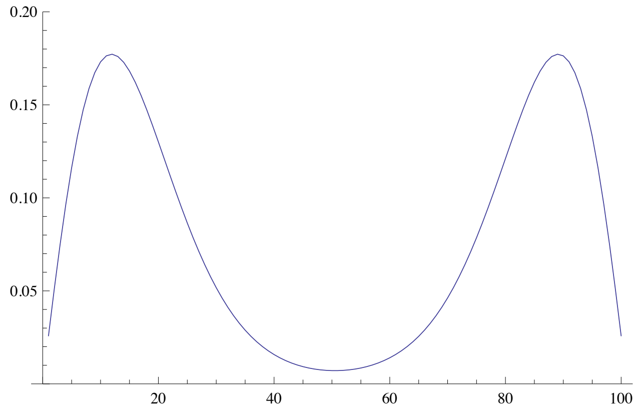
EIG = Eigenvalues[N[p]]

10201 * EIG
{41255., 41158.1, 41063.4, 40968.8, 40869.4, 40758.8, 40632., 40486.7, 40322.1,
 40138.4, 39935.6, 39714.1, 39474., 39215.7, 38939.5, 38645.5, 38334.2,
 38005.7, 37660.6, 37299., 36921.3, 36528., 36119.3, 35695.8, 35257.7,
 34805.6, 34339.9, 33860.9, 33369.3, 32865.4, 32349.7, 31822.8, 31285.1,
 30737.3, 30179.7, 29613., 29037.7, 28454.3, 27863.4, 27265.6, 26661.5,
 26051.7, 25436.7, 24817.1, 24193.6, 23566.7, 22937., 22305.2, 21671.9,
 21037.6, 20403.1, 19768.8, 19135.5, 18503.7, 17874.1, 17247.2, 16623.6,
 16004., 15389., 14779.2, 14175.1, 13577.3, 12986.5, 12403.1, 11827.8,
 11261.1, 10703.5, 10155.6, 9617.98, 9091.08, 8575.44, 8071.55, 7579.91,
 7100.98, 6635.24, 6183.13, 5745.1, 5321.57, 4912.95, 4519.64, 4142.02, 3780.47,
 3435.34, 3106.97, 2795.68, 2501.8, 2225.62, 1967.43, 1727.51, 1506.15, 1303.63,
 1120.24, 956.36, 812.457, 689.191, 590.237, 499.854, 476.163, 304.8, 304.66}
```

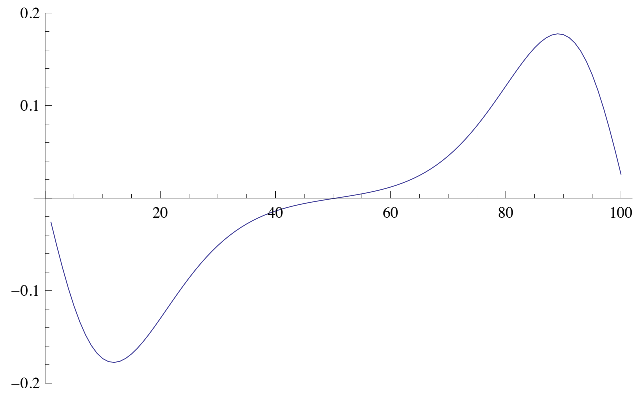
So the lowest three energies are $\boxed{304.66\ V_0,\ 304.8\ V_0, \text{ and } 476.163\,V_0.}$ Notice that the ground state is almost degenerate—essentially we have two separated wells with a huge barrier in between them, and the particle can be either in the left one or in the right one (or the even and odd linear combinations thereof).

```
EVE = Eigenvectors[N[p]]
```

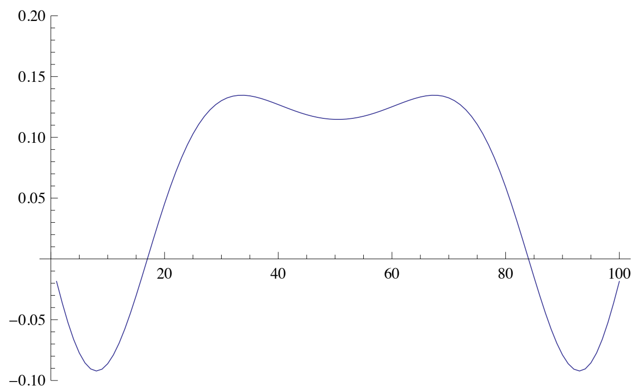
```
ListLinePlot[EVE[[100]], PlotRange → {0, 0.2}]
```




```
ListLinePlot[EVE[[99]], PlotRange → {-.2, 0.2}]
```




```
ListLinePlot[EVE[[98]], PlotRange → {-.1, 0.2}]
```



Notice that the central barrier pushes the wave function out to the wings.

Problem 2.63

(a) $-\frac{\partial}{\partial\beta}\ln(Z) = -\frac{1}{Z}\frac{\partial Z}{\partial\beta} = -\frac{1}{Z}\sum_n(-E_n)e^{-\beta E_n} = \sum_n E_n P(n).$ ✓

(b) Geometric series: $1 + x + x^2 + x^3 + \cdots = \frac{1}{1-x}$. Here $x = e^{-\beta\hbar\omega}$:

$$Z = \sum_{n=0}^{\infty} e^{-\beta(n+\frac{1}{2})\hbar\omega} = e^{-\beta\hbar\omega/2}\sum_{n=0}^{\infty} e^{(-\beta\hbar\omega)n} = e^{-\beta\hbar\omega/2}\frac{1}{1-e^{-\beta\hbar\omega}}. \quad ✓$$

(c)

$$\ln Z = \ln\left(e^{-\beta\hbar\omega/2)}\right) - \ln\left(1 - e^{-\beta\hbar\omega}\right) = -\frac{\beta\hbar\omega}{2} - \ln\left(1 - e^{-\beta\hbar\omega}\right),$$

$$\frac{\partial}{\partial\beta}\ln Z = -\frac{\hbar\omega}{2} - \frac{\hbar\omega e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} = -\left(\frac{\hbar\omega}{2}\right)\frac{1-e^{-\beta\hbar\omega}+2e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} \quad\Rightarrow\quad \bar{E} = \left(\frac{\hbar\omega}{2}\right)\frac{1+e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}. \quad ✓$$

(d)

$$\frac{\partial\bar{E}}{\partial T} = \frac{\partial\bar{E}}{\partial\beta}\frac{d\beta}{dT} = -\frac{1}{k_BT^2}\frac{\partial\bar{E}}{\partial\beta}.$$

$$\frac{\partial\bar{E}}{\partial\beta} = \left(\frac{\hbar\omega}{2}\right)\frac{\left(1-e^{-\beta\hbar\omega}\right)\left(-\hbar\omega e^{-\beta\hbar\omega}\right) - \left(1+e^{-\beta\hbar\omega}\right)\left(\hbar\omega e^{-\beta\hbar\omega}\right)}{\left(1-e^{-\beta\hbar\omega}\right)^2} = \left(\frac{\hbar\omega}{2}\right)\frac{-2\hbar\omega e^{-\beta\hbar\omega}}{\left(1-e^{-\beta\hbar\omega}\right)^2} = -\frac{(\hbar\omega)^2 e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^2}.$$

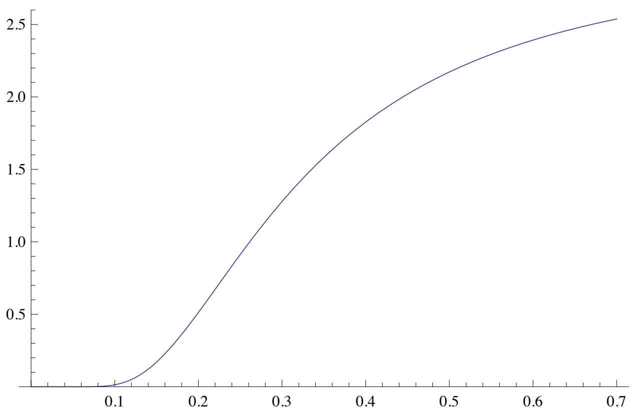
$$C = 3\left(\frac{1}{k_BT^2}\right)(\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^2}.$$

Or, using $\beta = 1/k_BT$ and $\hbar\omega = k_B\theta_E$,

$$C = 3\left(\frac{1}{k_BT^2}\right)(k_B\theta_E)^2\frac{e^{\theta_E/T}}{\left(e^{\theta_E/T}-1\right)^2} = 3k_B\left(\frac{\theta_E}{T}\right)^2\frac{e^{\theta_E/T}}{\left(e^{\theta_E/T}-1\right)^2}. \quad ✓$$

(e)

```
Plot[3 * (x^(-2)) * Exp[1 / x] / (Exp[1 / x] - 1)^2, {x, 0, .7}, PlotRange → {0, 2.6}]
```



Incidentally, comparing the graphs suggests that $x = 0.7$ corresponds to $T = 1000\,\mathrm{K}$, so $\theta_E = 1000/0.7\,\mathrm{K} = 1400\,\mathrm{K}$. Then $\hbar\omega = (1400k_B)\mathrm{K} = (1400)(8.6\times10^{-5})\,\mathrm{eV} = 0.12\,\mathrm{eV}$.

Problem 2.64

(a) Plugging into the differential equation we have

$$\sum_{n=2}^{\infty} a_n\, n\,(n-1)\,x^{n-2} - \sum_{n=2}^{\infty} a_n\, n\,(n-1)\,x^{n} - 2\sum_{n=1}^{\infty} a_n\, n\, x^n + \ell\,(\ell+1)\sum_{n=0}^{\infty} a_n\, x^n = 0\,.$$

Reindexing the sums so that all the powers of x match we have

$$\sum_{p=0}^{\infty} a_{p+2}\,(p+2)\,(p+1)\,x^p - \sum_{p=2}^{\infty} a_p\, p\,(p-1)\;x^p - 2\sum_{p=1}^{\infty} a_p\, p\, x^p + \ell\,(\ell+1)\sum_{p=0}^{\infty} a_p\, x^p = 0\,.$$

We can then combine the sums (extending the second and third sums to begin at $p = 0$) to get

$$\sum_{p=0}^{\infty} \left\{(p+2)\,(p+1)\;a_{p+2} - \left[p\,(p-1) + 2\,p - \ell\,(\ell+1)\right]\,a_p\right\}\,x^p = 0\,.$$

From this we read off the recursion relation

$$\boxed{a_{p+2} = \frac{p\,(p+1) - \ell\,(\ell+1)}{(p+2)\,(p+1)}\,a_p\,.}$$

(b) For large values of p,

$$a_{p+2} \approx \frac{p}{p+2}\,a_p\,.$$

with the (approximate) solution

$$a_p \approx \frac{C}{p}\,.$$

and this gives the behavior

$$f(x) \approx C\sum \frac{1}{p}\,x^p \approx \log\left(\frac{1}{1-x}\right)$$

which diverges at $x = 1$. (There will be finite corrections coming from the low values of p, but these cannot fix the divergence.)

(c) For $\ell = 0$ we need the even function ($a_1 = 0$) and the recursion relation gives $a_2 = 0$ so that

$$P_0(x) = a_0\,.$$

For $\ell = 1$ we need the odd function ($a_0 = 0$) and the recursion relation gives $a_3 = 0$ so that

$$P_1(x) = a_1\,x\,.$$

For $\ell = 2$ we need the even function again and the recursion relation gives $a_2 = -3\,a_0$ and $a_4 = 0$ so that

$$P_2(x) = a_0\left(1 - 3\,x^2\right)\,.$$

For $\ell = 3$ we need the odd function again and the recursion relation gives $a_3 = -5/3\,a_1$ and $a_5 = 0$ so that

$$P_3(x) = a_1\left(x - \frac{5}{3}\,x^3\right)\,.$$

Chapter 3

Formalism

Problem 3.1

(a) All conditions are trivial except Eq. A.1: we need to show that the sum of two square-integrable functions is itself square-integrable. Let $h(x) = f(x) + g(x)$, so that $|h|^2 = (f+g)^*(f+g) = |f|^2 + |g|^2 + f^*g + g^*f$ and hence

$$\int |h|^2\,dx = \int |f|^2\,dx + \int |g|^2\,dx + \int f^*g\,dx + \left(\int f^*g\,dx\right)^*.$$

If $f(x)$ and $g(x)$ are square-integrable, then the first two terms are finite, and (by Eq. 3.7) so too are the last two. So $\int |h|^2 dx$ is finite. QED

The set of all *normalized* functions is certainly *not* a vector space: it doesn't include 0, and the sum of two normalized functions is not (in general) normalized—in fact, if $f(x)$ is normalized, then the square integral of $2f(x)$ is 4.

(b) Equation A.19 is trivial:

$$\langle g|f\rangle = \int_a^b g(x)^* f(x)\,dx = \left(\int_a^b f(x)^* g(x)\,dx\right)^* = \langle f|g\rangle^*.$$

Equation A.20 holds (see Eq. 3.9) subject to the understanding in footnote 6. As for Eq. A.21, this is pretty obvious:

$$\langle f|(b|g\rangle + c|h\rangle) = \int f(x)^*\,(bg(x) + ch(x))\,dx = b\int f^*g\,dx + c\int f^*h\,dx = b\langle f|g\rangle + c\langle f|h\rangle.$$

Problem 3.2

(a)

$$\langle f|f\rangle = \int_0^1 x^{2\nu}\,dx = \frac{1}{2\nu+1}x^{2\nu+1}\Big|_0^1 = \frac{1}{2\nu+1}\left(1 - 0^{2\nu+1}\right).$$

Now $0^{2\nu+1}$ is finite (in fact, *zero*) provided $(2\nu+1) > 0$, which is to say, $\boxed{\nu > -\frac{1}{2}.}$ If $(2\nu+1) < 0$ the integral definitely blows up. As for the critical case $\nu = -\frac{1}{2}$, this must be handled separately:

$$\langle f|f\rangle = \int_0^1 x^{-1}\,dx = \ln x\Big|_0^1 = \ln 1 - \ln 0 = 0 + \infty.$$

So $f(x)$ is in Hilbert space only for ν strictly *greater* than -1/2.

(b) For $\nu = 1/2$, we know from (a) that $f(x)$ *is* in Hilbert space: $\boxed{\text{yes.}}$

Since $xf = x^{3/2}$, we know from (a) that it *is* in Hilbert space: $\boxed{\text{yes.}}$

For $df/dx = \frac{1}{2}x^{-1/2}$, we know from (a) that it is *not* in Hilbert space: $\boxed{\text{no.}}$

[*Moral:* Simple operations, such as differentiating (or multiplying by $1/x$), can carry a function *out* of Hilbert space.]

Problem 3.3

Suppose $\langle h|\hat{Q}h\rangle = \langle\hat{Q}h|h\rangle$ for all functions $h(x)$. Let $h(x) = f(x) + cg(x)$ for some arbitrary constant c. Then

$$\begin{aligned}\langle h|\hat{Q}h\rangle &= \langle(f+cg)|\hat{Q}(f+cg)\rangle = \langle f|\hat{Q}f\rangle + c\langle f|\hat{Q}g\rangle + c^*\langle g|\hat{Q}f\rangle + |c|^2\langle g|\hat{Q}g\rangle;\\ \langle\hat{Q}h|h\rangle &= \langle\hat{Q}(f+cg)|(f+cg)\rangle = \langle\hat{Q}f|f\rangle + c\langle\hat{Q}f|g\rangle + c^*\langle\hat{Q}g|f\rangle + |c|^2\langle\hat{Q}g|g\rangle.\end{aligned}$$

Equating the two and noting that $\langle f|\hat{Q}f\rangle = \langle\hat{Q}f|f\rangle$ and $\langle g|\hat{Q}g\rangle = \langle\hat{Q}g|g\rangle$ leaves

$$c\langle f|\hat{Q}g\rangle + c^*\langle g|\hat{Q}f\rangle = c\langle\hat{Q}f|g\rangle + c^*\langle\hat{Q}g|f\rangle.$$

In particular, choosing $c = 1$:

$$\langle f|\hat{Q}g\rangle + \langle g|\hat{Q}f\rangle = \langle\hat{Q}f|g\rangle + \langle\hat{Q}g|f\rangle,$$

whereas if $c = i$:

$$\langle f|\hat{Q}g\rangle - \langle g|\hat{Q}f\rangle = \langle\hat{Q}f|g\rangle - \langle\hat{Q}g|f\rangle.$$

Adding the last two equations:

$$\langle f|\hat{Q}g\rangle = \langle\hat{Q}f|g\rangle. \quad \text{QED}$$

Problem 3.4

(a) $\langle f|(\hat{H}+\hat{K})g\rangle = \langle f|\hat{H}g\rangle + \langle f|\hat{K}g\rangle = \langle\hat{H}f|g\rangle + \langle\hat{K}f|g\rangle = \langle(\hat{H}+\hat{K})f|g\rangle.$ ✓

(b) $\langle f|\alpha\hat{Q}g\rangle = \alpha\langle f|\hat{Q}g\rangle$; $\langle\alpha\hat{Q}f|g\rangle = \alpha^*\langle\hat{Q}f|g\rangle$. Hermitian $\Leftrightarrow$ $\boxed{\alpha \text{ is real.}}$

(c) $\langle f|\hat{H}\hat{K}g\rangle = \langle\hat{H}f|\hat{K}g\rangle = \langle\hat{K}\hat{H}f|g\rangle$, so $\hat{H}\hat{K}$ is hermitian $\Leftrightarrow$ $\hat{H}\hat{K} = \hat{K}\hat{H}$, or $\boxed{[\hat{H},\hat{K}] = 0.}$

(d) $\langle f|\hat{x}g\rangle = \int f^*(xg)\,dx = \int(xf)^*g\,dx = \langle\hat{x}f|g\rangle.$ ✓

$$\langle f|\hat{H}g\rangle = \int f^*\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right)g\,dx = -\frac{\hbar^2}{2m}\int f^*\frac{d^2g}{dx^2}\,dx + \int f^*Vg\,dx.$$

Integrating by parts (twice):

$$\int_{-\infty}^{\infty} f^*\frac{d^2g}{dx^2}\,dx = f^*\frac{dg}{dx}\bigg|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{df^*}{dx}\frac{dg}{dx}\,dx = f^*\frac{dg}{dx}\bigg|_{-\infty}^{\infty} - \frac{df^*}{dx}g\bigg|_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\frac{d^2f^*}{dx^2}g\,dx.$$

But for functions $f(x)$ and $g(x)$ in Hilbert space the boundary terms vanish, so $\int_{-\infty}^{\infty} f^*\frac{d^2g}{dx^2}\,dx = \int_{-\infty}^{\infty}\frac{d^2f^*}{dx^2}g\,dx$, and hence (assuming that $V(x)$ is real):

$$\langle f|\hat{H}g\rangle = \int_{-\infty}^{\infty}\left(-\frac{\hbar^2}{2m}\frac{d^2f}{dx^2} + Vf\right)^* g\,dx = \langle\hat{H}f|g\rangle. \quad ✓$$

Problem 3.5

(a) $\langle f|xg\rangle = \int f^*(xg)\,dx = \int (xf)^* g\,dx = \langle xf|g\rangle$, so $\boxed{x^\dagger = x.}$

$\langle f|ig\rangle = \int f^*(ig)\,dx = \int (-if)^* g\,dx = \langle -if|g\rangle$, so $\boxed{i^\dagger = -i.}$

$$\langle f|\frac{dg}{dx}\rangle = \int_{-\infty}^{\infty} f^* \frac{dg}{dx}\,dx = f^*g\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left(\frac{df}{dx}\right)^* g\,dx = -\langle\frac{df}{dx}|g\rangle, \text{ so } \boxed{\left(\frac{d}{dx}\right)^\dagger = -\frac{d}{dx}.}$$

(b) $a_+ = \dfrac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x)$. But p and x are hermitian, and $i^\dagger = -i$, so $(a_+)^\dagger = \dfrac{1}{\sqrt{2\hbar m\omega}}(ip + m\omega x)$, or $\boxed{(a_+)^\dagger = (a_-).}$

(c) $\langle f|(\hat{Q}\hat{R})g\rangle = \langle \hat{Q}^\dagger f|\hat{R}g\rangle = \langle \hat{R}^\dagger\hat{Q}^\dagger f|g\rangle = \langle(\hat{Q}\hat{R})^\dagger f|g\rangle$, so $(\hat{Q}\hat{R})^\dagger = \hat{R}^\dagger\hat{Q}^\dagger$. ✓

Problem 3.6

$$\langle f|\hat{Q}g\rangle = \int_0^{2\pi} f^*\frac{d^2g}{d\phi^2}\,d\phi = f^*\frac{dg}{d\phi}\Big|_0^{2\pi} - \int_0^{2\pi}\frac{df^*}{d\phi}\frac{dg}{d\phi}\,d\phi = f^*\frac{dg}{d\phi}\Big|_0^{2\pi} - \frac{df^*}{d\phi}g\Big|_0^{2\pi} + \int_0^{2\pi}\frac{d^2f^*}{d\phi^2}g\,d\phi.$$

As in Example 3.1, for periodic functions (Eq. 3.26) the boundary terms vanish, and we conclude that $\langle f|\hat{Q}g\rangle = \langle\hat{Q}f|g\rangle$, so $\hat{Q}$ is hermitian: $\boxed{\text{yes.}}$

$$\hat{Q}f = qf \Rightarrow \frac{d^2f}{d\phi^2} = qf \Rightarrow f_\pm(\phi) = \boxed{Ae^{\pm\sqrt{q}\phi}.}$$

The periodicity condition (Eq. 3.26) requires that $\sqrt{q}(2\pi) = 2n\pi i$, or $\sqrt{q} = in$, so the eigenvalues are $\boxed{q = -n^2,\ (n = 0, 1, 2, \ldots).}$ The spectrum is $\boxed{\text{doubly degenerate;}}$ for a given n there are *two* eigenfunctions (the plus sign or the minus sign, in the exponent), except for the special case $n = 0$, which is not degenerate.

Problem 3.7

(a) Suppose $\hat{Q}f = qf$ and $\hat{Q}g = qg$. Let $h(x) = af(x) + bg(x)$, for arbitrary constants a and b. Then

$$\hat{Q}h = \hat{Q}(af + bg) = a(\hat{Q}f) + b(\hat{Q}g) = a(qf) + b(qg) = q(af + bg) = qh. \quad ✓$$

(b) $\dfrac{d^2f}{dx^2} = \dfrac{d^2}{dx^2}(e^x) = \dfrac{d}{dx}(e^x) = e^x = f, \quad \dfrac{d^2g}{dx^2} = \dfrac{d^2}{dx^2}\left(e^{-x}\right) = \dfrac{d}{dx}\left(-e^{-x}\right) = e^{-x} = g.$

So both of them are eigenfunctions, with the same eigenvalue 1. The simplest orthogonal linear combinations are

$$\boxed{\sinh x = \frac{1}{2}\left(e^x - e^{-x}\right) = \frac{1}{2}(f - g) \quad \text{and} \quad \cosh x = \frac{1}{2}\left(e^x + e^{-x}\right) = \frac{1}{2}(f + g).}$$

(They are clearly orthogonal, since $\sinh x$ is odd while $\cosh x$ is even.)

Problem 3.8

(a) The eigenvalues (Eq. 3.29) are $0, \pm 1, \pm 2, \ldots$, which are obviously real. ✓ For any two eigenfunctions, $f = A_q e^{-iq\phi}$ and $g = A_{q'} e^{-iq'\phi}$ (Eq. 3.28), we have

$$\langle f|g\rangle = A_q^* A_{q'} \int_0^{2\pi} e^{iq\phi} e^{-iq'\phi}\, d\phi = A_q^* A_{q'} \left.\frac{e^{i(q-q')\phi}}{i(q-q')}\right|_0^{2\pi} = \frac{A_q^* A_{q'}}{i(q-q')} \left[e^{i(q-q')2\pi} - 1\right].$$

But q and q' are *integers*, so $e^{i(q-q')2\pi} = 1$, and hence $\langle f|g\rangle = 0$ (provided $q \neq q'$, so the denominator is nonzero). ✓

(b) In Problem 3.6 the eigenvalues are $q = -n^2$, with $n = 0, 1, 2, \ldots$, which are obviously real. ✓ For any two eigenfunctions, $f = A_q e^{\pm in\phi}$ and $g = A_{q'} e^{\pm in'\phi}$, we have

$$\langle f|g\rangle = A_q^* A_{q'} \int_0^{2\pi} e^{\mp in\phi} e^{\pm in'\phi}\, d\phi = A_q^* A_{q'} \left.\frac{e^{\pm i(n'-n)\phi}}{\pm i(n'-n)}\right|_0^{2\pi} = \frac{A_q^* A_{q'}}{\pm i(n'-n)} \left[e^{\pm i(n'-n)2\pi} - 1\right] = 0$$

(provided $n \neq n'$).

Problem 3.9

(a) $\boxed{\text{Infinite square well}}$ (Eq. 2.22).

(b) $\boxed{\text{Delta-function barrier}}$ (Fig. 2.15), or the finite rectangular barrier (Prob. 2.33).

(c) $\boxed{\text{Delta-function well}}$ (Eq. 2.114), or the finite square well (Eq. 2.148) or the sech^2 potential (Prob. 2.52).

Problem 3.10

From Eq. 2.31, with $n = 1$:

$$\hat{p}\,\psi_1(x) = \frac{\hbar}{i}\frac{d}{dx}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right) = \frac{\hbar}{i}\sqrt{\frac{2}{a}}\frac{\pi}{a}\cos\left(\frac{\pi}{a}x\right) = \left[-i\frac{\pi\hbar}{a}\cot\left(\frac{\pi}{a}x\right)\right]\psi_1(x).$$

Since $\hat{p}\,\psi_1$ is *not* a (constant) multiple of ψ_1, ψ_1 is not an eigenfunction of $\hat{p}$: $\boxed{\text{no.}}$

Problem 3.11

$$\Psi_0(x,t) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} e^{-i\omega t/2}; \quad \Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-i\omega t/2}\int_{-\infty}^{\infty} e^{-ipx/\hbar} e^{-\frac{m\omega}{2\hbar}x^2}\, dx.$$

From Problem 2.21(b):

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-i\omega t/2}\sqrt{\frac{2\pi\hbar}{m\omega}}\, e^{-p^2/2m\omega\hbar} = \boxed{\frac{1}{(\pi m\omega\hbar)^{1/4}} e^{-p^2/2m\omega\hbar} e^{-i\omega t/2}.}$$

$$|\Phi(p,t)|^2 = \frac{1}{\sqrt{\pi m\omega\hbar}} e^{-p^2/m\omega\hbar}.\quad \text{Maximum classical momentum: } \frac{p^2}{2m} = E = \frac{1}{2}\hbar\omega \Longrightarrow p = \sqrt{m\omega\hbar}.$$

So the probability it's outside classical range is:

$$P = \int_{-\infty}^{-\sqrt{m\omega\hbar}} |\Phi|^2 dp + \int_{\sqrt{m\omega\hbar}}^{\infty} |\Phi|^2 dp = 1 - 2\int_0^{\sqrt{m\omega\hbar}} |\Phi|^2 dp. \quad \text{Now}$$

$$\int_0^{\sqrt{m\omega\hbar}} |\Phi|^2 dp = \frac{1}{\sqrt{\pi m\omega\hbar}} \int_0^{\sqrt{m\omega\hbar}} e^{-p^2/m\omega\hbar}\, dp. \quad \text{Let } z \equiv \sqrt{\frac{2}{m\omega\hbar}}\, p, \text{ so } dp = \sqrt{\frac{m\omega\hbar}{2}}\, dz.$$

$$= \frac{1}{\sqrt{2\pi}} \int_0^{\sqrt{2}} e^{-z^2/2} dz = F(\sqrt{2}) - \frac{1}{2}, \text{ in CRC Table notation.}$$

$$P = 1 - 2\left[(F(\sqrt{2}) - \frac{1}{2}\right] = 1 - 2F(\sqrt{2}) + 1 = 2\left[1 - F(\sqrt{2})\right] = 0.157.$$

To two digits: $\boxed{0.16}$ (compare Prob. 2.14).

Problem 3.12

Let $k \equiv p/\hbar$ in Equation 2.101:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(p/\hbar) e^{i(px/\hbar)} e^{-ip^2t/2m}\, \frac{dp}{\hbar}.$$

Comparing Equation 3.55, read off

$$\boxed{\Phi(p,t) = \frac{1}{\hbar} e^{-ip^2t/2m}\, \phi(p/\hbar).}$$

Note that $|\Phi(p,t)|^2 = \frac{1}{\hbar}|\phi(p/\hbar)|^2$ is independent of t.

Alternatively, plug 2.101 into 3.54, and reverse the order of integration:

$$\begin{aligned}
\Phi(p,t) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \hbar^2k^2t/2m)}\, dk \right\} dx \\
&= \frac{1}{\sqrt{\hbar}} \int_{-\infty}^{\infty} \phi(k) e^{-i\hbar^2k^2t/2m} \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-p/\hbar)x}\, dx \right\} dk \\
&= \frac{1}{\sqrt{\hbar}} \int_{-\infty}^{\infty} \phi(k) e^{-i\hbar^2k^2t/2m}\, \delta\left(k - p/\hbar\right) dk = \frac{1}{\sqrt{\hbar}} e^{-ip^2t/2m} \phi(p/\hbar)
\end{aligned}$$

(I used Equation 2.147 in the third line).

Problem 3.13

From Eq. 3.55: $\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \Phi(p,t) dp.$

$$\langle x \rangle = \int \Psi^* x \Psi dx = \int \left[\frac{1}{\sqrt{2\pi\hbar}} \int e^{-ip'x/\hbar} \Phi^*(p',t) dp' \right] x \left[\frac{1}{\sqrt{2\pi\hbar}} \int e^{+ipx/\hbar} \Phi(p,t) dp \right] dx.$$

But $xe^{ipx/\hbar} = -i\hbar\dfrac{d}{dp}\left(e^{ipx/\hbar}\right)$, so (integrating by parts):

$$x\int e^{ipx/\hbar}\Phi\,dp = \int \frac{\hbar}{i}\frac{d}{dp}\left(e^{ipx/\hbar}\right)\Phi\,dp = \int e^{ipx/\hbar}\left[-\frac{\hbar}{i}\frac{\partial}{\partial p}\Phi(p,t)\right]dp.$$

So $\langle x\rangle = \dfrac{1}{2\pi\hbar}\displaystyle\iiint \left\{e^{-ip'x/\hbar}\Phi^*(p',t)e^{ipx/\hbar}\left[-\frac{\hbar}{i}\frac{\partial}{\partial p}\Phi(p,t)\right]\right\}dp'\,dp\,dx.$

Do the x integral first, letting $y \equiv x/\hbar$:

$$\frac{1}{2\pi\hbar}\int e^{-ip'x/\hbar}e^{ipx/\hbar}dx = \frac{1}{2\pi}\int e^{i(p-p')y}dy = \delta(p-p'),\ \text{(Eq. 2.144), so}$$

$$\langle x\rangle = \iint \Phi^*(p',t)\delta(p-p')\left[-\frac{\hbar}{i}\frac{\partial}{\partial p}\Phi(p,t)\right]dp'dp = \int \Phi^*(p,t)\left[-\frac{\hbar}{i}\frac{\partial}{\partial p}\Phi(p,t)\right]dp. \quad \text{QED}$$

Problem 3.14

(a)

$$[\hat{A}+\hat{B},\hat{C}] = (\hat{A}+\hat{B})\hat{C} - \hat{C}(\hat{A}+\hat{B}) = \hat{A}\hat{C} + \hat{B}\hat{C} - \hat{C}\hat{A} - \hat{C}\hat{B} = [\hat{A},\hat{C}] + \hat{B},\hat{C}] \quad \checkmark$$

$$[\hat{A}\hat{B},\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{C}\hat{A}\hat{B} = \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B} + \hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B} = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B}. \quad \checkmark$$

(b) Introducing a test function $g(x)$, as in Eq. 2.51:

$$[x^n,\hat{p}]g = x^n\frac{\hbar}{i}\frac{dg}{dx} - \frac{\hbar}{i}\frac{d}{dx}(x^n g) = x^n\frac{\hbar}{i}\frac{dg}{dx} - \frac{\hbar}{i}\left(nx^{n-1}g + x^n\frac{dg}{dx}\right) = i\hbar n x^{n-1}g.$$

So, dropping the test function, $[x^n,\hat{p}] = i\hbar n x^{n-1}$. $\checkmark$

(c) $[f,\hat{p}]g = f\dfrac{\hbar}{i}\dfrac{dg}{dx} - \dfrac{\hbar}{i}\dfrac{d}{dx}(fg) = f\dfrac{\hbar}{i}\dfrac{dg}{dx} - \dfrac{\hbar}{i}\left(\dfrac{df}{dx}g + f\dfrac{dg}{dx}\right) = i\hbar\dfrac{df}{dx}g \Rightarrow [f,\hat{p}] = i\hbar\dfrac{df}{dx}.$ $\checkmark$

(d)

$$[\hat{H},\hat{a}_\pm] = [\hbar\omega(\hat{a}_-\hat{a}_+ - \tfrac{1}{2}),\hat{a}_\pm] = \hbar\omega\left\{[\hat{a}_-\hat{a}_+,\hat{a}_\pm] - \cancel{[\tfrac{1}{2},\hat{a}_\pm]}\right\} = \hbar\omega\left\{\hat{a}_-[\hat{a}_+,\hat{a}_\pm] + [\hat{a}_-,\hat{a}_\pm]\hat{a}_+\right\}.$$

So, using $[\hat{a}_-,\hat{a}_+] = 1$ (Equation 2.56),

$$[\hat{H},\hat{a}_+] = \hbar\omega\left\{\hat{a}_-\cancel{[\hat{a}_+,\hat{a}_+]} + [\hat{a}_-,\hat{a}_+]\hat{a}_+\right\} = \hbar\omega\hat{a}_+, \quad \text{and}$$

$$[\hat{H},\hat{a}_-] = \hbar\omega\left\{\hat{a}_-[\hat{a}_+,\hat{a}_-] + \cancel{[\hat{a}_-,\hat{a}_-]}\hat{a}_+\right\} = \hbar\omega(-\hat{a}_-), \quad \text{or, combining them}$$

$$[\hat{H},\hat{a}_\pm] = \pm\hbar\omega\hat{a}_\pm. \quad \checkmark$$

Problem 3.15

$$\left[x,\frac{p^2}{2m}+V\right] = \frac{1}{2m}\left[x,p^2\right] + [x,V]; \quad \left[x,p^2\right] = xp^2 - p^2x = xp^2 - pxp + pxp - p^2x = [x,p]p + p[x,p].$$

Using Eq. 2.52: $\left[x,p^2\right] = i\hbar p + pi\hbar = 2i\hbar p$. And $[x,V] = 0$, so $\left[x,\dfrac{p^2}{2m}+V\right] = \dfrac{1}{2m}2i\hbar p = \dfrac{i\hbar p}{m}.$

The generalized uncertainty principle (Eq. 3.62) says, in this case,

$$\sigma_x^2\sigma_H^2 \geq \left(\frac{1}{2i}\frac{i\hbar}{m}\langle p\rangle\right)^2 = \left(\frac{\hbar}{2m}\langle p\rangle\right)^2 \Rightarrow \sigma_x\sigma_H \geq \frac{\hbar}{2m}|\langle p\rangle|. \quad \text{QED}$$

For stationary states $\sigma_H = 0$ and $\langle p\rangle = 0$, so it just says $0 \geq 0$.

Problem 3.16

Suppose $\hat{P}f_n = \lambda_n f_n$ and $\hat{Q}f_n = \mu_n f_n$ (that is: $f_n(x)$ is an eigenfunction both of $\hat{P}$ and of $\hat{Q}$), and the set $\{f_n\}$ is complete, so that any function $f(x)$ (in Hilbert space) can be expressed as a linear combination: $f = \sum c_n f_n$. Then

$$[\hat{P},\hat{Q}]f = (\hat{P}\hat{Q} - \hat{Q}\hat{P})\sum c_n f_n = \hat{P}\left(\sum c_n\mu_n f_n\right) - \hat{Q}\left(\sum c_n\lambda_n f_n\right) = \sum c_n\mu_n\lambda_n f_n - \sum c_n\lambda_n\mu_n f_n = 0.$$

Since this is true for *any* function f, it follows that $[\hat{P},\hat{Q}] = 0$.

Problem 3.17

$$\frac{d\Psi}{dx} = \frac{i}{\hbar}(iax - ia\langle x\rangle + \langle p\rangle)\Psi = \frac{a}{\hbar}\left(-x + \langle x\rangle + \frac{i}{a}\langle p\rangle\right)\Psi.$$

$$\frac{d\Psi}{\Psi} = \frac{a}{\hbar}\left(-x + \langle x\rangle + \frac{i\langle p\rangle}{a}\right)dx \Rightarrow \ln\Psi = \frac{a}{\hbar}\left(-\frac{x^2}{2} + \langle x\rangle x + \frac{i\langle p\rangle}{a}x\right) + \textit{constant}.$$

Let *constant* $= -\dfrac{\langle x\rangle^2 a}{2\hbar} + B$ (B a new constant). Then $\ln\Psi = -\dfrac{a}{2\hbar}(x - \langle x\rangle)^2 + \dfrac{i\langle p\rangle}{\hbar}x + B.$

$$\Psi = e^{-\frac{a}{2\hbar}(x-\langle x\rangle)^2}e^{i\langle p\rangle x/\hbar}e^B = Ae^{-a(x-\langle x\rangle)^2/2\hbar}e^{i\langle p\rangle x/\hbar}, \text{ where } A \equiv e^B.$$

Problem 3.18

(a) 1 commutes with everything, so $\boxed{\dfrac{d}{dt}\langle\Psi|\Psi\rangle = 0}$ (this is the conservation of normalization, which we originally proved in Eq. 1.27).

(b) Anything commutes with itself, so $[H,H] = 0$, and hence $\boxed{\dfrac{d}{dt}\langle H\rangle = 0}$ (assuming H has no explicit time dependence); this is conservation of energy, in the sense of the comment following Eq. 2.21.

(c) $[H,x] = -\dfrac{i\hbar p}{m}$ (see Problem 3.15). So $\dfrac{d\langle x\rangle}{dt} = \dfrac{i}{\hbar}\left(-\dfrac{i\hbar\langle p\rangle}{m}\right) = \boxed{\dfrac{\langle p\rangle}{m}}$ (Eq. 1.33).

(d) $[H,p] = \left[\dfrac{p^2}{2m} + V, p\right] = [V,p] = i\hbar\dfrac{\partial V}{\partial x}$ (Problem 3.14(c)). So $\dfrac{d\langle p\rangle}{dt} = \dfrac{i}{\hbar}\left(i\hbar\left\langle\dfrac{\partial V}{\partial x}\right\rangle\right) = \boxed{-\left\langle\dfrac{\partial V}{\partial x}\right\rangle.}$

This is Ehrenfest's theorem (Eq. 1.38).

Problem 3.19

(a) Problem 3.18(d) says $\frac{d\langle p\rangle}{dt} = -\left\langle\frac{\partial V}{\partial x}\right\rangle = 0$, so $\langle p\rangle = p_0$, a constant (independent of t). Then Problem 3.18(c) says $\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m} = \frac{p_0}{m}$, and hence $\langle x\rangle = \frac{p_0}{m}t + x_0$ (where x_0 is another constant). So $\langle x\rangle$ moves at constant velocity ($v_0 = p_0/m$). QED

(b) In the same way,

$$\frac{d\langle p\rangle}{dt} = -\left\langle\frac{\partial V}{\partial x}\right\rangle = -\langle m\omega^2 x\rangle = -m\omega^2\langle x\rangle.$$

$$\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m} \Rightarrow \frac{d^2\langle x\rangle}{dt^2} = \frac{1}{m}\frac{d\langle p\rangle}{dt} = \frac{1}{m}(-m\omega^2)\langle x\rangle = -\omega^2\langle x\rangle.$$

So $\langle x\rangle$ satisfies the classical harmonic oscillator equation, and the general solution is

$$\langle x\rangle = A\sin(\omega t) + B\cos(\omega t);$$

it oscillates at the classical frequency. QED

Problem 3.20

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_1 e^{-iE_1t/\hbar} + \psi_2 e^{-E_2t/\hbar}\right). \quad H^2\Psi = \frac{1}{\sqrt{2}}\left[(H^2\psi_1)e^{-E_1t/\hbar} + (H^2\psi_2)e^{-iE_2t/\hbar}\right].$$

$$H\psi_1 = E_1\psi_1 \Rightarrow H^2\psi_1 = E_1 H\psi_1 = E_1^2\psi_1, \quad \text{and } H^2\psi_2 = E_2^2\psi_2, \quad \text{so}$$

$$\begin{aligned}
\langle H^2\rangle &= \frac{1}{2}\langle\left(\psi_1 e^{-iE_1t/\hbar} + \psi_2 e^{-iE_2t/\hbar}\right)|\left(E_1^2\psi_1 e^{-iE_1t/\hbar} + E_2^2\psi_2 e^{-iE_2t/\hbar}\right)\rangle \\
&= \frac{1}{2}\big(\langle\psi_1|\psi_1\rangle e^{iE_1t/\hbar}E_1^2 e^{-iE_1t/\hbar} + \langle\psi_1|\psi_2\rangle e^{iE_1t/\hbar}E_2^2 e^{-iE_2t/\hbar} \\
&\quad + \langle\psi_2|\psi_1\rangle e^{iE_2t/\hbar}E_1^2 e^{-iE_1t/\hbar} + \langle\psi_2|\psi_2\rangle e^{iE_2t/\hbar}E_2^2 e^{-iE_2t/\hbar}\big) = \frac{1}{2}\left(E_1^2 + E_2^2\right).
\end{aligned}$$

Similarly, $\langle H\rangle = \frac{1}{2}(E_1 + E_2)$ (Problem 2.5(e)).

$$\begin{aligned}
\sigma_H^2 &= \langle H^2\rangle - \langle H\rangle^2 = \frac{1}{2}\left(E_1^2 + E_2^2\right) - \frac{1}{4}(E_1 + E_2)^2 = \frac{1}{4}\left(2E_1^2 + 2E_2^2 - E_2^2 - E_1^2 - 2E_1E_2\right) \\
&= \frac{1}{4}\left(E_1^2 - 2E_1E_2 + E_2^2\right) = \frac{1}{4}(E_2 - E_1)^2. \quad \boxed{\sigma_H = \frac{1}{2}(E_2 - E_1).}
\end{aligned}$$

$$\langle x^2\rangle = \frac{1}{2}\left[\langle\psi_1|x^2|\psi_1\rangle + \langle\psi_2|x^2|\psi_2\rangle + \langle\psi_1|x^2|\psi_2\rangle e^{i(E_1-E_2)t/\hbar} + \langle\psi_2|x^2|\psi_1\rangle e^{i(E_2-E_1)t/\hbar}\right].$$

$$\langle\psi_n|x^2|\psi_m\rangle = \frac{2}{a}\int_0^a x^2\sin\left(\frac{n\pi}{a}x\right)\sin\left(\frac{m\pi}{a}x\right)dx = \frac{1}{a}\int_0^a x^2\left[\cos\left(\frac{n-m}{a}\pi x\right) - \cos\left(\frac{n+m}{a}\pi x\right)\right]dx.$$

$$\begin{aligned}
\text{Now } \int_0^a x^2\cos\left(\frac{k}{a}\pi x\right)dx &= \left\{\frac{2a^2x}{k^2\pi^2}\cos\left(\frac{k}{a}\pi x\right) + \left(\frac{a}{k\pi}\right)^3\left[\left(\frac{k\pi x}{a}\right)^2 - 2\right]\sin\left(\frac{k}{a}\pi x\right)\right\}\Bigg|_0^a \\
&= \frac{2a^3}{k^2\pi^2}\cos(k\pi) = \frac{2a^3}{k^2\pi^2}(-1)^k \quad \text{(for } k = \text{nonzero integer).}
\end{aligned}$$

$$\therefore \langle\psi_n|x^2|\psi_m\rangle = \frac{2a^2}{\pi^2}\left[\frac{(-1)^{n-m}}{(n-m)^2} - \frac{(-1)^{n+m}}{(n+m)^2}\right] = \frac{2a^2}{\pi^2}(-1)^{n+m}\frac{4nm}{(n^2-m^2)^2}.$$

So $\langle\psi_1|x^2|\psi_2\rangle = \langle\psi_2|x^2|\psi_1\rangle = -\dfrac{16a^2}{9\pi^2}$. Meanwhile, from Problem 2.4, $\langle\psi_n|x^2|\psi_n\rangle = a^2\left[\dfrac{1}{3} - \dfrac{1}{2(n\pi)^2}\right]$.

Thus $\langle x^2\rangle = \dfrac{1}{2}\left\{a^2\left[\dfrac{1}{3} - \dfrac{1}{2\pi^2}\right] + a^2\left[\dfrac{1}{3} - \dfrac{1}{8\pi^2}\right] - \dfrac{16a^2}{9\pi^2}\left[\underbrace{e^{i(E_2-E_1)t/\hbar} + e^{-i(E_2-E_1)t/\hbar}}_{2\cos\left(\frac{E_2-E_1}{\hbar}t\right)}\right]\right\}$.

$\dfrac{E_2 - E_1}{\hbar} = \dfrac{(4-1)\pi^2\hbar^2}{2ma^2\hbar} = \dfrac{3\pi^2\hbar}{2ma^2} = 3\omega$ [in the notation of Problem 2.5(b)].

$\langle x^2\rangle = \dfrac{a^2}{2}\left[\dfrac{2}{3} - \dfrac{5}{8\pi^2} - \dfrac{32}{9\pi^2}\cos(3\omega t)\right]$. From Problem 2.5(c), $\langle x\rangle = \dfrac{a}{2}\left[1 - \dfrac{32}{9\pi^2}\cos(3\omega t)\right]$.

So $\sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2 = \dfrac{a^2}{4}\left[\dfrac{4}{3} - \dfrac{5}{4\pi^2} - \dfrac{64}{9\pi^2}\cos(3\omega t) - 1 + \dfrac{64}{9\pi^2}\cos(3\omega t) - \left(\dfrac{32}{9\pi^2}\right)^2\cos^2(3\omega t)\right]$.

$\boxed{\sigma_x^2 = \dfrac{a^2}{4}\left[\dfrac{1}{3} - \dfrac{5}{4\pi^2} - \left(\dfrac{32}{9\pi^2}\right)^2\cos^2(3\omega t)\right].}$ And, from Problem 2.5(d): $\boxed{\dfrac{d\langle x\rangle}{dt} = \dfrac{8\hbar}{3ma}\sin(3\omega t).}$

Meanwhile, the energy-time uncertainty principle (Eq. 3.74) says $\sigma_H^2\sigma_x^2 \geq \dfrac{\hbar^2}{4}\left(\dfrac{d\langle x\rangle}{dt}\right)^2$. Here

$$\sigma_H^2\sigma_x^2 = \frac{1}{4}(3\hbar\omega)^2\frac{a^2}{4}\left[\frac{1}{3} - \frac{5}{4\pi^2} - \left(\frac{32}{9\pi^2}\right)^2\cos^2(3\omega t)\right] = (\hbar\omega a)^2\left(\frac{3}{4}\right)^2\left[\frac{1}{3} - \frac{5}{4\pi^2} - \left(\frac{32}{9\pi^2}\right)^2\cos^2(3\omega t)\right].$$

$\dfrac{\hbar^2}{4}\left(\dfrac{d\langle x\rangle}{dt}\right)^2 = \left(\dfrac{\hbar}{2}\cdot\dfrac{8\hbar}{3ma}\right)^2\sin^2(3\omega t) = \left(\dfrac{8}{3\pi^2}\right)^2(\hbar\omega a)^2\sin^2(3\omega t)$, since $\dfrac{\hbar}{ma} = \dfrac{2a\omega}{\pi^2}$.

So the uncertainty principle holds if

$$\left(\frac{3}{4}\right)^2\left[\frac{1}{3} - \frac{5}{4\pi^2} - \left(\frac{32}{9\pi^2}\right)^2\cos^2(3\omega t)\right] \geq \left(\frac{8}{3\pi^2}\right)^2\sin^2(3\omega t),$$

which is to say, if

$$\frac{1}{3} - \frac{5}{4\pi^2} \geq \left(\frac{32}{9\pi^2}\right)^2\cos^2(3\omega t) + \left(\frac{4}{3}\frac{8}{3\pi^2}\right)^2\sin^2(3\omega t) = \left(\frac{32}{9\pi^2}\right)^2.$$

Evaluating both sides: $\dfrac{1}{3} - \dfrac{5}{4\pi^2} = 0.20668$; $\quad\left(\dfrac{32}{9\pi^2}\right)^2 = 0.12978$. So it holds. (Whew!)

Problem 3.21

From Problem 2.42, we have:

$$\langle x\rangle = \frac{\hbar l}{m}t, \text{ so } \boxed{\frac{d\langle x\rangle}{dt} = \frac{\hbar l}{m},}\ \sigma_x^2 = \frac{1}{4w^2} = \boxed{\frac{1+\theta^2}{4a},} \text{ where } \theta = \frac{2\hbar a t}{m};\ \langle H\rangle = \frac{1}{2m}\langle p^2\rangle = \frac{1}{2m}\hbar^2(a+l^2).$$

We need $\langle H^2\rangle$ (to get σ_H). Now, $H = \dfrac{p^2}{2m}$, so

$\langle H^2\rangle = \dfrac{1}{4m^2}\langle p^4\rangle = \dfrac{1}{4m^2}\displaystyle\int_{-\infty}^{\infty} p^4|\Phi(p,t)|^2dp$, where (Eq. 3.54): $\Phi(p,t) = \dfrac{1}{\sqrt{2\pi\hbar}}\displaystyle\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x,t)\,dx$.

From Problem 2.42: $\Psi(x,t) = \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{1+i\theta}} e^{-\frac{l^2}{4a}} e^{a\left(ix+\frac{l}{2a}\right)^2/(1+i\theta)}$.

$$\text{So } \Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\left(\frac{2a}{\pi}\right)^{1/4}\frac{1}{\sqrt{1+i\theta}}e^{-l^2/4a}\int_{-\infty}^{\infty} e^{-ipx/\hbar}e^{a\left(ix+\frac{l}{2a}\right)^2/(1+i\theta)}dx. \quad \text{Let } y \equiv x - \frac{il}{2a}.$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\left(\frac{2a}{\pi}\right)^{1/4}\frac{1}{\sqrt{1+i\theta}}e^{-l^2/4a}e^{pl/2a\hbar}\int_{-\infty}^{\infty} e^{-ipy/\hbar}e^{-ay^2/(1+i\theta)}dy.$$

[See Prob. 2.22(b) for the integral.]

$$= \frac{1}{\sqrt{2\pi\hbar}}\left(\frac{2a}{\pi}\right)^{1/4}\frac{1}{\sqrt{1+i\theta}}e^{-l^2/4a}e^{pl/2a\hbar}\sqrt{\frac{\pi(1+i\theta)}{a}}e^{-\frac{p^2(1+i\theta)}{4a\hbar^2}}$$

$$= \frac{1}{\sqrt{\hbar}}\left(\frac{1}{2a\pi}\right)^{1/4} e^{-\frac{l^2}{4a}} e^{\frac{pl}{2a\hbar}} e^{-\frac{p^2(1+i\theta)}{4a\hbar^2}}.$$

$$|\Phi(p,t)|^2 = \frac{1}{\sqrt{2a\pi}}\frac{1}{\hbar}e^{-l^2/2a}e^{pl/a\hbar}e^{-p^2/2a\hbar^2} = \frac{1}{\hbar\sqrt{2a\pi}}e^{-\frac{1}{2a}\left(l^2-\frac{2pl}{\hbar}+\frac{p^2}{\hbar^2}\right)} = \frac{1}{\hbar\sqrt{2a\pi}}e^{-(l-p/\hbar)^2/2a}.$$

$$\langle p^4\rangle = \frac{1}{\hbar\sqrt{2a\pi}}\int_{-\infty}^{\infty} p^4 e^{-(l-p/\hbar)^2/2a}dp. \quad \text{Let } \frac{p}{\hbar} - l \equiv z, \text{ so } p = \hbar(z+l).$$

$$= \frac{1}{\hbar\sqrt{2a\pi}}\hbar^5\int_{-\infty}^{\infty}(z+l)^4 e^{-z^2/2a}dz. \text{ Only even powers of } z \text{ survive:}$$

$$= \frac{\hbar^4}{\sqrt{2a\pi}}\int_{-\infty}^{\infty}\left(z^4+6z^2l^2+l^4\right)e^{-z^2/2a}dz = \frac{\hbar^4}{\sqrt{2a\pi}}\left[\frac{3(2a)^2}{4}\sqrt{2a\pi}+6l^2\frac{(2a)}{2}\sqrt{2a\pi}+l^4\sqrt{2a\pi}\right]$$

$$= \hbar^4\left(3a^2+6al^2+l^4\right). \quad \therefore \langle H^2\rangle = \frac{\hbar^4}{4m^2}\left(3a^2+6al^2+l^4\right).$$

$$\sigma_H^2 = \langle H^2\rangle - \langle H\rangle^2 = \frac{\hbar^4}{4m^2}\left(3a^2+6al^2+l^4-a^2-2al^2-l^4\right) = \frac{\hbar^4}{4m^2}\left(2a^2+4al^2\right) = \boxed{\frac{\hbar^4 a}{2m^2}\left(a+2l^2\right).}$$

$$\sigma_H^2\sigma_x^2 = \frac{\hbar^4 a}{2m^2}\left(a+2l^2\right)\frac{1}{4a}\left[1+\left(\frac{2\hbar at}{m}\right)^2\right] = \frac{\hbar^4 l^2}{4m^2}\left(1+\frac{a}{2l^2}\right)\left[1+\left(\frac{2\hbar at}{m}\right)^2\right]$$

$$\geq \frac{\hbar^4 l^2}{4m^2} = \frac{\hbar^2}{4}\left(\frac{\hbar l}{m}\right)^2 = \frac{\hbar^2}{4}\left(\frac{d\langle x\rangle}{dt}\right)^2, \text{ so it works.}$$

Problem 3.22

For $Q = x$, Eq. 3.74 says $\sigma_H\sigma_x \geq \frac{\hbar}{2}\left|\frac{d\langle x\rangle}{dt}\right|$. But $\langle p\rangle = m\frac{d\langle x\rangle}{dt}$, so $\sigma_x\sigma_H \geq \frac{\hbar}{2m}|\langle p\rangle|$, which is the Griffiths uncertainty principle of Problem 3.15.

Problem 3.23

$$P^2|\beta\rangle = P(P|\beta\rangle) = P(\langle\alpha|\beta\rangle|\alpha\rangle) = \langle\alpha|\beta\rangle(P|\alpha\rangle) = \langle\alpha|\beta\rangle\underbrace{\langle\alpha|\alpha\rangle}_{1}|\alpha\rangle = \langle\alpha|\beta\rangle|\alpha\rangle = P|\beta\rangle.$$

Since $P^2|\beta\rangle = P|\beta\rangle$ for *any* vector $|\beta\rangle$, $P^2 = P$. QED [*Note:* To say two operators are equal *means* that they have the same effect on all vectors.]

If $|\gamma\rangle$ is an eigenvector of $\hat{P}$ with eigenvalue λ, then $\hat{P}|\gamma\rangle = \lambda|\gamma\rangle$, and it follows that $\hat{P}^2|\gamma\rangle = \lambda\hat{P}|\gamma\rangle = \lambda^2|\gamma\rangle$. But $\hat{P}^2 = \hat{P}$, and $|\gamma\rangle \neq 0$, so $\lambda^2 = \lambda$, and hence the eigenvalues of $\hat{P}$ are $\boxed{\text{0 and 1.}}$ Any (complex) *multiple* of $|\alpha\rangle$ is an eigenvector of $\hat{P}$, with eigenvalue 1; any vector *orthogonal* to $|\alpha\rangle$ is an eigenvector of $\hat{P}$, with eigenvalue 0.

Problem 3.24

In the usual casual notation, write $\hat{Q}e_n$ as the name of the vector $\hat{Q}|e_n\rangle$. Then

$$Q_{mn} \equiv \langle e_m|\hat{Q}|e_n\rangle = \langle e_m|\hat{Q}e_n\rangle = \langle \hat{Q}e_m|e_n\rangle = \langle e_n|\hat{Q}e_m\rangle^* = \langle e_n|\hat{Q}|e_m\rangle^* = Q^*_{nm}. \quad \text{QED}$$

Problem 3.25

Write the eigenvector as $|\psi\rangle = c_1|1\rangle + c_2|2\rangle$, and call the eigenvalue E. The eigenvalue equation is

$$\begin{aligned}\hat{H}|\psi\rangle &= \epsilon\left(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\right)\left(c_1|1\rangle + c_2|2\rangle\right) = \epsilon\left(c_1|1\rangle + c_1|2\rangle - c_2|2\rangle + c_2|1\rangle\right) \\ &= \epsilon\left[(c_1 + c_2)|1\rangle + (c_1 - c_2)|2\rangle\right] = E|\psi\rangle = E(c_1|1\rangle + c_2|2\rangle).\end{aligned}$$

$$\epsilon(c_1 + c_2) = Ec_1 \Rightarrow c_2 = \left(\frac{E}{\epsilon} - 1\right)c_1; \quad \epsilon(c_1 - c_2) = Ec_2 \Rightarrow c_1 = \left(\frac{E}{\epsilon} + 1\right)c_2.$$

$$c_2 = \left(\frac{E}{\epsilon} - 1\right)\left(\frac{E}{\epsilon} + 1\right)c_2 \quad \Rightarrow \left(\frac{E}{\epsilon}\right)^2 - 1 = 1 \quad \Rightarrow \boxed{E = \pm\sqrt{2}\,\epsilon.}$$

The eigenvectors are: $c_2 = (\pm\sqrt{2} - 1)c_1 \Rightarrow \boxed{|\psi_\pm\rangle = c_1\left[|1\rangle + (\pm\sqrt{2} - 1)|2\rangle\right].}$

The Hamiltonian matrix is $\boxed{\mathsf{H} = \epsilon\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.}$

Problem 3.26

(a) $\boxed{\langle\alpha| = -i\langle 1| - 2\langle 2| + i\langle 3|; \quad \langle\beta| = -i\langle 1| + 2\langle 3|.}$

(b) $\langle\alpha|\beta\rangle = (-i\langle 1| - 2\langle 2| + i\langle 3|)\,(i|1\rangle + 2|3\rangle) = (-i)(i)\langle 1|1\rangle + (i)(2)\langle 3|3\rangle = \boxed{1 + 2i.}$

$\langle\beta|\alpha\rangle = (-i\langle 1| + 2\langle 3|)\,(i|1\rangle - 2|2\rangle - i|3\rangle) = (-i)(i)\langle 1|1\rangle + (2)(-i)\langle 3|3\rangle = \boxed{1 - 2i} = \langle\alpha|\beta\rangle^*.$ ✓

(c)

$$\begin{array}{llll} A_{11} = \langle 1|\alpha\rangle\langle\beta|1\rangle = (i)(-i) = 1; & A_{12} = \langle 1|\alpha\rangle\langle\beta|2\rangle = (i)(0) = 0; & A_{13} = \langle 1|\alpha\rangle\langle\beta|3\rangle = (i)(2) = 2i; \\ A_{21} = \langle 2|\alpha\rangle\langle\beta|1\rangle = (-2)(-i) = 2i; & A_{22} = \langle 2|\alpha\rangle\langle\beta|2\rangle = (-2)(0) = 0; & A_{23} = \langle 2|\alpha\rangle\langle\beta|3\rangle = (-2)(2) = -4; \\ A_{31} = \langle 3|\alpha\rangle\langle\beta|1\rangle = (-i)(-i) = -1; & A_{32} = \langle 3|\alpha\rangle\langle\beta|2\rangle = (-i)(0) = 0; & A_{33} = \langle 3|\alpha\rangle\langle\beta|3\rangle = (-i)(2) = -2i. \end{array}$$

$$\mathsf{A} = \begin{pmatrix} 1 & 0 & 2i \\ 2i & 0 & -4 \\ -1 & 0 & -2i \end{pmatrix}. \quad \boxed{\text{No,}} \text{ it's } \textit{not} \text{ hermitian.}$$

Problem 3.27

(a)

$$|\alpha\rangle = \sum_n c_n |e_n\rangle \Rightarrow \hat{Q}|\alpha\rangle = \sum_n c_n \hat{Q}|e_n\rangle = \sum_n \langle e_n|\alpha\rangle q_n |e_n\rangle = \left(\sum_n q_n |e_n\rangle\langle e_n|\right)|\alpha\rangle \Rightarrow \hat{Q} = \sum_n q_n |e_n\rangle\langle e_n|. \checkmark$$

(b) Noting that $\hat{Q}|e_n\rangle = q_n|e_n\rangle \Rightarrow \hat{Q}^2|e_n\rangle = q_n\hat{Q}|e_n\rangle = q_n^2|e_n\rangle \cdots \Rightarrow \hat{Q}^j|e_n\rangle = q_n^j|e_n\rangle$, we have

$$e^{\hat{Q}}|\alpha\rangle = \sum_{j=0}^{\infty} \frac{1}{j!}\hat{Q}^j \left(\sum_n |e_n\rangle\langle e_n|\right)|\alpha\rangle = \sum_n \left(\sum_j \frac{1}{j!}q_n^j\right)|e_n\rangle\langle e_n|\,|\alpha\rangle = \left(\sum_n e^{q_n}|e_n\rangle\langle e_n|\right)|\alpha\rangle,$$

so

$$e^{\hat{Q}} = \left(\sum_n e^{q_n}|e_n\rangle\langle e_n|\right). \quad \text{QED}$$

Problem 3.28

(a) The Taylor expansion of $\sin z$ is $z - \frac{1}{3!}z^3 + \frac{1}{5!}z^5 - \cdots$, so

$$(\sin\hat{D})x^5 = \left(\frac{d}{dx} - \frac{1}{3!}\frac{d^3}{dx^3} + \frac{1}{5!}\frac{d^5}{dx^5} - \cdots\right)x^5 = 5x^4 - \frac{1}{3!}5\cdot4\cdot3x^2 + \frac{1}{5!}5\cdot4\cdot3\cdot2\cdot1\,x^0$$
$$= \boxed{5x^4 - 10x^2 + 1.}$$

(b) $\dfrac{1}{1-z} = 1 + z + z^2 + z^3 + \cdots$, so

$$\left(\frac{1}{1-\hat{D}/2}\right)\cos x = \left(1 + \frac{1}{2}\frac{d}{dx} + \frac{1}{4}\frac{d^2}{dx^2} + \frac{1}{8}\frac{d^3}{dx^3} + \frac{1}{16}\frac{d^4}{dx^4} + \cdots\right)\cos x$$
$$= \cos x - \frac{1}{2}\sin x - \frac{1}{4}\cos x + \frac{1}{8}\sin x + \frac{1}{16}\cos x + \cdots$$
$$= \cos x\left(1 - \frac{1}{4} + \frac{1}{16} + \cdots\right) - \frac{1}{2}\sin x\left(1 - \frac{1}{4} + \frac{1}{16} + \cdots\right)$$
$$= (\cos x - \frac{1}{2}\sin x)\frac{1}{1+1/4} = \boxed{\tfrac{2}{5}(2\cos x - \sin x).}$$

Problem 3.29

(a) It's trivial for $n = 1$. Assume it is true for $(n-1)$ (i.e. $[\hat{A}^{n-1}, \hat{B}] = (n-1)\hat{A}^{n-2}\hat{C}$), and prove it then holds for n:

$$[\hat{A}^n, \hat{B}] = [\hat{A}(\hat{A}^{n-1}), \hat{B}] = \hat{A}[\hat{A}^{n-1}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}^{n-1} = \hat{A}(n-1)\hat{A}^{n-2}\hat{C} + \hat{C}\hat{A}^{n-1} = n\hat{A}^{n-1}\hat{C}.$$

(b)

$$\left[e^{\lambda\hat{A}}, \hat{B}\right] = \left[\sum_{n=0}^{\infty}\frac{1}{n!}\lambda^n\hat{A}^n, \hat{B}\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\lambda^n\left[\hat{A}^n, \hat{B}\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\lambda^n n\hat{A}^{n-1}\hat{C}$$
$$= \lambda\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\lambda^{n-1}\hat{A}^{n-1}\hat{C} = \lambda\sum_{m=0}^{\infty}\frac{1}{m!}\lambda^m\hat{A}^m\hat{C} = \lambda e^{\lambda\hat{A}}\hat{C}. \quad \text{QED}$$

(c) Note first that $\frac{d}{d\lambda}\left(e^{\lambda\hat{Q}}\right) = \frac{d}{d\lambda}\left(1 + \lambda\hat{Q} + \frac{1}{2}\lambda^2\hat{Q}^2 + \cdots\right) = \hat{Q} + \lambda\hat{Q}^2 + \frac{1}{2}\lambda^2\hat{Q}^3 + \cdots = \hat{Q}e^{\lambda\hat{Q}}$, so

$$\frac{d\hat{f}}{d\lambda} = (\hat{A} + \hat{B})e^{\lambda(\hat{A}+\hat{B})} = (\hat{A} + \hat{B})\hat{f}.$$

$$\frac{d\hat{g}}{d\lambda} = \hat{A}e^{\lambda\hat{A}}e^{\lambda\hat{B}}e^{-\lambda^2\hat{C}/2} + e^{\lambda\hat{A}}\hat{B}e^{\lambda\hat{B}}e^{-\lambda^2\hat{C}/2} + e^{\lambda\hat{A}}e^{\lambda\hat{B}}(-\lambda\hat{C})e^{-\lambda^2\hat{C}/2}.$$

In the second term on the right, we can move $\hat{B}$ to the left, using (b): $e^{\lambda\hat{A}}\hat{B} = \hat{B}e^{\lambda\hat{A}} + \lambda e^{\lambda\hat{A}}\hat{C}$. (Of course, $\hat{C}$ moves freely through the other terms, because it commutes with $\hat{A}$ and $\hat{B}$). Thus

$$\frac{d\hat{g}}{d\lambda} = (\hat{A} + \hat{B} + \lambda\hat{C} - \lambda\hat{C})e^{\lambda\hat{A}}e^{\lambda\hat{B}}e^{-\lambda^2\hat{C}/2} = (\hat{A} + \hat{B})\hat{g}.$$

Since $\hat{f}(\lambda)$ and $\hat{g}(\lambda)$ are equal for all λ, they are equal in particular for $\lambda = 1$:

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\hat{C}/2}.$$

This generalizes the old rule for *numbers* (as opposed to *operators*): $e^{x+y} = e^x e^y$.

Problem 3.30

Let $|n\rangle$ be the nth eigenstate of the Hamiltonian.

$$c_n(t) = \langle n|\mathcal{S}(t)\rangle = \langle n|\left(\int dx\,|x\rangle\langle x|\right)|\mathcal{S}(t)\rangle = \int dx\,\langle n|x\rangle\,\langle x|\mathcal{S}(t)\rangle.$$

But $\langle x|\mathcal{S}(t)\rangle = \Psi(x,t)$, and $\langle x|n\rangle$ is the nth energy eigenstate in position space, $\psi_n(x)$. So

$$\boxed{c_n(t) = \int \psi_n(x)^*\,\Psi(x,t)\,dx.}$$

Note that $c_n(t)$ here *includes* the wiggle factor, $e^{-iE_nt/\hbar}$.

Problem 3.31

$$|e_1\rangle = 1;\ \langle e_1|e_1\rangle = \int_{-1}^{1} 1\,dx = 2. \quad \text{So } \boxed{|e_1'\rangle = \frac{1}{\sqrt{2}}.}$$

$$|e_2\rangle = x;\ \langle e_1'|e_2\rangle = \frac{1}{\sqrt{2}}\int_{-1}^{1} x\,dx = 0;\ \langle e_2|e_2\rangle = \int_{-1}^{1} x^2 dx = \left.\frac{x^3}{3}\right|_{-1}^{1} = \frac{2}{3}. \quad \text{So } \boxed{|e_2'\rangle = \sqrt{\frac{3}{2}}\,x.}$$

$$|e_3\rangle = x^2;\ \langle e_1'|e_3\rangle = \frac{1}{\sqrt{2}}\int_{-1}^{1} x^2 dx = \frac{1}{\sqrt{2}}\frac{2}{3};\ \langle e_2'|e_3\rangle = \sqrt{\frac{2}{3}}\int_{-1}^{1} x^3 dx = 0.$$

So (Problem A.4): $\quad |e_3''\rangle = |e_3\rangle - \frac{1}{\sqrt{2}}\frac{2}{3}|e_1'\rangle = x^2 - \frac{1}{3}.$

$$\langle e_3''|e_3''\rangle = \int_{-1}^{1}\left(x^2 - \frac{1}{3}\right)^2 dx = \left.\left(\frac{x^5}{5} - \frac{2}{3}\cdot\frac{x^3}{3} + \frac{x}{9}\right)\right|_{-1}^{1} = \frac{2}{5} - \frac{4}{9} + \frac{2}{9} = \frac{8}{45}. \quad \text{So}$$

$$|e_3'\rangle = \sqrt{\frac{45}{8}}\left(x^2 - \frac{1}{3}\right) = \boxed{\sqrt{\frac{5}{2}}\left(\frac{3}{2}x^2 - \frac{1}{2}\right).}$$

$$|e_4\rangle = x^3. \quad \langle e_1'|e_4\rangle = \frac{1}{\sqrt{2}}\int_{-1}^{1} x^3 dx = 0; \quad \langle e_2'|e_4\rangle = \sqrt{\frac{3}{2}}\int_{-1}^{1} x^4 dx = \sqrt{\frac{3}{2}}\cdot\frac{2}{5};$$

$$\langle e_3'|e_4\rangle = \sqrt{\frac{5}{2}}\int_{-1}^{1}\left(\frac{3}{2}x^5 - \frac{1}{2}x^3\right)dx = 0. \quad |e_4''\rangle = |e_4\rangle - \langle e_2'|e_4\rangle|e_2'\rangle = x^3 - \sqrt{\frac{3}{2}}\frac{2}{5}\sqrt{\frac{3}{2}}\,x = x^3 - \frac{3}{5}x.$$

$$\langle e_4''|e_4''\rangle = \int_{-1}^{1}\left(x^3 - \frac{3}{5}x\right)^2 dx = \left[\frac{x^7}{7} - \frac{2\cdot 3}{5}\frac{x^5}{5} + \frac{9}{25}\frac{x^3}{3}\right]\Bigg|_{-1}^{1} = \frac{2}{7} - \frac{12}{25} + \frac{18}{75} = \frac{8}{7\cdot 25}.$$

$$|e_4'\rangle = \frac{5}{2}\sqrt{\frac{7}{2}}\left(x^3 - \frac{3}{5}x\right) = \boxed{\sqrt{\frac{7}{2}}\left(\frac{5}{2}x^3 - \frac{3}{2}x\right).}$$

Problem 3.32

(a) $\langle Q\rangle = \langle\psi|\hat{Q}\psi\rangle = \langle\hat{Q}^\dagger\psi|\psi\rangle = -\langle\hat{Q}\psi|\psi\rangle = -(\langle\psi|\hat{Q}\psi\rangle)^* = -\langle Q\rangle^*$, so $\langle Q\rangle$ is imaginary. ✓

(b) $\hat{Q}|\psi\rangle = \lambda|\psi\rangle \Rightarrow \langle\psi|\hat{Q}\psi\rangle = \lambda\langle\psi|\psi\rangle = -\langle\hat{Q}\psi|\psi\rangle = -\lambda^*\langle\psi|\psi\rangle$. Therefore $\lambda^* = -\lambda$, and hence λ is imaginary.

(c) If $\hat{Q}|\psi\rangle = \lambda|\psi\rangle$ and $\hat{Q}|\phi\rangle = \mu|\phi\rangle$, then $\langle\phi|\hat{Q}\psi\rangle = \lambda\langle\phi|\psi\rangle = -\langle\hat{Q}\phi|\psi\rangle = -\mu^*\langle\phi|\psi\rangle = \mu\langle\phi|\psi\rangle$. Therefore $(\lambda-\mu)\langle\phi|\psi\rangle = 0$, and if $\lambda \neq \mu$ the eigenvectors must be orthogonal.

(d) From Problem 3.5(b) we know that $(\hat{P}\hat{Q})^\dagger = \hat{Q}^\dagger\hat{P}^\dagger$, so if $\hat{P} = \hat{P}^\dagger$ and $\hat{Q} = \hat{Q}^\dagger$ then

$$[\hat{P},\hat{Q}]^\dagger = (\hat{P}\hat{Q} - \hat{Q}\hat{P})^\dagger = \hat{Q}^\dagger\hat{P}^\dagger - \hat{P}^\dagger\hat{Q}^\dagger = \hat{Q}\hat{P} - \hat{P}\hat{Q} = -[\hat{P},\hat{Q}]. \quad ✓$$

If $\hat{P} = -\hat{P}^\dagger$ and $\hat{Q} = -\hat{Q}^\dagger$, then $[\hat{P},\hat{Q}]^\dagger = \hat{Q}^\dagger\hat{P}^\dagger - \hat{P}^\dagger\hat{Q}^\dagger = (-\hat{Q})(-\hat{P}) - (-\hat{P})(-\hat{Q}) = -[\hat{P},\hat{Q}]$.

So in either case the commutator is antihermitian.

(e) Let $\hat{A} \equiv \frac{1}{2}(\hat{Q}+\hat{Q}^\dagger)$ and $\hat{B} \equiv \frac{1}{2}(\hat{Q}-\hat{Q}^\dagger)$. Clearly $\hat{Q} = \hat{A}+\hat{B}$. But $\hat{A}^\dagger = \frac{1}{2}(\hat{Q}^\dagger+\hat{Q}) = \hat{A}$, so $\hat{A}$ is hermitian, while $\hat{B}^\dagger = \frac{1}{2}(\hat{Q}^\dagger - \hat{Q}) = -\hat{B}$, so $\hat{B}$ is antihermitian

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Problem 3.33

(a) $\boxed{\psi_1.}$

(b) $\boxed{b_1 \text{ (with probability } 9/25) \text{ or } b_2 \text{ (with probability } 16/25).}$

(c) Right after the measurement of B:

- With probability 9/25 the particle is in state $\phi_1 = (3\psi_1 + 4\psi_2)/5$; in that case the probability of getting a_1 is 9/25.
- With probability 16/25 the particle is in state $\phi_2 = (4\psi_1 - 3\psi_2)/5$; in that case the probability of getting a_1 is 16/25.

So the total probability of getting a_1 is $\frac{9}{25}\cdot\frac{9}{25}+\frac{16}{25}\cdot\frac{16}{25}=\boxed{\frac{337}{625}=0.5392.}$

[*Note:* The measurment of B (even if we don't know the *outcome* of that measurement) collapses the wave function, and thereby alters the probabilities for the second measurment of A. If the graduate student inadvertantly neglected to measure B, the second measurement of A would be *certain* to reproduce the result a_1.]

Problem 3.34

(a) $\Psi_n(x,t)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)e^{-iE_nt/\hbar}$, with $E_n=\frac{n^2\pi^2\hbar^2}{2ma^2}$.

$$\begin{aligned}
\Phi_n(p,t) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{-ipx/\hbar}\Psi_n(x,t)\,dx = \frac{1}{\sqrt{2\pi\hbar}}\sqrt{\frac{2}{a}}e^{-iE_nt/\hbar}\int_0^a e^{-ipx/\hbar}\sin\left(\frac{n\pi}{a}x\right)dx\\
&= \frac{1}{\sqrt{\pi\hbar a}}e^{-iE_nt/\hbar}\frac{1}{2i}\int_0^a\left[e^{i(n\pi/a-p/\hbar)x}-e^{i(-n\pi/a-p/\hbar)x}\right]dx\\
&= \frac{1}{\sqrt{\pi\hbar a}}e^{-iE_nt/\hbar}\frac{1}{2i}\left[\frac{e^{i(n\pi/a-p/\hbar)x}}{i(n\pi/a-p/\hbar)}-\frac{e^{i(-n\pi/a-p/\hbar)x}}{i(-n\pi/a-p/\hbar)}\right]\Bigg|_0^a\\
&= \frac{-1}{2\sqrt{\pi\hbar a}}e^{-iE_nt/\hbar}\left[\frac{e^{i(n\pi-pa/\hbar)}-1}{(n\pi/a-p/\hbar)}+\frac{e^{-i(n\pi+pa/\hbar)}-1}{(n\pi/a+p/\hbar)}\right]\\
&= \frac{-1}{2\sqrt{\pi\hbar a}}e^{-iE_nt/\hbar}\left[\frac{(-1)^ne^{-ipa/\hbar}-1}{(n\pi-ap/\hbar)}a+\frac{(-1)^ne^{-ipa/\hbar}-1}{(n\pi+ap/\hbar)}a\right]\\
&= -\frac{1}{2}\sqrt{\frac{a}{\pi\hbar}}e^{-iE_nt/\hbar}\frac{2n\pi}{(n\pi)^2-(ap/\hbar)^2}\left[(-1)^ne^{-ipa/\hbar}-1\right]\\
&= \boxed{\sqrt{\frac{a\pi}{\hbar}}\frac{ne^{-iE_nt/\hbar}}{(n\pi)^2-(ap/\hbar)^2}\left[1-(-1)^ne^{-ipa/\hbar}\right].}
\end{aligned}$$

(b) Noting that

$$1-(-1)^ne^{-ipa/\hbar}=e^{-ipa/2\hbar}\left[e^{ipa/2\hbar}-(-1)^ne^{-ipa/2\hbar}\right]=2e^{-ipa/2\hbar}\begin{cases}\cos(pa/2\hbar) & (n \text{ odd}),\\ i\sin(pa/2\hbar) & (n \text{ even}),\end{cases}$$

we have

$$\boxed{|\Phi_n(p,t)|^2=\frac{4\pi a}{\hbar}\frac{n^2}{[(n\pi)^2-(ap/\hbar)^2]^2}\times\begin{cases}\cos^2(ap/2\hbar) & n \text{ odd},\\ \sin^2(ap/2\hbar) & n \text{ even}.\end{cases}}$$

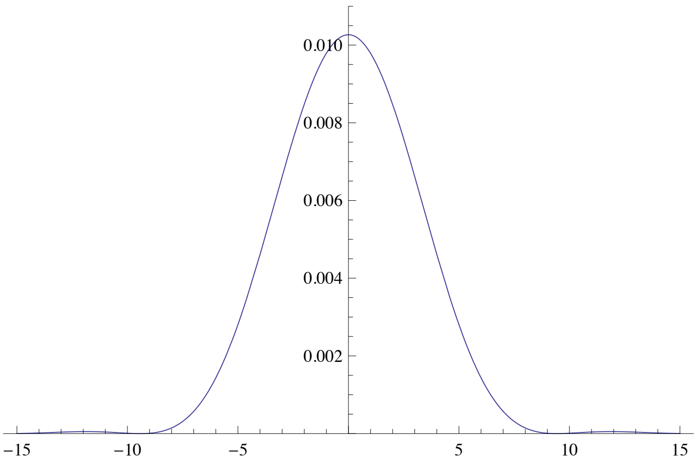
From the formula it looks as though the maxima should occur at $p=\pm(n\pi\hbar/a)$ (though since the numerator also vanishes there, the function itself is perfectly finite). Physically I would expect the most probable values of p to be given by $E_n=(n^2\pi^2\hbar^2)/(2ma^2)=p^2/2m$, or (again) $p=\pm(n\pi\hbar/a)$. For the graphs I used $a=1$ and $\hbar=1$, so the maxima should be at $n\pi=(3.1, 6.3, 15.7, 30.1)$; actually (by eyeball) they are at (0, 5, 15, 30). As n increases they get closer to the "expected" value, but the interesting thing is that there is a range of possible momenta, not just two discrete values, as one might naively have guessed (but in Problem 3.10 we already noted that the stationary states are not eigenstates of $\hat{p}$).

```
f[x_] := n^2 / ((n π)^2 - x^2)^2 (Cos[x / 2])^2

g[x_] := n^2 / ((n π)^2 - x^2)^2 (Sin[x / 2])^2

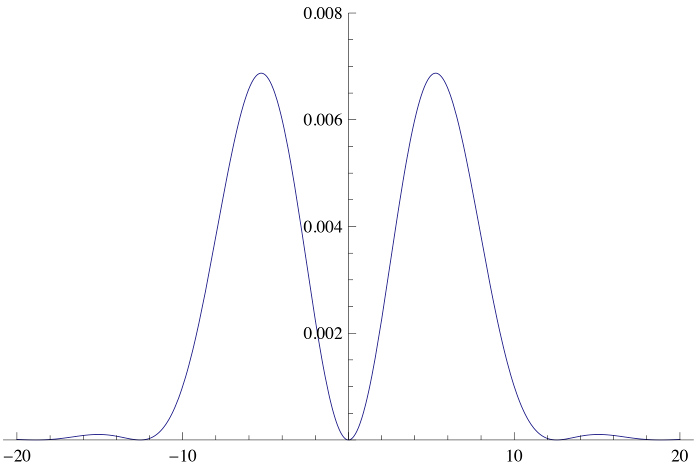
n = 1

Plot[f[x], {x, -15, 15}, PlotRange → {0, 0.011}]
```



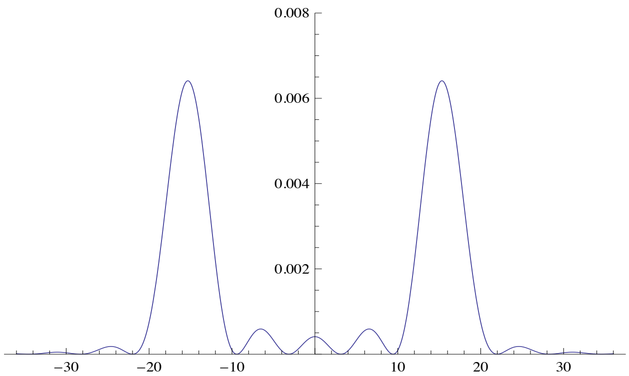

```
n = 2

Plot[g[x], {x, -20, 20}, PlotRange → {0, 0.008}]
```

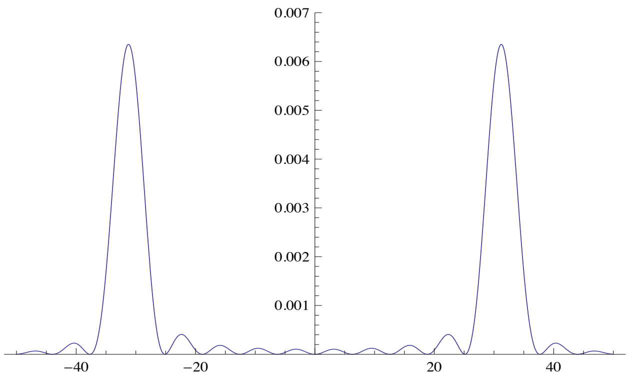



```
n = 5
```

```
Plot[f[x], {x, -36, 36}, PlotRange → {0, 0.008}]
```



```
n = 10
Plot[g[x], {x, -50, 50}, PlotRange → {0, 0.007}]
```



(c)

$$\langle p^2\rangle = \int_{-\infty}^{\infty} p^2|\Phi_n(p,t)|^2\,dp = \frac{4n^2\pi a}{\hbar}\int_{-\infty}^{\infty}\frac{p^2}{[(n\pi)^2-(ap/\hbar)^2]^2}\left\{\begin{matrix}\cos^2(pa/2\hbar)\\ \sin^2(pa/2\hbar)\end{matrix}\right\}dp \quad [\text{let } x\equiv \frac{ap}{n\pi\hbar}]$$

$$= \frac{4n\hbar^2}{a^2}\int_{-\infty}^{\infty}\frac{x^2}{(1-x^2)^2}T_n(x)\,dx = \frac{4n\hbar^2}{a^2}I_n,$$

where

$$T_n(x)\equiv\left\{\begin{matrix}\cos^2(n\pi x/2), & \text{if } n \text{ is odd,}\\ \sin^2(n\pi x/2), & \text{if } n \text{ is even.}\end{matrix}\right\}$$

The integral can be evaluated by partial fractions:

$$\frac{x^2}{(x^2-1)^2} = \frac{1}{4}\left[\frac{1}{(x-1)^2}+\frac{1}{(x+1)^2}+\frac{1}{(x-1)}-\frac{1}{(x+1)}\right] \Rightarrow$$

$$I_n = \frac{1}{4}\left[\int_{-\infty}^{\infty}\frac{1}{(x-1)^2}T_n(x)\,dx+\int_{-\infty}^{\infty}\frac{1}{(x+1)^2}T_n(x)\,dx+\int_{-\infty}^{\infty}\frac{1}{(x-1)}T_n(x)\,dx-\int_{-\infty}^{\infty}\frac{1}{(x+1)}T_n(x)\,dx\right].$$

For odd n:

$$\int_{-\infty}^{\infty}\frac{1}{(x\pm1)^k}\cos^2\left(\frac{n\pi x}{2}\right)dx = \int_{-\infty}^{\infty}\frac{1}{y^k}\cos^2\left[\frac{n\pi}{2}(y\mp1)\right]dy = \int_{-\infty}^{\infty}\frac{1}{y^k}\sin^2\left(\frac{n\pi y}{2}\right)dy.$$

For even n:

$$\int_{-\infty}^{\infty} \frac{1}{(x\pm 1)^k} \sin^2\left(\frac{n\pi x}{2}\right) dx = \int_{-\infty}^{\infty} \frac{1}{y^k} \sin^2\left[\frac{n\pi}{2}(y\mp 1)\right] dy = \int_{-\infty}^{\infty} \frac{1}{y^k} \sin^2\left(\frac{n\pi y}{2}\right) dy.$$

In either case, then,

$$I_n = \frac{1}{2}\int_{-\infty}^{\infty} \frac{1}{y^2} \sin^2\left(\frac{n\pi y}{2}\right) dy = \frac{n\pi}{4}\int_{-\infty}^{\infty} \frac{sin^2 u}{u^2} du = \frac{n\pi^2}{4}.$$

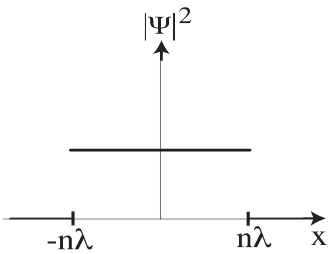
Therefore

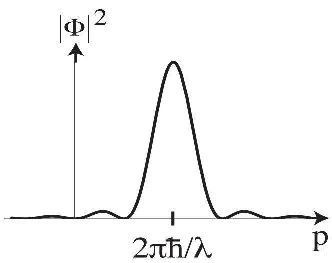
$$\langle p^2\rangle = \frac{4n\hbar^2}{a^2} I_n = \frac{4n\hbar^2}{a^2}\frac{n\pi^2}{4} = \left(\frac{n\pi\hbar}{a}\right)^2 \quad \text{(same as Problem 2.4).}$$

Problem 3.35

$$\begin{aligned}
\Phi(p,0) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x,0)\,dx = \frac{1}{2\sqrt{n\pi\hbar\lambda}}\int_{-n\lambda}^{n\lambda} e^{i(2\pi/\lambda - p/\hbar)x} dx \\
&= \frac{1}{2\sqrt{n\pi\hbar\lambda}} \frac{e^{i(2\pi/\lambda-p/\hbar)x}}{i(2\pi/\lambda - p/\hbar)}\bigg|_{-n\lambda}^{n\lambda} = \frac{1}{2\sqrt{n\pi\hbar\lambda}} \frac{e^{i2\pi n}e^{-ipn\lambda/\hbar)} - e^{-i2\pi n}e^{ipn\lambda/\hbar)}}{i(2\pi/\lambda - p/\hbar)} \\
&= \boxed{\sqrt{\frac{\hbar\lambda}{n\pi}}\frac{\sin(np\lambda/\hbar)}{(p\lambda - 2\pi\hbar)}.}
\end{aligned}$$

$$|\Psi(x,0)|^2 = \frac{1}{2n\lambda} \quad (-n\lambda < x < n\lambda); \quad |\Phi(p,0)|^2 = \frac{\lambda\hbar}{n\pi}\frac{\sin^2(np\lambda/\hbar)}{(p\lambda-2\pi\hbar)^2}.$$





The width of the $|\Psi|^2$ graph is $\boxed{w_x = 2n\lambda.}$ The $|\Phi|^2$ graph is a maximum at $2\pi\hbar/\lambda$, and goes to zero on either side at $\frac{2\pi\hbar}{\lambda}\left(1 \pm \frac{1}{2n}\right)$, so $\boxed{w_p = \frac{2\pi\hbar}{n\lambda}.}$ As $n\to\infty$, $w_x \to \infty$ and $w_p \to 0$; in this limit the particle has a well-defined momentum, but a completely indeterminate position. In general,

$$w_x w_p = (2n\lambda)\frac{2\pi\hbar}{n\lambda} = 4\pi\hbar > \hbar/2,$$

so the uncertainty principle is satisfied (using the widths as a measure of uncertainty). If we try to check the uncertainty principle more rigorously, using standard deviation as the measure, we get an uninformative result, because

$$\langle p^2\rangle = \frac{\lambda\hbar}{n\pi}\int_{-\infty}^{\infty} p^2 \frac{\sin^2(np\lambda/\hbar)}{(p\lambda-2\pi\hbar)^2} dp = \infty.$$

(At large $|p|$ the integrand is approximately $(1/\lambda^2)\sin^2(np\lambda/\hbar)$, so the integral blows up.) Meanwhile $\langle p\rangle$ is finite $(2\pi\hbar/\lambda)$, so $\sigma_p = \infty$, and the uncertainty principle tells us nothing. The source of the problem is the discontinuity in Ψ at the end points; here $\hat{p}\,\Psi = -i\hbar\, d\Psi/dx$ picks up a delta function, and $\langle\Psi|\hat{p}^2\Psi\rangle = \langle\hat{p}\,\Psi|\hat{p}\,\Psi\rangle \to \infty$ because the integral of the *square* of the delta function blows up. In general, if you want σ_p to be finite, you cannot allow discontinuities in Ψ.

Problem 3.36

(a)

$$1 = |A|^2 \int_{-\infty}^{\infty} \frac{1}{(x^2+a^2)^2}\,dx = 2|A|^2 \int_0^{\infty} \frac{1}{(x^2+a^2)^2}\,dx = 2|A|^2 \frac{1}{2a^2}\left[\frac{x}{x^2+a^2} + \frac{1}{a}\tan^{-1}\left(\frac{x}{a}\right)\right]\Bigg|_0^{\infty}$$
$$= \frac{1}{a^2}|A|^2\frac{1}{a}\tan^{-1}(\infty) = \frac{\pi}{2a^3}|A|^2 \quad \Rightarrow \quad \boxed{A = a\sqrt{\frac{2a}{\pi}}.}$$

(b)

$$\langle x\rangle = A^2 \int_{-\infty}^{\infty} \frac{x}{(a^2+x^2)^2}\,dx = \boxed{0.}$$
$$\langle x^2\rangle = 2A^2 \int_0^{\infty} \frac{x^2}{(a^2+x^2)^2}\,dx. \quad \left[\text{Let } y \equiv \frac{x^2}{a^2},\ x = a\sqrt{y},\ dx = \frac{a}{2\sqrt{y}}\,dy.\right]$$
$$= \frac{2a^2}{\pi}\int_0^{\infty}\frac{y^{1/2}}{(1+y)^2}\,dy = \frac{2a^2}{\pi}\frac{\Gamma(3/2)\Gamma(1/2)}{\Gamma(2)} = \frac{2a^2}{\pi}\frac{(\sqrt{\pi}/2)(\sqrt{\pi})}{1} = \boxed{a^2.}$$
$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \boxed{a.}$$

(c)

$$\Phi(p,0) = \frac{A}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\frac{1}{x^2+a^2}\,dx. \quad \left[\text{But } e^{-ipx/\hbar} = \cos\left(\frac{px}{\hbar}\right) - i\sin\left(\frac{px}{\hbar}\right), \text{ and sine is odd.}\right]$$
$$= \frac{2A}{\sqrt{2\pi\hbar}}\int_0^{\infty}\frac{\cos(px/\hbar)}{x^2+a^2}\,dx = \frac{2A}{\sqrt{2\pi\hbar}}\left(\frac{\pi}{2a}e^{-|p|a/\hbar}\right) = \boxed{\sqrt{\frac{a}{\hbar}}\,e^{-|p|a/\hbar}.}$$

$$\int_{-\infty}^{\infty}|\Phi(p,0)|^2\,dp = \frac{a}{\hbar}\int_{-\infty}^{\infty} e^{-2|p|a/\hbar}\,dp = \frac{2a}{\hbar}\left(\frac{e^{-2pa/\hbar}}{-2a/\hbar}\right)\Bigg|_0^{\infty} = 1. \quad \checkmark$$

(d)

$$\langle p\rangle = \frac{a}{\hbar}\int_{-\infty}^{\infty} pe^{-2|p|a/\hbar}\,dp = \boxed{0.}$$
$$\langle p^2\rangle = 2\frac{a}{\hbar}\int_0^{\infty} p^2e^{-2pa/\hbar}\,dp = \frac{2a}{\hbar}2\left(\frac{\hbar}{2a}\right)^3 = \boxed{\frac{\hbar^2}{2a^2}.} \quad \sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \boxed{\frac{\hbar}{\sqrt{2}\,a}.}$$

(e) $$\sigma_x\sigma_p = a\frac{\hbar}{\sqrt{2}\,a} = \sqrt{2}\frac{\hbar}{2} > \frac{\hbar}{2}. \quad \checkmark$$

Problem 3.37

Equation 3.73 $\Rightarrow \dfrac{d}{dt}\langle xp\rangle = \dfrac{i}{\hbar}\langle [H,xp]\rangle$; Eq. 3.65 $\Rightarrow [H,xp]=[H,x]p+x[H,p]$; Problem 3.15 $\Rightarrow [H,x] = -\dfrac{i\hbar p}{m}$; Problem 3.18(d) $\Rightarrow [H,p]=i\hbar\dfrac{\partial V}{\partial x}$. So

$$\frac{d}{dt}\langle xp\rangle = \frac{i}{\hbar}\left[-\frac{i\hbar}{m}\langle p^2\rangle + i\hbar\langle x\frac{\partial V}{\partial x}\rangle\right] = 2\langle\frac{p^2}{2m}\rangle - \langle x\frac{\partial V}{\partial x}\rangle = 2\langle T\rangle - \langle x\frac{\partial V}{\partial x}\rangle. \quad \text{QED}$$

In a stationary state all expectation values (at least, for operators that do not depend explicitly on t) are time-independent (see item 1 on p. 26), so $d\langle xp\rangle/dt = 0$, and we are left with Eq. 3.113.

For the harmonic oscillator:

$$V=\frac{1}{2}m\omega^2x^2 \Rightarrow \frac{dV}{dx}=m\omega^2x \Rightarrow x\frac{dV}{dx}=m\omega^2x^2=2V \Rightarrow 2\langle T\rangle = 2\langle V\rangle \Rightarrow \langle T\rangle=\langle V\rangle. \quad \text{QED}$$

In Problem 2.11(c) we found that $\langle T\rangle=\langle V\rangle=\frac{1}{4}\hbar\omega$ (for $n=0$); $\langle T\rangle=\langle V\rangle=\frac{3}{4}\hbar\omega$ (for $n=1$). ✓
In Problem 2.12 we found that $\langle T\rangle=\frac{1}{2}\left(n+\frac{1}{2}\right)\hbar\omega$, while $\langle x^2\rangle=(n+\frac{1}{2})\hbar/m\omega$, so $\langle V\rangle=\frac{1}{2}m\omega^2\langle x^2\rangle=\frac{1}{2}(n+\frac{1}{2})\hbar\omega$, and hence $\langle T\rangle=\langle V\rangle$ for *all* stationary states. ✓

Problem 3.38

$$\Psi(x,t)=\frac{1}{\sqrt{2}}\left(\psi_1e^{-iE_1t/\hbar}+\psi_2e^{-iE_2t/\hbar}\right); \qquad \langle\Psi(x,t)|\Psi(x,0)\rangle=0\Rightarrow$$

$$\frac{1}{2}\left(e^{iE_1t/\hbar}\langle\psi_1|\psi_1\rangle+e^{iE_1t/\hbar}\langle\psi_1|\psi_2\rangle+e^{iE_2t/\hbar}\langle\psi_2|\psi_1\rangle+e^{iE_2t/\hbar}\langle\psi_2|\psi_2\rangle\right)$$

$$=\frac{1}{2}\left(e^{iE_1t/\hbar}+e^{iE_2t/\hbar}\right)=0,\ \text{or}\ e^{iE_2t/\hbar}=-e^{iE_1t/\hbar},\ \text{so}\ e^{i(E_2-E_1)t/\hbar}=-1=e^{i\pi}.$$

Thus $(E_2-E_1)t/\hbar=\pi$ (orthogonality also at $3\pi,\ 5\pi$, etc., but this is the *first* occurrence).

$$\therefore \Delta t\equiv\frac{t}{\pi}=\frac{\hbar}{E_2-E_1}. \quad \text{But}\ \Delta E=\sigma_H=\frac{1}{2}(E_2-E_1)\ \text{(Problem 3.20).} \quad \text{So}\ \Delta t\,\Delta E=\frac{\hbar}{2}. \quad ✓$$

Problem 3.39

Equation 2.70: $x=\sqrt{\dfrac{\hbar}{2m\omega}}(a_++a_-)$, $p=i\sqrt{\dfrac{\hbar m\omega}{2}}(a_+-a_-)$; Eq. 2.67 : $\begin{cases} a_+|n\rangle = \sqrt{n+1}\,|n+1\rangle, \\ a_-|n\rangle = \sqrt{n}\,|n-1\rangle. \end{cases}$

$$\begin{aligned}\langle n|x|n'\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle n|(a_++a_-)|n'\rangle=\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n'+1}\,\langle n|n'+1\rangle+\sqrt{n'}\,\langle n|n'-1\rangle\right] \\ &= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n'+1}\,\delta_{n,n'+1}+\sqrt{n'}\,\delta_{n,n'-1}\right)=\boxed{\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\delta_{n',n-1}+\sqrt{n'}\,\delta_{n,n'-1}\right).} \\ \langle n|p|n'\rangle &= \boxed{i\sqrt{\frac{m\hbar\omega}{2}}\left(\sqrt{n}\,\delta_{n',n-1}-\sqrt{n'}\,\delta_{n,n'-1}\right).}\end{aligned}$$

Noting that n and n' run from zero to infinity, the matrices are:

$$\boxed{\mathsf{X} = \sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & 0 & \vdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \sqrt{5} & \\ & & & \cdots & & & \end{pmatrix}; \quad \mathsf{P} = i\sqrt{\frac{m\hbar\omega}{2}} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 & 0 & \vdots \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} & 0 & \\ 0 & 0 & 0 & \sqrt{4} & & -\sqrt{5} & \\ & & & \cdots & & & \end{pmatrix}.}$$

Squaring these matrices:

$$\mathsf{X}^2 = \frac{\hbar}{2m\omega} \begin{pmatrix} 1 & 0 & \sqrt{1\cdot 2} & 0 & 0 & 0 & \\ 0 & 3 & 0 & \sqrt{2\cdot 3} & 0 & 0 & \\ \sqrt{1\cdot 2} & 0 & 5 & 0 & \sqrt{3\cdot 4} & 0 & \vdots \\ 0 & \sqrt{2\cdot 3} & 0 & 7 & 0 & \sqrt{4\cdot 5} & \\ & & & \cdots & & & \end{pmatrix};$$

$$\mathsf{P}^2 = -\frac{m\hbar\omega}{2} \begin{pmatrix} -1 & 0 & \sqrt{1\cdot 2} & 0 & 0 & 0 & \\ 0 & -3 & 0 & \sqrt{2\cdot 3} & 0 & 0 & \\ \sqrt{1\cdot 2} & 0 & -5 & 0 & \sqrt{3\cdot 4} & 0 & \vdots \\ 0 & \sqrt{2\cdot 3} & 0 & -7 & 0 & \sqrt{4\cdot 5} & \\ & & & \cdots & & & \end{pmatrix}.$$

So the Hamiltonian, in matrix form, is

$$\begin{aligned} \mathsf{H} &= \frac{1}{2m}\mathsf{P}^2 + \frac{m\omega^2}{2}\mathsf{X}^2 \\ &= -\frac{\hbar\omega}{4} \begin{pmatrix} -1 & 0 & \sqrt{1\cdot 2} & 0 & 0 & 0 & \\ 0 & -3 & 0 & \sqrt{2\cdot 3} & 0 & 0 & \\ \sqrt{1\cdot 2} & 0 & -5 & 0 & \sqrt{3\cdot 4} & 0 & \vdots \\ 0 & \sqrt{2\cdot 3} & 0 & -7 & 0 & \sqrt{4\cdot 5} & \\ & & & \cdots & & & \end{pmatrix} \\ &+ \frac{\hbar\omega}{4} \begin{pmatrix} 1 & 0 & \sqrt{1\cdot 2} & 0 & 0 & 0 & \\ 0 & 3 & 0 & \sqrt{2\cdot 3} & 0 & 0 & \\ \sqrt{1\cdot 2} & 0 & 5 & 0 & \sqrt{3\cdot 4} & 0 & \vdots \\ 0 & \sqrt{2\cdot 3} & 0 & 7 & 0 & \sqrt{4\cdot 5} & \\ & & & \cdots & & & \end{pmatrix} = \boxed{\frac{\hbar\omega}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & \\ 0 & 3 & 0 & 0 & \\ 0 & 0 & 5 & 0 & \\ 0 & 0 & 0 & 7 & \\ & & & & \ddots \end{pmatrix}}. \end{aligned}$$

It's plainly diagonal, and the nonzero elements are $H_{nn} = \left(n + \frac{1}{2}\right)\hbar\omega$, as they should be.

Problem 3.40

Using Equation 3.114,

$$\langle x\rangle = \int\left(\sum_n c_n\psi_n e^{-iE_nt/\hbar}\right)^* x\left(\sum_{n'} c_{n'}\psi_{n'}e^{-iE_{n'}t/\hbar}\right)dx = \sum_n\sum_{n'} c_n^* c_{n'}e^{i(E_n-E_{n'})t/\hbar}\langle n|x|n'\rangle$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\sum_n\sum_{n'} c_n^* c_{n'}e^{i(E_n-E_{n'})t/\hbar}\left(\sqrt{n'}\,\delta_{n,n'-1}+\sqrt{n}\,\delta_{n',n-1}\right)$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\sum_n\left[\sqrt{n+1}\,c_n^*c_{n+1}e^{i(E_n-E_{n+1})t/\hbar}+\sqrt{n}\,c_n^*c_{n-1}e^{i(E_n-E_{n-1})t/\hbar}\right]$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\sum_{n=0}^{\infty}\sqrt{n+1}\,c_n^*c_{n+1}e^{-i\omega t}+\sum_{n=0}^{\infty}\sqrt{n}\,c_n^*c_{n-1}e^{i\omega t}\right].$$

In the last step I used

$$E_n-E_{n-1}=\left(n+\frac{1}{2}\right)\hbar\omega-\left(n-\frac{1}{2}\right)\hbar\omega=\hbar\omega,\quad E_n-E_{n+1}=\left(n+\frac{1}{2}\right)\hbar\omega-\left(n+\frac{3}{2}\right)\hbar\omega=-\hbar\omega.$$

Noting that $\sqrt{n}$ kills the $n=0$ term in the second sum, let $n\to n+1$ and run it from 0 to ∞:

$$\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\sum_{n=0}^{\infty}\sqrt{n+1}\left[c_n^*c_{n+1}e^{-i\omega t}+c_{n+1}^*c_ne^{i\omega t}\right]$$
$$= \left(\sqrt{\frac{\hbar}{2m\omega}}\sum_{n=0}^{\infty}\sqrt{n+1}\,c_n^*c_{n+1}\right)e^{-i\omega t}+\left(\sqrt{\frac{\hbar}{2m\omega}}\sum_{n=0}^{\infty}\sqrt{n+1}\,c_nc_{n+1}^*\right)e^{i\omega t}$$
$$= \frac{1}{2}\left(Ce^{i\phi}\right)e^{-i\omega t}+\frac{1}{2}\left(Ce^{-i\phi}\right)e^{i\omega t}=C\cos(\omega t-\phi).\quad\checkmark$$

In the case of Problem 2.40, $c_0=3/5, c_1=-2\sqrt{2}/5, c_2=2\sqrt{2}/5$ (and all the rest are zero) so

$$Ce^{-i\phi}=\sqrt{\frac{2\hbar}{m\omega}}\left(c_1^*c_0+\sqrt{2}\,c_2^*c_1\right)=\sqrt{\frac{2\hbar}{m\omega}}\left(\frac{(-2\sqrt{2})}{5}\frac{3}{5}+\sqrt{2}\,\frac{2\sqrt{2}}{5}\frac{(-2\sqrt{2})}{5}\right)=-\frac{28}{25}\sqrt{\frac{\hbar}{m\omega}}.$$

$$\boxed{C=\frac{28}{25}\sqrt{\frac{\hbar}{m\omega}},\quad \phi=\pi.}$$

Problem 3.41

Evidently $\Psi(x,t)=c_0\psi_0(x)e^{-iE_0t/\hbar}+c_1\psi_1(x)e^{-iE_1t/\hbar}$, with $|c_0|^2=|c_1|^2=1/2$, so $c_0=e^{i\theta_0}/\sqrt{2},\ c_1=e^{i\theta_1}/\sqrt{2}$, for some real θ_0,θ_1.

$$\langle p\rangle=|c_0|^2\langle\psi_0|p\psi_0\rangle+|c_1|^2\langle\psi_1|p\psi_1\rangle+c_0^*c_1e^{i(E_0-E_1)t/\hbar}\langle\psi_0|p\psi_1\rangle+c_1^*c_0e^{i(E_1-E_0)t/\hbar}\langle\psi_1|p\psi_0\rangle.$$

But $E_1-E_0=(\frac{3}{2}\hbar\omega)-(\frac{1}{2}\hbar\omega)=\hbar\omega$, and (Problem 2.11) $\langle\psi_0|p\psi_0\rangle=\langle\psi_1|p\psi_1\rangle=0$, while (Eqs. 2.70 and 2.67)

$$\langle\psi_0|p\psi_1\rangle=i\sqrt{\frac{\hbar m\omega}{2}}\langle\psi_0|(a_+-a_-)\psi_1\rangle=i\sqrt{\frac{\hbar m\omega}{2}}\left[\langle\psi_0|\sqrt{2}\psi_2\rangle-\langle\psi_0|\sqrt{1}\psi_0\rangle\right]=-i\sqrt{\frac{\hbar m\omega}{2}};\langle\psi_1|p\psi_0\rangle=i\sqrt{\frac{\hbar m\omega}{2}}.$$

$$\begin{aligned}\langle p\rangle &= \frac{1}{\sqrt{2}}e^{-i\theta_0}\frac{1}{\sqrt{2}}e^{i\theta_1}e^{-i\omega t}\left(-i\sqrt{\frac{\hbar m\omega}{2}}\right)+\frac{1}{\sqrt{2}}e^{-i\theta_1}\frac{1}{\sqrt{2}}e^{i\theta_0}e^{i\omega t}\left(i\sqrt{\frac{\hbar m\omega}{2}}\right)\\ &= \frac{i}{2}\sqrt{\frac{\hbar m\omega}{2}}\left[-e^{-i(\omega t-\theta_1+\theta_0)}+e^{i(\omega t-\theta_1+\theta_0)}\right]=-\sqrt{\frac{\hbar m\omega}{2}}\sin(\omega t+\theta_0-\theta_1).\end{aligned}$$

The maximum is $\boxed{\sqrt{\hbar m\omega/2};}$ it occurs at $t=0\Leftrightarrow\sin(\theta_0-\theta_1)=-1$, or $\theta_1=\theta_0+\pi/2$. We might as well pick $\theta_0=0,\ \theta_1=\pi/2$; then

$$\Psi(x,t)=\frac{1}{\sqrt{2}}\left[\psi_0e^{-i\omega t/2}+\psi_1e^{i\pi/2}e^{-3i\omega t/2}\right]=\boxed{\frac{1}{\sqrt{2}}e^{-i\omega t/2}\left(\psi_0+i\psi_1e^{-i\omega t}\right).}$$

Problem 3.42

(a) $\langle x\rangle=\langle\alpha|x\alpha\rangle=\sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|(a_++a_-)\alpha\rangle=\sqrt{\frac{\hbar}{2m\omega}}\left(\langle a_-\alpha|\alpha\rangle+\langle\alpha|a_-\alpha\rangle\right)=\boxed{\sqrt{\frac{\hbar}{2m\omega}}(\alpha+\alpha^*).}$

$$\begin{aligned}x^2 &= \frac{\hbar}{2m\omega}\left(a_+^2+a_+a_-+a_-a_++a_-^2\right).\quad\text{But } a_-a_+=[a_-,a_+]+a_+a_-=1+a_+a_-\quad\text{(Eq. 2.55).}\\ &= \frac{\hbar}{2m\omega}\left(a_+^2+2a_+a_-+1+a_-^2\right).\end{aligned}$$

$$\begin{aligned}\langle x^2\rangle &= \frac{\hbar}{2m\omega}\langle\alpha|\left(a_+^2+2a_+a_-+1+a_-^2\right)\alpha\rangle=\frac{\hbar}{2m\omega}\left(\langle a_-^2\alpha|\alpha\rangle+2\langle a_-\alpha|a_-\alpha\rangle+\langle\alpha|\alpha\rangle+\langle\alpha|a_-^2\alpha\rangle\right)\\ &= \frac{\hbar}{2m\omega}\left[(\alpha^*)^2+2(\alpha^*)\alpha+1+\alpha^2\right]=\boxed{\frac{\hbar}{2m\omega}\left[1+(\alpha+\alpha^*)^2\right].}\end{aligned}$$

$$\langle p\rangle=\langle\alpha|p\alpha\rangle=i\sqrt{\frac{\hbar m\omega}{2}}\langle\alpha|(a_+-a_-)\alpha\rangle=i\sqrt{\frac{\hbar m\omega}{2}}\left(\langle a_-\alpha|\alpha\rangle-\langle\alpha|a_-\alpha\rangle\right)=\boxed{-i\sqrt{\frac{\hbar m\omega}{2}}(\alpha-\alpha^*).}$$

$$p^2=-\frac{\hbar m\omega}{2}\left(a_+^2-a_+a_--a_-a_++a_-^2\right)=-\frac{\hbar m\omega}{2}\left(a_+^2-2a_+a_--1+a_-^2\right).$$

$$\begin{aligned}\langle p^2\rangle &= -\frac{\hbar m\omega}{2}\langle\alpha|\left(a_+^2-2a_+a_--1+a_-^2\right)\alpha\rangle=-\frac{\hbar m\omega}{2}\left(\langle a_-^2\alpha|\alpha\rangle-2\langle a_-\alpha|a_-\alpha\rangle-\langle\alpha|\alpha\rangle+\langle\alpha|a_-^2\alpha\rangle\right)\\ &= -\frac{\hbar m\omega}{2}\left[(\alpha^*)^2-2(\alpha^*)\alpha-1+\alpha^2\right]=\boxed{\frac{\hbar m\omega}{2}\left[1-(\alpha-\alpha^*)^2\right].}\end{aligned}$$

(b)

$$\begin{aligned}\sigma_x^2 &= \langle x^2\rangle-\langle x\rangle^2=\frac{\hbar}{2m\omega}\left[1+(\alpha+\alpha^*)^2-(\alpha+\alpha^*)^2\right]=\frac{\hbar}{2m\omega};\\ \sigma_p^2 &= \langle p^2\rangle-\langle p\rangle^2=\frac{\hbar m\omega}{2}\left[1-(\alpha-\alpha^*)^2+(\alpha-\alpha^*)^2\right]=\frac{\hbar m\omega}{2}.\quad\sigma_x\sigma_p=\sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{\hbar m\omega}{2}}=\frac{\hbar}{2}.\quad\text{QED}\end{aligned}$$

(c) Using Eq. 2.68 for ψ_n:

$$c_n = \langle\psi_n|\alpha\rangle = \frac{1}{\sqrt{n!}}\langle(a_+)^n\psi_0|\alpha\rangle = \frac{1}{\sqrt{n!}}\langle\psi_0|(a_-)^n\alpha\rangle = \frac{1}{\sqrt{n!}}\alpha^n\langle\psi_0|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}}c_0. \quad \checkmark$$

(d) $1 = \sum_{n=0}^{\infty}|c_n|^2 = |c_0|^2\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!} = |c_0|^2 e^{|\alpha|^2} \quad \Rightarrow \quad \boxed{c_0 = e^{-|\alpha|^2/2}.}$

(e) $|\alpha(t)\rangle = \sum_{n=0}^{\infty} c_n e^{-iE_n t/\hbar}|n\rangle = \sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-|\alpha|^2/2}e^{-i(n+\frac{1}{2})\omega t}|n\rangle = e^{-i\omega t/2}\sum_{n=0}^{\infty}\frac{\left(\alpha e^{-i\omega t}\right)^n}{\sqrt{n!}}e^{-|\alpha|^2/2}|n\rangle.$

Apart from the overall phase factor $e^{-i\omega t/2}$ (which doesn't affect its status as an eigenfunction of a_-, or its eigenvalue), $|\alpha(t)\rangle$ is the same as $|\alpha\rangle$, but with eigenvalue $\alpha(t) = e^{-i\omega t}\alpha$. ✓

(f) From (a), $\langle x\rangle = \sqrt{\hbar/2m\omega}[\alpha(t) + \alpha^*(t)]$. From (e), $\alpha(t) = e^{-i\omega t}\alpha$. So

$$\begin{aligned}\langle x\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left(\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(C\sqrt{\frac{m\omega}{2\hbar}}e^{i\phi}e^{-i\omega t} + C\sqrt{\frac{m\omega}{2\hbar}}e^{-i\phi}e^{i\omega t}\right)\\ &= \frac{1}{2}C\left(e^{-i(\omega t-\phi} + e^{i(\omega t-\phi)}\right) = \boxed{C\cos(\omega t-\phi)}.\end{aligned}$$

From (b), $\sigma_x = \boxed{\sqrt{\frac{\hbar}{2m\omega}}.}$ So the expectation value of x oscillates at the classical frequency (but this is true for *all* states of the harmonic oscillator—see Problem 3.40) and the wave packet maintains a constant width.

(g) Equation 2.59 says $a_-|\psi_0\rangle = 0$, so $\boxed{\text{yes,}}$ it *is* a coherent state, with eigenvalue $\boxed{\alpha = 0.}$

Problem 3.43

(a) Equation 3.60 becomes $|z|^2 = [\mathrm{Re}(z)]^2 + [\mathrm{Im}(z)]^2 = \left[\frac{1}{2}(z+z^*)\right]^2 + \left[\frac{1}{2i}(z-z^*)\right]^2$; Eq. 3.61 generalizes to

$$\sigma_A^2\sigma_B^2 \geq \left[\frac{1}{2}\left(\langle f|g\rangle + \langle g|f\rangle\right)\right]^2 + \left[\frac{1}{2i}\left(\langle f|g\rangle - \langle g|f\rangle\right)\right]^2.$$

But $\langle f|g\rangle - \langle g|f\rangle = \langle[\hat{A},\hat{B}]\rangle$ (p. 106), and, by the same argument,

$$\langle f|g\rangle + \langle g|f\rangle = \langle\hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle + \langle\hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle = \langle\hat{A}\hat{B} + \hat{B}\hat{A} - 2\langle A\rangle\langle B\rangle\rangle = \langle D\rangle.$$

So $\sigma_A^2\sigma_B^2 \geq \frac{1}{4}\left(\langle D\rangle^2 + \langle C\rangle^2\right)$. ✓

(b) If $\hat{B} = \hat{A}$, then $\hat{C} = 0$, $\hat{D} = 2\left(\hat{A}^2 - \langle A\rangle^2\right)$; $\langle D\rangle = 2\left(\langle\hat{A}^2\rangle - \langle A\rangle^2\right) = 2\sigma_A^2$. So Eq. 3.115 says $\sigma_A^2\sigma_A^2 \geq (1/4)4\sigma_A^4 = \sigma_A^4$, which is *true*, but not very informative.

Problem 3.44

First find the eigenvalues and eigenvectors of the Hamiltonian. The characteristic equation says

$$\begin{vmatrix} (a-E) & 0 & b \\ 0 & (c-E) & 0 \\ b & 0 & (a-E) \end{vmatrix} = (a-E)(c-E)(a-E) - b^2(c-E) = (c-E)\left[(a-E)^2 - b^2\right] = 0,$$

Either $E = c$, or else $(a-E)^2 = b^2 \;\Rightarrow\; E = a \pm b$. So the eigenvalues are

$$E_1 = c, \quad E_2 = a + b, \quad E_3 = a - b.$$

To find the corresponding eigenvectors, write

$$\begin{pmatrix} a & 0 & b \\ 0 & c & 0 \\ b & 0 & a \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = E_n \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}.$$

(1)

$$\left.\begin{aligned} a\alpha + b\gamma &= c\alpha \Rightarrow (a-c)\alpha + b\gamma = 0; \\ c\beta &= c\beta \qquad \text{(redundant)} \qquad ; \\ b\alpha + a\gamma &= c\gamma \Rightarrow (a-c)\gamma + b\alpha = 0. \end{aligned}\right\} \Rightarrow \left[(a-c)^2 - b^2\right]\alpha = 0.$$

So (excluding the degenerate case $a - c = \pm b$) $\alpha = 0$, and hence also $\gamma = 0$.

(2)

$$\begin{aligned} a\alpha + b\gamma &= (a+b)\alpha \Rightarrow & \alpha - \gamma &= 0; \\ c\beta &= (a+b)\beta \Rightarrow & \beta &= 0; \\ b\alpha + a\gamma &= (a+b)\gamma & \text{(redundant)}. \end{aligned}$$

So $\alpha = \gamma$ and $\beta = 0$.

(3)

$$\begin{aligned} a\alpha + b\gamma &= (a-b)\alpha \Rightarrow & \alpha + \gamma &= 0; \\ c\beta &= (a-b)\beta \Rightarrow & \beta &= 0; \\ b\alpha + a\gamma &= (a-b)\gamma & \text{(redundant)}. \end{aligned}$$

So $\alpha = -\gamma$ and $\beta = 0$.

Conclusion: The (normalized) eigenvectors of H are

$$|s_1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |s_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad |s_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}.$$

(a) Here $|\mathcal{S}(0)\rangle = |s_1\rangle$, so

$$|\mathcal{S}(t)\rangle = e^{-iE_1 t/\hbar}|s_1\rangle = \boxed{e^{-ict/\hbar} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.}$$

(b)

$$|\mathcal{S}(0)\rangle = \frac{1}{\sqrt{2}}\left(|s_2\rangle + |s_3\rangle\right).$$

$$|\mathcal{S}(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_2t/\hbar}|s_2\rangle + e^{-iE_3t/\hbar}|s_3\rangle\right) = \frac{1}{\sqrt{2}}\left[e^{-i(a+b)t/\hbar}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix} + e^{-i(a-b)t/\hbar}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}\right]$$

$$= \frac{1}{2}e^{-iat/\hbar}\begin{pmatrix}e^{-ibt/\hbar}+e^{ibt/\hbar}\\0\\e^{-ibt/\hbar}-e^{ibt/\hbar}\end{pmatrix} = \boxed{e^{-iat/\hbar}\begin{pmatrix}\cos(bt/\hbar)\\0\\-i\sin(bt/\hbar)\end{pmatrix}.}$$

Problem 3.45

$$\langle n|\hat{x}|\mathcal{S}(t)\rangle = \langle n|\hat{x}\left(\sum_{n'=0}^{\infty}|n'\rangle\langle n'|\right)|\mathcal{S}(t)\rangle = \sum_{n'=0}^{\infty}\langle n|\hat{x}|n'\rangle\,\langle n'|\mathcal{S}(t)\rangle.$$

From Equation 3.114, $\langle n|\hat{x}|n'\rangle = \sqrt{\hbar/2m\omega}\left(\sqrt{n'}\,\delta_{n,n'-1} + \sqrt{n}\,\delta_{n',n-1}\right)$, so

$$\langle n|\hat{x}|\mathcal{S}(t)\rangle = \sum_{n'=0}^{\infty}\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n'}\,\delta_{n,n'-1} + \sqrt{n}\,\delta_{n',n-1}\right)c_{n'}(t) = \boxed{\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,c_{n+1}(t) + \sqrt{n}\,c_{n-1}(t)\right).}$$

Problem 3.46

(a) H:

$$\boxed{E_1 = \hbar\omega,\ E_2 = E_3 = 2\hbar\omega;\quad |h_1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix},\ |h_2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix},\ |h_3\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}.}$$

A:

$$\begin{vmatrix}-a & \lambda & 0\\ \lambda & -a & 0\\ 0 & 0 & (2\lambda-a)\end{vmatrix} = a^2(2\lambda-a) - (2\lambda-a)\lambda^2 = 0 \Rightarrow \boxed{a_1 = 2\lambda,\ a_2 = \lambda,\ a_3 = -\lambda.}$$

$$\lambda\begin{pmatrix}0&1&0\\1&0&0\\0&0&2\end{pmatrix}\begin{pmatrix}\alpha\\\beta\\\gamma\end{pmatrix} = a\begin{pmatrix}\alpha\\\beta\\\gamma\end{pmatrix} \Rightarrow \begin{cases}\lambda\beta = a\alpha\\ \lambda\alpha = a\beta\\ 2\lambda\gamma = a\gamma\end{cases}$$

(1)

$$\left.\begin{aligned}\lambda\beta &= 2\lambda\alpha \ \Rightarrow\ \beta = 2\alpha,\\ \lambda\alpha &= 2\lambda\beta \ \Rightarrow\ \alpha = 2\beta,\\ 2\lambda\gamma &= 2\lambda\gamma;\end{aligned}\right\}\quad \alpha = \beta = 0;\quad \boxed{|a_1\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}.}$$

(2)

$$\left.\begin{aligned} \lambda\beta &= \lambda\alpha \;\Rightarrow\; \beta = \alpha, \\ \lambda\alpha &= \lambda\beta \;\Rightarrow\; \alpha = \beta, \\ 2\lambda\gamma &= \lambda\gamma; \Rightarrow\; \gamma = 0. \end{aligned}\right\} \quad \boxed{|a_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix}.}$$

(3)

$$\left.\begin{aligned} \lambda\beta &= -\lambda\alpha \;\Rightarrow\; \beta = -\alpha, \\ \lambda\alpha &= -\lambda\beta \;\Rightarrow\; \alpha = -\beta, \\ 2\lambda\gamma &= -\lambda\gamma; \Rightarrow\; \gamma = 0. \end{aligned}\right\} \quad \boxed{|a_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\\0\end{pmatrix}.}$$

B:

$$\begin{vmatrix} (2\mu-b) & 0 & 0 \\ 0 & -b & \mu \\ 0 & \mu & -b \end{vmatrix} = b^2(2\mu-b) - (2\mu-b)\mu^2 = 0 \Rightarrow \boxed{b_1 = 2\mu,\; b_2 = \mu,\; b_3 = -\mu.}$$

$$\mu\begin{pmatrix}2&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}\alpha\\\beta\\\gamma\end{pmatrix} = b\begin{pmatrix}\alpha\\\beta\\\gamma\end{pmatrix} \Rightarrow \left\{\begin{aligned} 2\mu\alpha &= b\alpha \\ \mu\gamma &= b\beta \\ \mu\beta &= b\gamma \end{aligned}\right.$$

(1)

$$\left.\begin{aligned} 2\mu\alpha &= 2\mu\alpha, \\ \mu\gamma &= 2\mu\beta \;\Rightarrow\; \gamma = 2\beta, \\ \mu\beta &= 2\mu\gamma \;\Rightarrow\; \beta = 2\gamma; \end{aligned}\right\} \quad \beta = \gamma = 0; \quad \boxed{|b_1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}.}$$

(2)

$$\left.\begin{aligned} 2\mu\alpha &= \mu\alpha \;\Rightarrow\; \alpha = 0, \\ \mu\gamma &= \mu\beta \;\Rightarrow\; \gamma = \beta, \\ \mu\beta &= \mu\gamma; \Rightarrow\; \beta = \gamma. \end{aligned}\right\} \quad \boxed{|b_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\end{pmatrix}.}$$

(3)

$$\left.\begin{aligned} 2\mu\alpha &= -\mu\alpha \;\Rightarrow\; \alpha = 0, \\ \mu\gamma &= -\mu\beta \;\Rightarrow\; \gamma = -\beta, \\ \mu\beta &= -\mu\gamma; \Rightarrow\; \beta = -\gamma. \end{aligned}\right\} \quad \boxed{|b_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\end{pmatrix}.}$$

(b)

$$\begin{aligned}
\langle H\rangle &= \langle \mathcal{S}(0)|H|\mathcal{S}(0)\rangle = \hbar\omega\begin{pmatrix}c_1^* & c_2^* & c_3^*\end{pmatrix}\begin{pmatrix}1&0&0\\0&2&0\\0&0&2\end{pmatrix}\begin{pmatrix}c_1\\c_2\\c_3\end{pmatrix} = \boxed{\hbar\omega\left(|c_1|^2 + 2|c_2|^2 + 2|c_3|^2\right).} \\
\langle A\rangle &= \langle \mathcal{S}(0)|A|\mathcal{S}(0)\rangle = \lambda\begin{pmatrix}c_1^* & c_2^* & c_3^*\end{pmatrix}\begin{pmatrix}0&1&0\\1&0&0\\0&0&2\end{pmatrix}\begin{pmatrix}c_1\\c_2\\c_3\end{pmatrix} = \boxed{\lambda\left(c_1^*c_2 + c_2^*c_1 + 2|c_3|^2\right).} \\
\langle B\rangle &= \langle \mathcal{S}(0)|B|\mathcal{S}(0)\rangle = \mu\begin{pmatrix}c_1^* & c_2^* & c_3^*\end{pmatrix}\begin{pmatrix}2&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}c_1\\c_2\\c_3\end{pmatrix} = \boxed{\mu\left(2|c_1|^2 + c_2^*c_3 + c_3^*c_2\right).}
\end{aligned}$$

(c)

$$\begin{aligned}|\mathcal{S}(0)\rangle &= c_1|h_1\rangle + c_2|h_2\rangle + c_3|h_3\rangle \quad \Rightarrow\\ |\mathcal{S}(t)\rangle &= c_1 e^{-iE_1t/\hbar}|h_1\rangle + c_2 e^{-iE_2t/\hbar}|h_2\rangle + c_3 e^{-iE_3t/\hbar}|h_3\rangle = c_1 e^{-i\omega t}|h_1\rangle + c_2 e^{-2i\omega t}|h_2\rangle + c_3 e^{-2i\omega t}|h_3\rangle\\ &= e^{-2i\omega t}\left[c_1 e^{i\omega t}\begin{pmatrix}1\\0\\0\end{pmatrix} + c_2\begin{pmatrix}0\\1\\0\end{pmatrix} + c_3\begin{pmatrix}0\\0\\1\end{pmatrix}\right] = \boxed{e^{-2i\omega t}\begin{pmatrix}c_1 e^{i\omega t}\\ c_2\\ c_3\end{pmatrix}.}\end{aligned}$$

H: $\boxed{h_1 = \hbar\omega,\ \text{probability } |c_1|^2; \quad h_2 = h_3 = 2\hbar\omega,\ \text{probability } (|c_2|^2 + |c_3|^2).}$

A: $\boxed{a_1 = 2\lambda,}$ $\langle a_1|\mathcal{S}(t)\rangle = e^{-2i\omega t}\begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}c_1 e^{i\omega t}\\ c_2\\ c_3\end{pmatrix} = e^{-2i\omega t}c_3 \Rightarrow \boxed{\text{probability } |c_3|^2.}$

$\boxed{a_2 = \lambda,}$ $\langle a_2|\mathcal{S}(t)\rangle = e^{-2i\omega t}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1 & 0\end{pmatrix}\begin{pmatrix}c_1 e^{i\omega t}\\ c_2\\ c_3\end{pmatrix} = \frac{1}{\sqrt{2}}e^{-2i\omega t}\left(c_1 e^{i\omega t} + c_2\right) \Rightarrow$

$$\text{probability} = \frac{1}{2}\left(c_1^* e^{-i\omega t} + c_2^*\right)\left(c_1 e^{i\omega t} + c_2\right) = \boxed{\frac{1}{2}\left(|c_1|^2 + |c_2|^2 + c_1^* c_2 e^{-i\omega t} + c_2^* c_1 e^{i\omega t}\right).}$$

$\boxed{a_3 = -\lambda,}$ $\langle a_3|\mathcal{S}(t)\rangle = e^{-2i\omega t}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1 & 0\end{pmatrix}\begin{pmatrix}c_1 e^{i\omega t}\\ c_2\\ c_3\end{pmatrix} = \frac{1}{\sqrt{2}}e^{-2i\omega t}\left(c_1 e^{i\omega t} - c_2\right) \Rightarrow$

$$\text{probability} = \frac{1}{2}\left(c_1^* e^{-i\omega t} - c_2^*\right)\left(c_1 e^{i\omega t} - c_2\right) = \boxed{\frac{1}{2}\left(|c_1|^2 + |c_2|^2 - c_1^* c_2 e^{-i\omega t} - c_2^* c_1 e^{i\omega t}\right).}$$

Note that the sum of the probabilities is 1.

B: $\boxed{b_1 = 2\mu,}$ $\langle b_1|\mathcal{S}(t)\rangle = e^{-2i\omega t}\begin{pmatrix}1 & 0 & 0\end{pmatrix}\begin{pmatrix}c_1 e^{i\omega t}\\ c_2\\ c_3\end{pmatrix} = e^{-i\omega t}c_1 \Rightarrow \boxed{\text{probability } |c_1|^2.}$

$\boxed{b_2 = \mu,}$ $\langle b_2|\mathcal{S}(t)\rangle = e^{-2i\omega t}\frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1 & 1\end{pmatrix}\begin{pmatrix}c_1 e^{i\omega t}\\ c_2\\ c_3\end{pmatrix} = \frac{1}{\sqrt{2}}e^{-2i\omega t}(c_2 + c_3) \Rightarrow$

$$\text{probability} = \frac{1}{2}(c_2^* + c_3^*)(c_2 + c_3) = \boxed{\frac{1}{2}\left(|c_2|^2 + |c_3|^2 + c_2^* c_3 + c_3^* c_2\right).}$$

$\boxed{b_3 = -\mu,}$ $\langle b_3|\mathcal{S}(t)\rangle = e^{-2i\omega t}\frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1 & -1\end{pmatrix}\begin{pmatrix}c_1 e^{i\omega t}\\ c_2\\ c_3\end{pmatrix} = \frac{1}{\sqrt{2}}e^{-2i\omega t}(c_2 - c_3) \Rightarrow$

$$\text{probability} = \frac{1}{2}(c_2^* - c_3^*)(c_2 - c_3) = \boxed{\frac{1}{2}\left(|c_2|^2 + |c_3|^2 - c_2^* c_3 - c_3^* c_2\right).}$$

Again, the sum of the probabilities is 1.

Problem 3.47

(a)

$$\hat{H}_1 = \hat{A}^\dagger\hat{A} = \left(-i\frac{\hat{p}}{\sqrt{2m}} + W\right)\left(i\frac{\hat{p}}{\sqrt{2m}} + W\right) = \frac{\hat{p}^2}{2m} + \frac{i}{\sqrt{2m}}(W\hat{p} - \hat{p}W) + W^2 = \frac{\hat{p}^2}{2m} + V_1.$$

So $V_1 = W^2 + \frac{i}{\sqrt{2m}}[W,\hat{p}]$. To calculate the commutator, use a test function $f(x)$:

$$[W,\hat{p}]f(x) = W(-i\hbar\frac{df}{dx} + i\hbar\frac{d}{dx}(Wf) = i\hbar\left(-W\frac{df}{dx} + \frac{dW}{dx}f + W\frac{df}{dx}\right) = i\hbar\frac{dW}{dx}f \Rightarrow [W,\hat{p}] = i\hbar\frac{dW}{dx}.$$

$$\boxed{V_1 = W^2 - \frac{\hbar}{\sqrt{2m}}\frac{dW}{dx}.}$$

$$\hat{H}_2 = \hat{A}\hat{A}^\dagger = \left(i\frac{\hat{p}}{\sqrt{2m}} + W\right)\left(-i\frac{\hat{p}}{\sqrt{2m}} + W\right) = \frac{\hat{p}^2}{2m} - \frac{i}{\sqrt{2m}}(W\hat{p} - \hat{p}W) + W^2 = \frac{\hat{p}^2}{2m} + V_2.$$

So $V_2 = W^2 - \frac{i}{\sqrt{2m}}[W,\hat{p}]$, and hence $\boxed{V_2 = W^2 + \frac{\hbar}{\sqrt{2m}}\frac{dW}{dx}.}$

(b)

$$\hat{H}_1\psi_n^{(1)} = E_n^{(1)}\psi_n^{(1)} \Rightarrow \hat{A}^\dagger\hat{A}\psi_n^{(1)} = E_n^{(1)}\psi_n^{(1)} \Rightarrow \hat{H}_2\left(\hat{A}\psi_n^{(1)}\right) = \hat{A}\hat{A}^\dagger\hat{A}\psi_n^{(1)} = \hat{A}E_n^{(1)}\psi_n^{(1)} = E_n^{(1)}\left(\hat{A}\psi_n^{(1)}\right). \quad \checkmark$$

$$\hat{H}_2\psi_n^{(2)} = E_n^{(2)}\psi_n^{(2)} \Rightarrow \hat{A}\hat{A}^\dagger\psi_n^{(2)} = E_n^{(2)}\psi_n^{(2)} \Rightarrow \hat{H}_1\left(\hat{A}^\dagger\psi_n^{(2)}\right) = \hat{A}^\dagger\hat{A}\hat{A}^\dagger\psi_n^{(2)} = \hat{A}^\dagger E_n^{(2)}\psi_n^{(2)} = E_n^{(2)}\left(\hat{A}^\dagger\psi_n^{(2)}\right). \quad \checkmark$$

(c)

$$\hat{A}\psi_0^{(1)}(x) = 0 \Rightarrow \left(\frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + W\right)\psi_0^{(1)}(x) = 0 \Rightarrow \boxed{W(x) = -\frac{\hbar}{\sqrt{2m}}\frac{(d\psi_0^{(1)}/dx)}{\psi_0^{(1)}} = -\frac{\hbar}{\sqrt{2m}}\frac{d}{dx}\left[\ln\left(\psi_0^{(1)}\right)\right].}$$

(d)

$$W(x) = -\frac{\hbar}{\sqrt{2m}}\frac{d}{dx}\left[\ln\left(\frac{\sqrt{m\alpha}}{\hbar}\right) - \frac{m\alpha}{\hbar^2}|x|\right] = \frac{\hbar}{\sqrt{2m}}\frac{m\alpha}{\hbar^2}\operatorname{sign}(x) = \boxed{\sqrt{\frac{m}{2}}\frac{\alpha}{\hbar}\operatorname{sign}(x).}$$

$$V_2 = W^2 + \frac{\hbar}{\sqrt{2m}}\frac{dW}{dx} = \frac{m\alpha^2}{2\hbar^2} + \frac{\hbar}{\sqrt{2m}}\sqrt{\frac{m}{2}}\frac{\alpha}{\hbar}\frac{d}{dx}(\operatorname{sign}(x)) = \boxed{\frac{m\alpha^2}{2\hbar^2} + \alpha\delta(x).}$$

I used the fact that

$$\operatorname{sign}(x) = -1 + 2\theta(x) = \begin{cases} -1, & (x < 0) \\ +1, & (x > 0) \end{cases}$$

and $d\theta/dx = \delta(x)$ (Problem 2.23(b)).

Problem 3.48

(a) Integrate by parts:

$$\langle g|\hat{p}f\rangle = \int_0^a g^*\left(-i\hbar\frac{df}{dx}\right)dx = -i\hbar\, g^* f\Big|_0^a + i\hbar\int_0^a \frac{dg^*}{dx}f\,dx = \int_0^a\left(-i\hbar\frac{dg}{dx}\right)^* f\,dx = \langle\hat{p}g|f\rangle. \quad \checkmark$$

The boundary term drops out because $f(0) = f(a) = 0$, *regardless* of what $g(x)$ does at the end points. $\boxed{\text{No.}}$ It's *not* self-adjoint, because the domain of $\hat{p}^\dagger$ (the set of allowable g's) is not the same as that of $\hat{p}$ (the allowed f's).

(b) For the boundary term to vanish we need

$$g^* f\Big|_0^a = g^*(a)\,f(a) - g^*(0)\,f(0) = g^*(a)\lambda f(0) - g^*(0)\,f(0) = [\lambda g^*(a) - g^*(0)]\,f(0) = 0.$$

But $f(0)$ is *not* necessarily zero—else we are back to part (a)—so we need

$$\lambda g^*(a) = g^*(0), \quad \text{or} \quad \boxed{g(a) = \frac{1}{\lambda^*} g(0).}$$

The two domains will be identical if $1/\lambda^* = \lambda$, or $|\lambda|^2 = 1$, which is to say, $\boxed{\lambda = e^{i\phi}}$ for some real number ϕ.

(c) For $f(x)$ and $g(x)$ to be in $L^2(0,\infty)$, $f(\infty) = g(\infty) = 0$, so to kill the boundary term we need $g^*(0)\,f(0) = 0$. Either $f(0) = 0$, in which case $g(0)$ can be anything, or else $g(0) = 0$, in which case $f(0)$ can be anything; there is no way to make the two domains equal. $\boxed{\text{No,}}$ there is no self-adjoint momentum operator on the semi-infinite interval.

Problem 3.49

(a) For the free particle, $V(x) = 0$, so the time-dependent Schrödinger equation reads

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}. \qquad \Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{ipx/\hbar}\Phi(p,t)\,dp \;\Rightarrow$$

$$\frac{\partial\Psi}{\partial t} = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{ipx/\hbar}\frac{\partial\Phi}{\partial t}\,dp, \qquad \frac{\partial^2\Psi}{\partial x^2} = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(-\frac{p^2}{\hbar^2}\right)e^{ipx/\hbar}\Phi\,dp. \quad \text{So}$$

$$\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{ipx/\hbar}\left[i\hbar\frac{\partial\Phi}{\partial t}\right]dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{ipx/\hbar}\left[\frac{p^2}{2m}\Phi\right]dp.$$

But two functions with the same Fourier transform are equal (as you can easily prove using Plancherel's theorem), so

$$\boxed{i\hbar\frac{\partial\Phi}{\partial t} = \frac{p^2}{2m}\Phi.} \quad \frac{1}{\Phi}\,d\Phi = -\frac{ip^2}{2m\hbar}\,dt \quad \Rightarrow \quad \boxed{\Phi(p,t) = e^{-ip^2t/2m\hbar}\Phi(p,0).}$$

(b)

$$\Psi(x,0) = Ae^{-ax^2}e^{ilx}, \quad A = \left(\frac{2a}{\pi}\right)^{1/4} \quad \text{(Problem 2.42(a)).}$$

$$\Phi(p,0) = \frac{1}{\sqrt{2\pi\hbar}}\left(\frac{2a}{\pi}\right)^{1/4}\int_{-\infty}^{\infty} e^{-ipx/\hbar}e^{-ax^2}e^{ilx}\,dx = \frac{1}{(2\pi a\hbar^2)^{1/4}}e^{-(l-p/\hbar)^2/4a} \quad \text{(Problem 2.42(b)).}$$

$$\boxed{\Phi(p,t) = \frac{1}{(2\pi a\hbar^2)^{1/4}}e^{-(l-p/\hbar)^2/4a}e^{-ip^2t/2m\hbar}; \qquad |\Phi(p,t)|^2 = \frac{1}{\sqrt{2\pi a}\,\hbar}e^{-(l-p/\hbar)^2/2a}.}$$

(c)

$$\begin{aligned}
\langle p\rangle &= \int_{-\infty}^{\infty} p|\Phi(p,t)|^2\,dp = \frac{1}{\sqrt{2\pi a}\,\hbar}\int_{-\infty}^{\infty} pe^{-(l-p/\hbar)^2/2a}\,dp \\
&\qquad \text{[Let } y\equiv(p/\hbar)-l,\ \text{so } p=\hbar(y+l) \text{ and } dp=\hbar\,dy.\text{]} \\
&= \frac{\hbar}{\sqrt{2\pi a}}\int_{-\infty}^{\infty}(y+l)e^{-y^2/2a}\,dy \quad \text{[but the first term is odd]} \\
&= \frac{2\hbar l}{\sqrt{2\pi a}}\int_{0}^{\infty} e^{-y^2/2a}\,dy = \frac{2\hbar l}{\sqrt{2\pi a}}\sqrt{\frac{\pi a}{2}} = \boxed{\hbar l} \quad \text{[as in Problem 2.42(d)].}
\end{aligned}$$

$$\begin{aligned}
\langle p^2\rangle &= \int_{-\infty}^{\infty} p^2|\Phi(p,t)|^2\,dp = \frac{1}{\sqrt{2\pi a}\,\hbar}\int_{-\infty}^{\infty} p^2e^{-(l-p/\hbar)^2/2a}\,dp = \frac{\hbar^2}{\sqrt{2\pi a}}\int_{-\infty}^{\infty}(y^2+2yl+l^2)e^{-y^2/2a}\,dy \\
&= \frac{2\hbar^2}{\sqrt{2\pi a}}\left[\int_0^{\infty} y^2e^{-y^2/2a}\,dy + l^2\int_0^{\infty} e^{-y^2/2a}\,dy\right] \\
&= \frac{2\hbar^2}{\sqrt{2\pi a}}\left[2\sqrt{\pi}\left(\sqrt{\frac{a}{2}}\right)^3 + l^2\sqrt{\frac{\pi a}{2}}\right] = \boxed{(a+l^2)\hbar^2} \quad \text{[as in Problem 2.42(d)].}
\end{aligned}$$

(d) $H = \dfrac{p^2}{2m}$; $\langle H\rangle = \dfrac{1}{2m}\langle p^2\rangle = \dfrac{\hbar^2}{2m}(l^2+a) = \dfrac{1}{2m}\langle p\rangle^2 + \dfrac{\hbar^2 a}{2m}$. But $\langle H\rangle_0 = \dfrac{1}{2m}\langle p^2\rangle_0 = \dfrac{\hbar^2 a}{2m}$ (Problem 2.21(d)). So $\langle H\rangle = \dfrac{1}{2m}\langle p\rangle^2 + \langle H\rangle_0$. QED *Comment:* The energy of the traveling gaussian is the energy of the same gaussian at rest, plus the kinetic energy ($\langle p\rangle^2/2m$) associated with the motion of the wave packet as a whole.

Chapter 4

Quantum Mechanics in Three Dimensions

Problem 4.1

(a)

$$[x,y] = xy - yx = 0, \text{ etc., so } \boxed{[r_i, r_j] = 0.}$$

$$[p_x, p_y]f = \frac{\hbar}{i}\frac{\partial}{\partial x}\left(\frac{\hbar}{i}\frac{\partial f}{\partial y}\right) - \frac{\hbar}{i}\frac{\partial}{\partial y}\left(\frac{\hbar}{i}\frac{\partial f}{\partial x}\right) = -\hbar^2\left(\frac{\partial^2 f}{\partial x \partial y} - \frac{\partial^2 f}{\partial y \partial x}\right) = 0$$

(by the equality of cross-derivatives), so $\boxed{[p_i, p_j] = 0.}$

$$[x, p_x]f = \frac{\hbar}{i}\left(x\frac{\partial f}{\partial x} - \frac{\partial}{\partial x}(xf)\right) = \frac{\hbar}{i}\left(x\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial x} - f\right) = i\hbar f,$$

so $[x, p_x] = i\hbar$ (likewise $[y, p_y] = i\hbar$ and $[z, p_z] = i\hbar$).

$$[y, p_x]f = \frac{\hbar}{i}\left(y\frac{\partial f}{\partial x} - \frac{\partial}{\partial x}(yf)\right) = \frac{\hbar}{i}\left(y\frac{\partial f}{\partial x} - y\frac{\partial f}{\partial y}\right) = 0 \text{ (since } \frac{\partial y}{\partial x} = 0\text{). So } [y, p_x] = 0,$$

and same goes for the other "mixed" commutators. Thus $\boxed{[r_i, p_j] = -[p_j, r_i] = i\hbar\delta_{ij}.}$

(b) The derivation of Eq. 3.73 is identical in three dimensions, so $\dfrac{d\langle x\rangle}{dt} = \dfrac{i}{\hbar}\langle[H, x]\rangle$;

$$[H, x] = \left[\frac{p^2}{2m} + V, x\right] = \frac{1}{2m}[p_x^2 + p_y^2 + p_z^2, x] = \frac{1}{2m}[p_x^2, x]$$
$$= \frac{1}{2m}\left(p_x[p_x, x] + [p_x, x]p_x\right) = \frac{1}{2m}\left[(-i\hbar)p_x + (-i\hbar)p_x\right] = -i\frac{\hbar}{m}p_x.$$

$$\therefore \frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\left(-i\frac{\hbar}{m}\langle p_x\rangle\right) = \frac{1}{m}\langle p_x\rangle. \text{ The same goes for } y \text{ and } z\text{, so: } \boxed{\frac{d\langle \mathbf{r}\rangle}{dt} = \frac{1}{m}\langle \mathbf{p}\rangle.}$$

$$\frac{d\langle p_x\rangle}{dt} = \frac{i}{\hbar}\langle[H,p_x]\rangle; \quad [H,p_x] = \left[\frac{p^2}{2m}+V,p_x\right] = [V,p_x] = i\hbar\frac{\partial V}{\partial x} \text{ (Eq. 3.65)}$$

$$= \frac{i}{\hbar}(i\hbar)\left\langle\frac{\partial V}{\partial x}\right\rangle = \left\langle-\frac{\partial V}{\partial x}\right\rangle. \quad \text{Same for } y \text{ and } z, \text{ so: } \boxed{\frac{d\langle\mathbf{p}\rangle}{dt} = \langle-\nabla V\rangle.}$$

(c) From Eq. 3.62: $\sigma_x\sigma_{p_x} \geq \left|\frac{1}{2i}\langle[x,p_x]\rangle\right| = \left|\frac{1}{2i}i\hbar\right| = \frac{\hbar}{2}$. Generally, $\boxed{\sigma_{r_i}\sigma_{p_j} \geq \frac{\hbar}{2}\delta_{ij}.}$

Problem 4.2

(a) Equation 4.8 $\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right) = E\psi$ (inside the box). Separable solutions: $\psi(x,y,z) = X(x)Y(y)Z(z)$. Put this in, and divide by XYZ:

$$\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{Z}\frac{d^2Z}{dz^2} = -\frac{2m}{\hbar^2}E.$$

The three terms on the left are functions of x, y, and z, respectively, so each must be a constant. Call the separation constants k_x^2, k_y^2, and k_z^2 (as we'll soon seen, they must be positive).

$$\frac{d^2X}{dx^2} = -k_x^2X; \quad \frac{d^2Y}{dy^2} = -k_y^2Y; \quad \frac{d^2Z}{dz^2} = -k_z^2Z, \quad \text{with} \quad E = \frac{\hbar^2}{2m}(k_x^2+k_y^2+k_z^2).$$

Solution:

$$X(x) = A_x\sin k_xx + B_x\cos k_xx; \quad Y(y) = A_y\sin k_yy + B_y\cos k_yy; \quad Z(z) = A_z\sin k_zz + B_z\cos k_zz.$$

But $X(0)=0$, so $B_x=0$; $Y(0)=0$, so $B_y=0$; $Z(0)=0$, so $B_z=0$. And $X(a)=0 \Rightarrow \sin(k_xa)=0 \Rightarrow k_x = n_x\pi/a$ ($n_x = 1,2,3,\ldots$). [As before (page 32), $n_x \neq 0$, and negative values are redundant.] Likewise $k_y = n_y\pi/a$ and $k_z = n_z\pi/a$. So

$$\psi(x,y,z) = A_xA_yA_z\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right)\sin\left(\frac{n_z\pi}{a}z\right), \quad E = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}(n_x^2+n_y^2+n_z^2).$$

We might as well normalize $X, Y,$ and Z separately: $A_x = A_y = A_z = \sqrt{2/a}$. *Conclusion:*

$$\boxed{\psi(x,y,z) = \left(\frac{2}{a}\right)^{3/2}\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right)\sin\left(\frac{n_z\pi}{a}z\right); \quad E = \frac{\pi^2\hbar^2}{2ma^2}(n_x^2+n_y^2+n_z^2); \quad n_x,n_y,n_z = 1,2,3,\ldots}$$

(b)

n_x	n_y	n_z	$(n_x^2+n_y^2+n_z^2)$
1	1	1	3
1	1	2	6
1	2	1	6
2	1	1	6
1	2	2	9
2	1	2	9
2	2	1	9
1	1	3	11
1	3	1	11
3	1	1	11
2	2	2	12
1	2	3	14
1	3	2	14
2	1	3	14
2	3	1	14
3	1	2	14
3	2	1	14

Energy	Degeneracy
$E_1 = 3\dfrac{\pi^2\hbar^2}{2ma^2};$	$d = 1$
$E_2 = 6\dfrac{\pi^2\hbar^2}{2ma^2};$	$d = 3.$
$E_3 = 9\dfrac{\pi^2\hbar^2}{2ma^2};$	$d = 3.$
$E_4 = 11\dfrac{\pi^2\hbar^2}{2ma^2};$	$d = 3.$
$E_5 = 12\dfrac{\pi^2\hbar^2}{2ma^2};$	$d = 1.$
$E_6 = 14\dfrac{\pi^2\hbar^2}{2ma^2};$	$d = 6.$

(c) The next combinations are: $E_7(322)$, $E_8(411)$, $E_9(331)$, $E_{10}(421)$, $E_{11}(332)$, $E_{12}(422)$, $E_{13}(431)$, and $E_{14}(333 \text{ and } 511)$. The degeneracy of E_{14} is $\boxed{4.}$ Simple combinatorics accounts for degeneracies of 1 ($n_x = n_y = n_z$), 3 (two the same, one different), or 6 (all three different). But in the case of E_{14} there is a numerical "accident": $3^2+3^2+3^2 = 27$, but $5^2+1^2+1^2$ is *also* 27, so the degeneracy is greater than combinatorial reasoning alone would suggest.

Problem 4.3

(a) Using Equations 4.8 and 4.13,

$$-\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right)\right\} + V\psi = E\psi, \quad \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) = \frac{1}{r^2}\left[r^2\frac{d^2\psi}{dr^2} + 2r\frac{d\psi}{dr}\right] = \frac{d^2\psi}{dr^2} + \frac{2}{r}\frac{d\psi}{dr} = \frac{1}{a^2}\psi - \frac{2}{ra}\psi.$$

$$-\frac{\hbar^2}{2m}\left(\frac{1}{a^2}\psi - \frac{2}{ra}\psi\right) + V\psi = E\psi \quad \Rightarrow \quad -\frac{\hbar^2}{2ma^2} + \frac{\hbar^2}{mar} + V(r) = E.$$

At $r \to \infty$ we get $\boxed{E = -\dfrac{\hbar^2}{2ma^2},}$ so $\boxed{V(r) = -\dfrac{\hbar^2}{mar}.}$

(b) This time

$$\frac{d\psi}{dr} = -\frac{2r}{a^2}\psi, \quad \frac{d^2\psi}{dr^2} = -\frac{2}{a^2}\psi + \left(\frac{2r}{a^2}\right)^2\psi,$$

so

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) = -\frac{2}{a^2}\psi + \frac{4r^2}{a^4}\psi + \frac{2}{r}\left(-\frac{2r}{a^2}\psi\right) = -\frac{6}{a^2}\psi + \frac{4r^2}{a^4}\psi.$$

$$-\frac{\hbar^2}{2m}\left(-\frac{6}{a^2} + \frac{4r^2}{a^4}\right) + V(r) = E.$$

At $r = 0$ we get $\boxed{E = \frac{3\hbar^2}{ma^2},}$ so $\boxed{V(r) = \frac{2\hbar^2}{ma^4}r^2.}$

Problem 4.4

Eq. 4.32 $\Rightarrow Y_0^0 = \frac{1}{\sqrt{4\pi}}P_0^0(\cos\theta)$; Eq. 4.27 $\Rightarrow P_0^0(x) = P_0(x)$; Eq. 4.28 $\Rightarrow P_0(x) = 1$. $\boxed{Y_0^0 = \frac{1}{\sqrt{4\pi}}.}$

$$Y_2^1 = \sqrt{\frac{5}{4\pi}\frac{1}{3\cdot 2}}\,e^{i\phi}P_2^1(\cos\theta); \quad P_2^1(x) = -\sqrt{1-x^2}\frac{d}{dx}P_2(x);$$

$$P_2(x) = \frac{1}{4\cdot 2}\left(\frac{d}{dx}\right)^2\left(x^2-1\right)^2 = \frac{1}{8}\frac{d}{dx}\left[2(x^2-1)2x\right] = \frac{1}{2}\left[x^2-1+x(2x)\right] = \frac{1}{2}\left(3x^2-1\right);$$

$$P_2^1(x) = -\sqrt{1-x^2}\frac{d}{dx}\left[\frac{3}{2}x^2 - \frac{1}{2}\right] = -\sqrt{1-x^2}\,3x;\; P_2^1(\cos\theta) = -3\cos\theta\sin\theta.\; \boxed{Y_2^1 = -\sqrt{\frac{15}{8\pi}}\,e^{i\phi}\sin\theta\cos\theta.}$$

Normalization: $\displaystyle\iint |Y_0^0|^2\sin\theta\,d\theta\,d\phi = \frac{1}{4\pi}\left[\int_0^\pi \sin\theta\,d\theta\right]\left[\int_0^{2\pi} d\phi\right] = \frac{1}{4\pi}(2)(2\pi) = 1.$ ✓

$$\iint |Y_2^1|^2\sin\theta\,d\theta\,d\phi = \frac{15}{8\pi}\int_0^\pi \sin^2\theta\cos^2\theta\sin\theta\,d\theta\int_0^{2\pi} d\phi = \frac{15}{4}\int_0^\pi \cos^2\theta(1-\cos^2\theta)\sin\theta\,d\theta$$

$$= \frac{15}{4}\left[-\frac{\cos^3\theta}{3} + \frac{\cos^5\theta}{5}\right]\Bigg|_0^\pi = \frac{15}{4}\left[\frac{2}{3} - \frac{2}{5}\right] = \frac{5}{2} - \frac{3}{2} = 1 \text{ ✓}$$

Orthogonality: $\displaystyle\iint Y_0^{0*}Y_2^1\sin\theta\,d\theta\,d\phi = -\frac{1}{\sqrt{4\pi}}\sqrt{\frac{15}{8\pi}}\underbrace{\left[\int_0^\pi \sin\theta\cos\theta\sin\theta\,d\theta\right]}_{(\sin^3\theta)/3|_0^\pi=0}\underbrace{\left[\int_0^{2\pi} e^{i\phi}d\phi\right]}_{(e^{i\phi})/i|_0^{2\pi}=0} = 0.$ ✓

Problem 4.5

$$\frac{d\Theta}{d\theta} = \frac{A}{\tan(\theta/2)}\frac{1}{2}\sec^2(\theta/2) = \frac{A}{2}\frac{1}{\sin(\theta/2)\cos(\theta/2)} = \frac{A}{\sin\theta}. \quad \text{Therefore} \quad \frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = \frac{d}{d\theta}(A) = 0.$$

With $\ell = m = 0$, Eq. 4.25 reads: $\displaystyle\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = 0.$ So $A\ln[\tan(\theta/2)]$ *does* satisfy Eq. 4.25. However,

$\Theta(0) = A\ln(0) = A(-\infty);\; \Theta(\pi) = A\ln\left(\tan\frac{\pi}{2}\right) = A\ln(\infty) = A(\infty).$ $\boxed{\Theta \text{ blows up at } \theta = 0 \text{ and at } \theta = \pi.}$

[In truth, this is not as decisive as it appears, since $\int_0^\pi [(\ln[\tan(\theta/2)])^2\sin\theta\,d\theta = \pi^2/6$, which is perfectly finite; Θ itself blows up at 0 and π, but $\sin\theta$ tames it.]

Problem 4.6

$$Y_\ell^{-m} = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}\, e^{-im\phi}\, P_\ell^{-m}(\cos\theta); \quad P_\ell^{-m}(\cos\theta) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(\cos\theta);$$

$$Y_\ell^{-m} = (-1)^m \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, e^{-im\phi}\, P_\ell^m(\cos\theta) = (-1)^m \left(Y_\ell^m\right)^*. \quad \text{QED}$$

Problem 4.7

$$Y_\ell^\ell = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{1}{(2\ell)!}}\, e^{i\ell\phi} P_\ell^\ell(\cos\theta). \quad P_\ell^\ell(x) = (-1)^\ell (1-x^2)^{\ell/2}\left(\frac{d}{dx}\right)^\ell P_\ell(x).$$

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell, \quad \text{so } P_\ell^\ell(x) = \frac{(-1)^\ell}{2^\ell \ell!}(1-x^2)^{\ell/2}\left(\frac{d}{dx}\right)^{2\ell}(x^2-1)^\ell.$$

Now $(x^2-1)^\ell = x^{2\ell} + \cdots$, where all the other terms involve powers of x *less* than 2ℓ, and hence give zero when differentiated 2ℓ times. So

$$P_\ell^\ell(x) = \frac{(-1)^\ell}{2^\ell \ell!}(1-x^2)^{\ell/2}\left(\frac{d}{dx}\right)^{2\ell} x^{2\ell}. \quad \text{But } \left(\frac{d}{dx}\right)^n x^n = n!, \quad \text{so } P_\ell^\ell(x) = (-1)^\ell \frac{(2\ell)!}{2^\ell \ell!}(1-x^2)^{\ell/2}.$$

$$\therefore Y_\ell^\ell = (-1)^\ell \sqrt{\frac{(2\ell+1)}{4\pi(2\ell)!}}\, e^{i\ell\phi}\frac{(2\ell)!}{2^\ell \ell!}(\sin\theta)^\ell = \boxed{\frac{1}{\ell!}\sqrt{\frac{(2\ell+1)!}{4\pi}}\left(-\frac{1}{2}e^{i\phi}\sin\theta\right)^\ell.}$$

$$Y_3^2 = \sqrt{\frac{7}{4\pi}\cdot\frac{1}{5!}}\, e^{2i\phi} P_3^2(\cos\theta); \quad P_3^2(\cos\theta) = 15\sin^2\theta\,\cos\theta; \quad \text{so}$$

$$Y_3^2 = \sqrt{\frac{7}{4\pi}\frac{1}{5!}}\, 15 e^{2i\phi}\cos\theta\sin^2\theta = \boxed{\frac{1}{4}\sqrt{\frac{105}{2\pi}}\, e^{2i\phi}\sin^2\theta\cos\theta.}$$

Check that Y_ℓ^ℓ satisfies Eq. 4.18: Let $\displaystyle \frac{1}{\ell!}\sqrt{\frac{(2\ell+1)!}{4\pi}}\left(-\frac{1}{2}\right)^\ell \equiv A$, so $\quad Y_\ell^\ell = A(e^{i\phi}\sin\theta)^\ell$.

$$\frac{\partial Y_\ell^\ell}{\partial\theta} = A e^{i\ell\phi}\ell(\sin\theta)^{\ell-1}\cos\theta; \quad \sin\theta\frac{\partial Y_\ell^\ell}{\partial\theta} = \ell\cos\theta Y_\ell^\ell;$$

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y_\ell^\ell}{\partial\theta}\right) = \ell\cos\theta\left(\sin\theta\frac{\partial Y_\ell^\ell}{\partial\theta}\right) - \ell\sin^2\theta Y_\ell^\ell = \left(\ell^2\cos^2\theta - \ell\sin^2\theta\right)Y_\ell^\ell. \quad \frac{\partial^2 Y_\ell^\ell}{\partial\phi^2} = -\ell^2 Y_\ell^\ell.$$

So the left side of Eq. 4.18 is $\left[\ell^2(1-\sin^2\theta) - \ell\sin^2\theta - \ell^2\right]Y_\ell^\ell = -\ell(\ell+1)\sin^2\theta\, Y_\ell^\ell$, which matches the right side.

Check that Y_3^2 satisfies Eq. 4.18: Let $B \equiv \displaystyle\frac{1}{4}\sqrt{\frac{105}{2\pi}}$, so $Y_3^2 = Be^{2i\phi}\sin^2\theta\cos\theta$.

$$\frac{\partial Y_3^2}{\partial\theta} = Be^{2i\phi}\left(2\sin\theta\cos^2\theta - \sin^3\theta\right); \quad \sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y_3^2}{\partial\theta}\right) = Be^{2i\phi}\sin\theta\frac{\partial}{\partial\theta}\left(2\sin^2\theta\cos^2\theta - \sin^4\theta\right)$$

$$= Be^{2i\phi}\sin\theta\left(4\sin\theta\cos^3\theta - 4\sin^3\theta\cos\theta - 4\sin^3\theta\cos\theta\right) = 4Be^{2i\phi}\sin^2\theta\cos\theta\left(\cos^2\theta - 2\sin^2\theta\right)$$

$= 4(\cos^2\theta - 2\sin^2\theta)Y_3^2$. $\dfrac{\partial^2 Y_3^2}{\partial\phi^2} = -4Y_3^2$. So the left side of Eq. 4.18 is

$$4(\cos^2\theta - 2\sin^2\theta - 1)Y_3^2 = 4(-3\sin^2\theta)Y_3^2 = -\ell(\ell+1)\sin^2\theta\, Y_3^2,$$

where $\ell = 3$, so it fits the right side of Eq. 4.18.

Problem 4.8

$$\int_{-1}^{1} P_\ell(x)P_{\ell'}(x)dx = \frac{1}{2^\ell \ell!}\frac{1}{2^{\ell'}\ell'!}\int_{-1}^{1}\left[\left(\frac{d}{dx}\right)^{\ell}(x^2-1)^\ell\right]\left[\left(\frac{d}{dx}\right)^{\ell'}(x^2-1)^{\ell'}\right]dx.$$

If $\ell \neq \ell'$, we may as well let ℓ be the larger of the two ($\ell > \ell'$). Integrate by parts, pulling successively each derivative off the first term onto the second:

$$\begin{aligned}
2^\ell \ell! 2^{\ell'}\ell'!\int_{-1}^{1} P_\ell(x)P_{\ell'}(x)dx &= \left[\left(\frac{d}{dx}\right)^{\ell-1}(x^2-1)^\ell\right]\left[\left(\frac{d}{dx}\right)^{\ell'}(x^2-1)^{\ell'}\right]\Bigg|_{-1}^{1} \\
&\quad - \int_{-1}^{1}\left[\left(\frac{d}{dx}\right)^{\ell-1}(x^2-1)^\ell\right]\left[\left(\frac{d}{dx}\right)^{\ell'+1}(x^2-1)^{\ell'}\right]dx \\
&= \ldots(\text{boundary terms})\ldots + (-1)^\ell\int_{-1}^{1}(x^2-1)^\ell\left(\frac{d}{dx}\right)^{\ell'+\ell}(x^2-1)^{\ell'}dx.
\end{aligned}$$

But $(d/dx)^{\ell'+\ell}(x^2-1)^{\ell'} = 0$, because $(x^2-1)^{\ell'}$ is a polynomial whose highest power is $2\ell'$, so more than $2\ell'$ derivatives will kill it, and $\ell' + \ell > 2\ell'$. Now, the boundary terms are of the form:

$$\left[\left(\frac{d}{dx}\right)^{\ell-n}(x^2-1)^\ell\right]\left[\left(\frac{d}{dx}\right)^{\ell'+n-1}(x^2-1)^{\ell'}\right]\Bigg|_{-1}^{+1}, \quad n = 1, 2, 3, \ldots, \ell.$$

Look at the first term: $(x^2-1)^\ell = (x^2-1)(x^2-1)\ldots(x^2-1)$; ℓ factors. So $0, 1, 2, \ldots, \ell-1$ derivatives will still leave at least one overall factor of (x^2-1). [Zero derivatives leaves ℓ factors; one derivative leaves $\ell-1$: $d/dx(x^2-1)^\ell = 2\ell x(x^2-1)^{\ell-1}$; two derivatives leaves $\ell-2$: $d^2/dx^2(x^2-1)^\ell = 2\ell(x^2-1)^{\ell-1} + 2\ell(\ell-1)2x^2(x^2-1)^{\ell-2}$, and so on.] So the boundary terms are all zero, and hence $\int_{-1}^{1} P_\ell(x)P_{\ell'}(x)dx = 0$.

This leaves only the case $\ell = \ell'$. Again the boundary terms vanish, but this time the remaining integral does *not*:

$$\begin{aligned}
(2^\ell \ell!)^2\int_{-1}^{1}[P_\ell(x)]^2 dx &= (-1)^\ell\int_{-1}^{1}(x^2-1)^\ell\underbrace{\left(\frac{d}{dx}\right)^{2\ell}(x^2-1)^\ell}_{(d/dx)^{2\ell}(x^{2\ell})=(2\ell)!}dx \\
&= (-1)^\ell(2\ell)!\int_{-1}^{1}(x^2-1)^\ell dx = 2(2\ell)!\int_0^1(1-x^2)^\ell dx.
\end{aligned}$$

Let $x \equiv \cos\theta$, so $dx = -\sin\theta\, d\theta$, $\quad (1-x^2) = \sin^2\theta$, $\quad \theta : \pi/2 \to 0$. Then

$$\begin{aligned}
\int_0^1(1-x^2)^\ell dx &= \int_{\pi/2}^{0}(\sin\theta)^{2\ell}(-\sin\theta)d\theta = \int_0^{\pi/2}(\sin\theta)^{2\ell+1}d\theta \\
&= \frac{(2)(4)\cdots(2\ell)}{(1)(3)(5)\cdots(2\ell+1)} = \frac{(2^\ell \ell!)^2}{1\cdot 2\cdot 3\cdot\cdots\cdot(2\ell+1)} = \frac{(2^\ell \ell!)^2}{(2\ell+1)!}.
\end{aligned}$$

$$\therefore \int_{-1}^{1}[P_\ell(x)]^2dx = \frac{1}{(2^\ell \ell!)^2}2(2\ell)!\frac{(2^\ell \ell!)^2}{(2\ell+1)!} = \frac{2}{2\ell+1}. \quad \text{So } \int_{-1}^{1} P_\ell(x)P_{\ell'}(x)dx = \frac{2}{2\ell+1}\delta_{\ell\ell'}. \quad \text{QED}$$

Problem 4.9

(a)

$$n_1(x) = -(-x)\frac{1}{x}\frac{d}{dx}\left(\frac{\cos x}{x}\right) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}.$$

$$\begin{aligned}
n_2(x) &= -(-x)^2\left(\frac{1}{x}\frac{d}{dx}\right)^2\frac{\cos x}{x} = -x^2\left(\frac{1}{x}\frac{d}{dx}\right)\left[\frac{1}{x}\frac{d}{dx}\left(\frac{\cos x}{x}\right)\right] \\
&= -x\frac{d}{dx}\left(\frac{1}{x}\cdot\frac{-x\sin x - \cos x}{x^2}\right) = x\frac{d}{dx}\left(\frac{\sin x}{x^2} + \frac{\cos x}{x^3}\right) \\
&= x\left(\frac{x^2\cos x - 2x\sin x}{x^4} + \frac{-x^3\sin x - 3x^2\cos x}{x^6}\right) \\
&= \frac{\cos x}{x} - 2\frac{\sin x}{x^2} - \frac{\sin x}{x^2} - \frac{3\cos x}{x^3} = \boxed{-\left(\frac{3}{x^3} - \frac{1}{x}\right)\cos x - \frac{3}{x^2}\sin x.}
\end{aligned}$$

(b) Letting $\sin x \approx x$ and $\cos x \approx 1$, and keeping only the lowest power of x:

$$n_1(x) \approx -\frac{1}{x^2} - \frac{1}{x}x \approx \boxed{-\frac{1}{x^2}.} \quad \text{As } x \to 0, \text{ this blows up.}$$

$$n_2(x) \approx -\left(\frac{3}{x^3} - \frac{1}{x}\right) - \frac{3}{x^2}x \approx \boxed{-\frac{3}{x^3},} \text{ which again blows up at the origin.}$$

Problem 4.10

(a)

$$u = Arj_1(kr) = A\left[\frac{\sin(kr)}{k^2r} - \frac{\cos(kr)}{k}\right] = \frac{A}{k}\left[\frac{\sin(kr)}{(kr)} - \cos(kr)\right].$$

$$\frac{du}{dr} = \frac{A}{k}\left[\frac{k^2r\cos(kr) - k\sin(kr)}{(kr)^2} + k\sin(kr)\right] = A\left[\frac{\cos(kr)}{kr} - \frac{\sin(kr)}{(kr)^2} + \sin(kr)\right].$$

$$\begin{aligned}
\frac{d^2u}{dr^2} &= A\left[\frac{-k^2r\sin(kr) - k\cos(kr)}{(kr)^2} - \frac{k^3r^2\cos(kr) - 2k^2r\sin(kr)}{(kr)^4} + k\cos(kr)\right] \\
&= Ak\left[-\frac{\sin(kr)}{(kr)} - \frac{\cos(kr)}{(kr)^2} - \frac{\cos(kr)}{(kr)^2} + 2\frac{\sin(kr)}{(kr)^3} + \cos(kr)\right] \\
&= Ak\left[\left(1 - \frac{2}{(kr)^2}\right)\cos(kr) + \left(\frac{2}{(kr)^3} - \frac{1}{(kr)}\right)\sin(kr)\right].
\end{aligned}$$

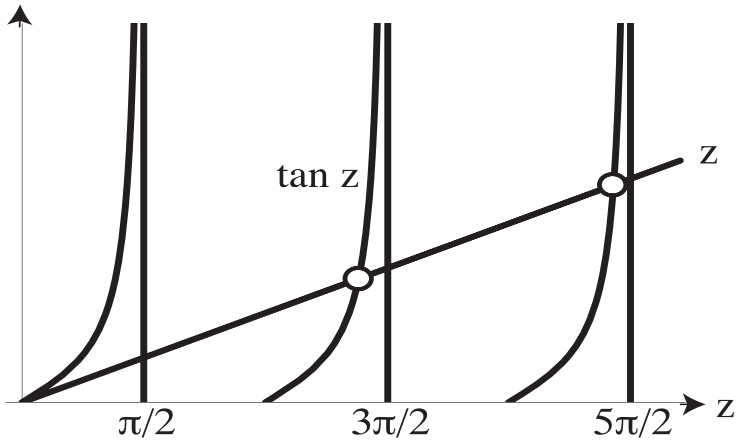
With $V = 0$ and $\ell = 1$, Eq. 4.37 reads: $\dfrac{d^2u}{dr^2} - \dfrac{2}{r^2}u = -\dfrac{2mE}{\hbar^2}u = -k^2u$. In this case the left side is

$$Ak\left[\left(1-\frac{2}{(kr)^2}\right)\cos(kr)+\left(\frac{2}{(kr)^3}-\frac{1}{(kr)}\right)\sin(kr)-\frac{2}{(kr)^2}\left(\frac{\sin(kr)}{(kr)}-\cos(kr)\right)\right]$$

$$= Ak\left[\cos(kr)-\frac{\sin(kr)}{kr}\right] = -k^2u. \quad \text{So this } u \text{ does satisfy Eq. 4.37.}$$

(b) Equation 4.48 $\Rightarrow j_1(z) = 0$, where $z = ka$. Thus $\frac{\sin z}{z^2} - \frac{\cos z}{z} = 0$, or $\boxed{\tan z = z.}$ For high z (large n, if $n = 1, 2, 3, \ldots$ counts the allowed energies in increasing order), the intersections occur slightly below $z = (n + \frac{1}{2})\pi$.

$$\therefore E = \frac{\hbar^2k^2}{2m} = \frac{\hbar^2z^2}{2ma^2} = \frac{\hbar^2\pi^2}{2ma^2}\left(n+\frac{1}{2}\right)^2. \quad \text{QED}$$



Problem 4.11

For $r \le a$, $u(r) = A\sin(kr)$, with $k \equiv \sqrt{2m(E+V_0)}/\hbar$. For $r \ge a$, Eq. 4.37 with $\ell = 0, V = 0$, and (for a bound state) $E < 0 \quad \Rightarrow$:

$$\frac{d^2u}{dr^2} = -\frac{2m}{\hbar^2}Eu = \kappa^2u, \text{ with } \kappa \equiv \sqrt{-2mE}/\hbar \Rightarrow u(r) = Ce^{\kappa r} + De^{-\kappa r}.$$

But the $Ce^{\kappa r}$ term blows up as $r \to \infty$, so $u(r) = De^{-\kappa r}$.

$$\left.\begin{array}{l}\text{Continuity of } u \text{ at } \quad r = a: A\sin(ka) = De^{-\kappa a}\\ \text{Continuity of } u' \text{ at } \quad r = a: Ak\cos(ka) = -D\kappa e^{-\kappa a}\end{array}\right\}\text{divide: } \frac{1}{k}\tan(ka) = -\frac{1}{\kappa}, \text{ or } -\cot ka = \frac{\kappa}{k}.$$

Let $ka \equiv z$; $\dfrac{\kappa}{k} = \dfrac{\sqrt{2mV_0a^2/\hbar^2 - z^2}}{z}$. Let $z_0 \equiv \dfrac{\sqrt{2mV_0}}{\hbar}a$. $\boxed{-\cot z = \sqrt{(z_0/z)^2 - 1}.}$ This is exactly the same transcendental equation we encountered in Problem 2.29—see graph there. There is no solution if $z_0 < \pi/2$, which is to say, if $2mV_0a^2/\hbar^2 < \pi^2/4$, or $V_0a^2 < \pi^2\hbar^2/8m$. Otherwise, the ground state energy occurs somewhere between $z = \pi/2$ and $z = \pi$:

$$E + V_0 = \frac{\hbar^2k^2a^2}{2ma^2} = \frac{\hbar^2}{2ma^2}z^2, \text{ so } \boxed{\frac{\hbar^2\pi^2}{8ma^2} < (E_0+V_0) < \frac{\hbar^2\pi^2}{2ma^2}} \quad \text{(precise value depends on } V_0).$$

Problem 4.12

R_{30} $(n=3,\ell=0)$: Eq. 4.62 $\Rightarrow v(\rho)=\sum_{j=0} c_j\rho^j$.

$$\text{Eq. 4.76} \Rightarrow c_1=\frac{2(1-3)}{(1)(2)}c_0=-2c_0; \quad c_2=\frac{2(2-3)}{(2)(3)}c_1=-\frac{1}{3}c_1=\frac{2}{3}c_0; \quad c_3=\frac{2(3-3)}{(3)(4)}c_2=0.$$

$$\text{Eq. 4.73} \Rightarrow \rho=\frac{r}{3a}; \quad \text{Eq. 4.75} \Rightarrow R_{30}=\frac{1}{r}\rho e^{-\rho}v(\rho)=\frac{1}{r}\frac{r}{3a}e^{-r/3a}\left[c_0-2c_0\frac{r}{3a}+\frac{2}{3}c_0\left(\frac{r}{3a}\right)^2\right]$$

$$R_{30}=\boxed{\left(\frac{c_0}{3a}\right)\left[1-\frac{2}{3}\left(\frac{r}{a}\right)+\frac{2}{27}\left(\frac{r}{a}\right)^2\right]e^{-r/3a}.}$$

$$R_{31}\ (n=3,\ell=1):\ c_1=\frac{2(2-3)}{(1)(4)}c_0=-\frac{1}{2}c_0; \quad c_2=\frac{2(3-3)}{(2)(5)}c_1=0.$$

$$R_{31}=\frac{1}{r}\left(\frac{r}{3a}\right)^2e^{-r/3a}\left(c_0-\frac{1}{2}c_0\frac{r}{3a}\right)=\boxed{\left(\frac{c_0}{9a^2}\right)r\left[1-\frac{1}{6}\left(\frac{r}{a}\right)\right]e^{-r/3a}.}$$

$$R_{32}\ (n=3,\ell=2):\ c_1=\frac{2(3-3)}{(1)(6)}c_0=0. \quad R_{32}=\frac{1}{r}\left(\frac{r}{3a}\right)^3e^{-r/3a}(c_0)=\boxed{\left(\frac{c_0}{27a^3}\right)r^2e^{-r/3a}.}$$

Problem 4.13

(a)

$$\text{Eq. 4.31} \Rightarrow \int_0^\infty |R|^2r^2dr=1. \quad \text{Eq. 4.82} \Rightarrow R_{20}=\left(\frac{c_0}{2a}\right)\left(1-\frac{r}{2a}\right)e^{-r/2a}. \quad \text{Let } z\equiv\frac{r}{a}.$$

$$1=\left(\frac{c_0}{2a}\right)^2a^3\int_0^\infty\left(1-\frac{z}{2}\right)^2e^{-z}z^2\,dz=\frac{c_0^2a}{4}\int_0^\infty\left(z^2-z^3+\frac{1}{4}z^4\right)e^{-z}dz=\frac{c_0^2a}{4}\left(2-6+\frac{24}{4}\right)=\frac{a}{2}c_0^2.$$

$$\therefore \boxed{c_0=\sqrt{\frac{2}{a}}.} \quad \text{Eq. 4.74} \Rightarrow \psi_{200}=R_{20}Y_0^0. \quad \text{Table 4.3} \Rightarrow Y_0^0=\frac{1}{\sqrt{4\pi}}.$$

$$\therefore \psi_{200}=\frac{1}{\sqrt{4\pi}}\sqrt{\frac{2}{a}}\frac{1}{2a}\left(1-\frac{r}{2a}\right)e^{-r/2a} \quad \Rightarrow \boxed{\psi_{200}=\frac{1}{\sqrt{2\pi a}}\frac{1}{2a}\left(1-\frac{r}{2a}\right)e^{-r/2a}.}$$

(b)

$$R_{21}=\frac{c_0}{4a^2}re^{-r/2a}; \quad 1=\left(\frac{c_0}{4a^2}\right)^2a^5\int_0^\infty z^4e^{-z}dz=\frac{c_0^2a}{16}24=\frac{3}{2}ac_0^2, \text{ so } \boxed{c_0=\sqrt{\frac{2}{3a}}.}$$

$$R_{21}=\frac{1}{\sqrt{6a}}\frac{1}{2a^2}re^{-r/2a}; \quad \psi_{21\pm1}=\frac{1}{\sqrt{6a}}\frac{1}{2a^2}re^{-r/2a}\left(\mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}\right)=\boxed{\mp\frac{1}{\sqrt{\pi a}}\frac{1}{8a^2}re^{-r/2a}\sin\theta e^{\pm i\phi};}$$

$$\psi_{210}=\frac{1}{\sqrt{6a}}\frac{1}{2a^2}re^{-r/2a}\left(\sqrt{\frac{3}{4\pi}}\cos\theta\right)=\boxed{\frac{1}{\sqrt{2\pi a}}\frac{1}{4a^2}re^{-r/2a}\cos\theta.}$$

Problem 4.14

(a)

$$L_0 = e^x e^{-x} = \boxed{1.} \quad L_1 = e^x \frac{d}{dx}\left(e^{-x}x\right) = e^x\left[e^{-x} - e^{-x}x\right] = \boxed{1 - x.}$$

$$\begin{aligned} L_2 &= \frac{e^x}{2}\left(\frac{d}{dx}\right)^2\left(e^{-x}x^2\right) = \frac{e^x}{2}\frac{d}{dx}\left(2xe^{-x} - e^{-x}x^2\right) \\ &= \frac{e^x}{2}\left(2e^{-x} - 2xe^{-x} + e^{-x}x^2 - 2xe^{-x}\right) = \boxed{1 - 2x + \tfrac{1}{2}x^2.} \end{aligned}$$

$$\begin{aligned} L_3 &= \frac{e^x}{6}\left(\frac{d}{dx}\right)^3\left(e^{-x}x^3\right) = \frac{e^x}{6}\left(\frac{d}{dx}\right)^2\left(-e^{-x}x^3 + 3x^2e^{-x}\right) \\ &= \frac{e^x}{6}\frac{d}{dx}\left(e^{-x}x^3 - 3x^2e^{-x} - 3x^2e^{-x} + 6xe^{-x}\right) \\ &= \frac{e^x}{6}\left(-e^{-x}x^3 + 3x^2e^{-x} + 6x^2e^{-x} - 12xe^{-x} - 6xe^{-x} + 6e^{-x}\right) \\ &= \boxed{1 - 3x + \tfrac{3}{2}x^2 - \tfrac{1}{6}x^3.} \end{aligned}$$

(b)

$$v(\rho) = L_2^5(2\rho); \quad L_2^5(x) = (-1)^5\left(\frac{d}{dx}\right)^5 L_7(x).$$

$$\begin{aligned} L_7(x) &= \frac{e^x}{7!}\left(\frac{d}{dx}\right)^7\left(x^7e^{-x}\right) = \frac{e^x}{7!}\left(\frac{d}{dx}\right)^6\left(7x^6e^{-x} - x^7e^{-x}\right) \\ &= \frac{e^x}{7!}\left(\frac{d}{dx}\right)^5\left(42x^5e^{-x} - 7x^6e^{-x} - 7x^6e^{-x} + x^7e^{-x}\right) \\ &= \frac{e^x}{7!}\left(\frac{d}{dx}\right)^4\left(210x^4e^{-x} - 42x^5e^{-x} - 84x^5e^{-x} + 14x^6e^{-x} + 7x^6e^{-x} - x^7e^{-x}\right) \\ &= \frac{e^x}{7!}\left(\frac{d}{dx}\right)^3\Big[840x^3e^{-x} - (210+630)x^4e^{-x} \\ &\quad + (126+126)x^5e^{-x} - (21+7)x^6e^{-x} + x^7e^{-x}\Big] \\ &= \frac{e^x}{7!}\left(\frac{d}{dx}\right)^2\Big(2520x^2e^{-x} - (840+3360)x^3e^{-x} \\ &\quad + (840+1260)x^4e^{-x} - (252+168)x^5e^{-x} + (28+7)x^6e^{-x} - x^7e^{-x}\Big) \\ &= \frac{e^x}{7!}\left(\frac{d}{dx}\right)\Big[5040xe^{-x} - (2520+12600)x^2e^{-x} + (4200+8400)x^3e^{-x} \\ &\quad - (2100+2100)x^4e^{-x} + (420+210)x^5e^{-x} - (35+7)x^6e^{-x} + x^7e^{-x}\Big]. \end{aligned}$$

$$L_7(x) = \frac{e^x}{7!}\Big[5040e^{-x} - (5040 + 30240)xe^{-x} + (15120 + 37800)x^2e^{-x}$$
$$- (12600 + 8400 + 8400)x^3e^{-x} + (2100 + 2100 + 3150)x^4e^{-x}$$
$$- (630 + 252)x^5e^{-x} + (42 + 7)x^6e^{-x} - x^7e^{-x}\Big]$$
$$= \frac{1}{7!}\left(5040 - 35280x + 52920x^2 - 29400x^3 + 7350x^4 - 882x^5 + 49x^6 - x^7\right).$$

$$L_2^5 = -\frac{1}{7!}\left(\frac{d}{dx}\right)^5\left(-882x^5 + 49x^6 - x^7\right)$$
$$= -\frac{1}{7!}\left[-882(5\cdot 4\cdot 3\cdot 2) + 49(6\cdot 5\cdot 4\cdot 3\cdot 2)x - 7\cdot 6\cdot 5\cdot 4\cdot 3x^2\right]$$
$$= \frac{60}{5040}\left[(882\times 2) - (49\times 12)x + 42x^2\right] = 21 - 7x + \tfrac{1}{2}x^2.$$

$$v(\rho) = \boxed{21 - 14\rho + 2\rho^2.}$$

(c)

$$\text{Eq. 4.62} \Rightarrow v(\rho) = \sum_{j=0}^{\infty} c_j\rho^j. \quad \text{Eq. 4.76} \Rightarrow c_1 = \frac{2(3-5)}{(1)(6)}c_0 = -\frac{2}{3}c_0.$$

$$c_2 = \frac{2(4-5)}{(2)(7)}c_1 = -\frac{1}{7}c_1 = \frac{2}{21}c_0; \quad c_3 = \frac{2(5-5)}{(3)(8)}c_2 = 0.$$

$$v(\rho) = c_0 - \frac{2}{3}c_0\rho + \frac{2}{21}c_0\rho^2 = \boxed{\frac{c_0}{21}\left(21 - 14\rho + 2\rho^2\right).} \quad \checkmark$$

Problem 4.15

(a)

$$\psi = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}, \quad \text{so } \langle r^n\rangle = \frac{1}{\pi a^3}\int r^n e^{-2r/a}\left(r^2\sin\theta\,dr\,d\theta\,d\phi\right) = \frac{4\pi}{\pi a^3}\int_0^\infty r^{n+2}e^{-2r/a}dr.$$

$$\langle r\rangle = \frac{4}{a^3}\int_0^\infty r^3e^{-2r/a}dr = \frac{4}{a^3}3!\left(\frac{a}{2}\right)^4 = \boxed{\frac{3}{2}a;} \quad \langle r^2\rangle = \frac{4}{a^3}\int_0^\infty r^4e^{-2r/a}dr = \frac{4}{a^3}4!\left(\frac{a}{2}\right)^5 = \boxed{3a^2.}$$

(b)

$$\boxed{\langle x\rangle = 0;} \quad \langle x^2\rangle = \frac{1}{3}\langle r^2\rangle = \boxed{a^2.}$$

(c)

$$\psi_{211} = R_{21}Y_1^1 = -\frac{1}{\sqrt{\pi a}}\frac{1}{8a^2}re^{-r/2a}\sin\theta e^{i\phi} \quad \text{(Problem 4.13(b))}.$$

$$\begin{aligned}\langle x^2\rangle &= \frac{1}{\pi a}\frac{1}{(8a^2)^2}\int\left(r^2e^{-r/a}\sin^2\theta\right)\left(r^2\sin^2\theta\cos^2\phi\right)r^2\sin\theta\,dr\,d\theta\,d\phi\\ &= \frac{1}{64\pi a^5}\int_0^\infty r^6e^{-r/a}\,dr\int_0^\pi\sin^5\theta\,d\theta\int_0^{2\pi}\cos^2\phi\,d\phi\\ &= \frac{1}{64\pi a^5}\left(6!a^7\right)\left(2\frac{2\cdot 4}{1\cdot 3\cdot 5}\right)\left(\frac{1}{2}\cdot 2\pi\right) = \boxed{12a^2.}\end{aligned}$$

Problem 4.16

$\psi = \frac{1}{\sqrt{\pi a^3}}e^{-r/a};\quad P = |\psi|^2 4\pi r^2\,dr = \frac{4}{a^3}e^{-2r/a}r^2\,dr = p(r)\,dr;\quad p(r) = \frac{4}{a^3}r^2e^{-2r/a}.$

$\frac{dp}{dr} = \frac{4}{a^3}\left[2re^{-2r/a} + r^2\left(-\frac{2}{a}e^{-2r/a}\right)\right] = \frac{8r}{a^3}e^{-2r/a}\left(1-\frac{r}{a}\right) = 0 \Rightarrow \boxed{r = a.}$

Problem 4.17

$$[z,[H,z]] = z(Hz - zH) - (Hz - zH)z = 2zHz - z^2H - Hz^2,\ \Rightarrow\ zHz = \frac{1}{2}\left\{[z,[H,z]] + z^2H + Hz^2\right\},$$

$$[H,z] = \left[\frac{p^2}{2m}+V,z\right] = \frac{1}{2m}\left[(p_x^2+p_y^2+p_z^2),z\right] = \frac{1}{2m}[p_z^2,z] = \frac{1}{2m}\left(p_z[p_z,z]+[p_z,z]p_z\right) = -\frac{i\hbar}{m}p_z.$$

$$[z,[H,z]] = -\frac{i\hbar}{m}[z,p_z] = -\frac{i\hbar}{m}(i\hbar) = \frac{\hbar^2}{m},\quad \text{so}\quad zHz = \frac{1}{2}\left(\frac{\hbar^2}{m} + Hz^2 + z^2H\right).\quad \text{Using Problem 4.18(b)}:$$

$$\langle zHz\rangle = \frac{1}{2}\left(\frac{\hbar^2}{m} + \langle\psi|Hz^2|\psi\rangle + \langle\psi|z^2H|\psi\rangle\right) = \frac{\hbar^2}{2m} + E_1\langle z^2\rangle = \frac{\hbar^2}{2m} - \frac{\hbar^2}{2ma^2}a^2 = \boxed{0.}$$

Problem 4.18

(a) $\Psi(\mathbf{r},t) = \frac{1}{\sqrt{2}}\left(\psi_{2\,1\,1}e^{-iE_2t/\hbar} + \psi_{2\,1\,-1}e^{-iE_2t/\hbar}\right) = \frac{1}{\sqrt{2}}\left(\psi_{2\,1\,1}+\psi_{2\,1\,-1}\right)e^{-iE_2t/\hbar};\quad E_2 = \frac{E_1}{4} = -\frac{\hbar^2}{8ma^2}.$

From Problem 4.13(b):

$\psi_{2\,1\,1}+\psi_{2\,1\,-1} = -\frac{1}{\sqrt{\pi a}}\frac{1}{8a^2}re^{-r/2a}\sin\theta\left(e^{i\phi}-e^{-i\phi}\right) = -\frac{i}{\sqrt{\pi a}\,4a^2}re^{-r/2a}\sin\theta\,\sin\phi.$

$$\boxed{\Psi(\mathbf{r},t) = -\frac{i}{\sqrt{2\pi a}\,4a^2}re^{-r/2a}\sin\theta\,\sin\phi\,e^{-iE_2t/\hbar}.}$$

(b)

$$\begin{aligned}\langle V\rangle &= \int|\Psi|^2\left(-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}\right)d^3\mathbf{r} = \frac{1}{(2\pi a)(16a^4)}\left(-\frac{e^2}{4\pi\epsilon_0}\right)\int\left(r^2e^{-r/a}\sin^2\theta\,\sin^2\phi\right)\frac{1}{r}r^2\sin\theta\,dr\,d\theta\,d\phi\\ &= \frac{1}{32\pi a^5}\left(-\frac{\hbar^2}{ma}\right)\int_0^\infty r^3e^{-r/a}\,dr\int_0^\pi\sin^3\theta\,d\theta\int_0^{2\pi}\sin^2\phi\,d\phi = -\frac{\hbar^2}{32\pi ma^6}\left(3!a^4\right)\left(\frac{4}{3}\right)(\pi)\\ &= \boxed{-\frac{\hbar^2}{4ma^2} = \frac{1}{2}E_1 = \frac{1}{2}(-13.6\text{eV}) = -6.8\text{eV}}\quad \text{(independent of } t\text{).}\end{aligned}$$

Problem 4.19

$$\boxed{E_n(Z) = Z^2 E_n; \quad E_1(Z) = Z^2 E_1; \quad a(Z) = a/Z; \quad R(Z) = Z^2 R.}$$

Lyman lines range from $n_i = 2$ to $n_i = \infty$ (with $n_f = 1$); the wavelengths range from
$\frac{1}{\lambda_2} = R\left(1 - \frac{1}{4}\right) = \frac{3}{4}R \Rightarrow \lambda_2 = \frac{4}{3R}$ down to $\frac{1}{\lambda_1} = R\left(1 - \frac{1}{\infty}\right) = R \Rightarrow \lambda_1 = \frac{1}{R}$.

For $Z = 2$: $\lambda_1 = \frac{1}{4R} = \frac{1}{4(1.097 \times 10^7)} = \boxed{2.28 \times 10^{-8}\text{m}}$ to $\lambda_2 = \frac{1}{3R} = \boxed{3.04 \times 10^{-8}\text{ m},}$ $\boxed{\text{ultraviolet.}}$

For $Z = 3$: $\lambda_1 = \frac{1}{9R} = \boxed{1.01 \times 10^{-8}\text{ m}}$ to $\lambda_2 = \frac{4}{27R} = \boxed{1.35 \times 10^{-8}\text{ m},}$ also $\boxed{\text{ultraviolet.}}$

Problem 4.20

(a) $\boxed{V(r) = -G\frac{Mm}{r}.}$ So $\frac{e^2}{4\pi\epsilon_0} \to GMm$ translates hydrogen results to the gravitational analogs.

(b) Equation 4.72: $a = \left(\frac{4\pi\epsilon_0}{e^2}\right)\frac{\hbar^2}{m}$, so $\boxed{a_g = \frac{\hbar^2}{GMm^2}}$

$$= \frac{(1.0546 \times 10^{-34}\text{ Js})^2}{(6.6726 \times 10^{-11}\text{ m}^3/\text{kg}\cdot\text{s}^2)(1.9892 \times 10^{30}\text{ kg})(5.98 \times 10^{24}\text{kg})^2} = \boxed{2.34 \times 10^{-138}\text{ m.}}$$

(c) Equation 4.70 $\Rightarrow$ $\boxed{E_n = -\left[\frac{m}{2\hbar^2}(GMm)^2\right]\frac{1}{n^2}.}$

$$E_c = \frac{1}{2}mv^2 - G\frac{Mm}{r_o}. \quad \text{But } G\frac{Mm}{r_o^2} = \frac{mv^2}{r_o} \Rightarrow \frac{1}{2}mv^2 = \frac{GMm}{2r_o}, \text{ so}$$

$$E_c = -\frac{GMm}{2r_o} = -\left[\frac{m}{2\hbar^2}(GMm)^2\right]\frac{1}{n^2} \Rightarrow n^2 = \frac{GMm^2}{\hbar^2}r_o = \frac{r_o}{a_g} \Rightarrow \boxed{n = \sqrt{\frac{r_o}{a_g}}.}$$

$$r_o = \text{earth-sun distance} = 1.496 \times 10^{11}\text{ m} \Rightarrow n = \sqrt{\frac{1.496 \times 10^{11}}{2.34 \times 10^{-138}}} = \boxed{2.53 \times 10^{74}.}$$

(d)

$$\Delta E = -\left[\frac{G^2M^2m^3}{2\hbar^2}\right]\left[\frac{1}{(n+1)^2} - \frac{1}{n^2}\right]. \qquad \frac{1}{(n+1)^2} = \frac{1}{n^2(1+1/n)^2} \approx \frac{1}{n^2}\left(1 - \frac{2}{n}\right).$$

$$\text{So } \left[\frac{1}{(n+1)^2} - \frac{1}{n^2}\right] \approx \frac{1}{n^2}\left(1 - \frac{2}{n} - 1\right) = -\frac{2}{n^3}; \quad \Delta E = \frac{G^2M^2m^3}{\hbar^2 n^3}.$$

$$\Delta E = \frac{(6.67 \times 10^{-11})^2(1.99 \times 10^{30})^2(5.98 \times 10^{24})^3}{(1.055 \times 10^{-34})^2(2.53\times^{74})^3} = \boxed{2.09 \times 10^{-41}\text{J.}} \quad E_p = \Delta E = h\nu = \frac{hc}{\lambda}.$$

$$\lambda = (3 \times 10^8)(6.63 \times 10^{-34})/(2.09 \times 10^{-41}) = \boxed{9.52 \times 10^{15}\text{ m.}}$$

But 1 ly $= 9.46 \times 10^{15}$ m. Is it a coincidence that $\lambda \approx 1$ ly? No: From part (c), $n^2 = GMm^2 r_o/\hbar^2$, so

$$\lambda = \frac{ch}{\Delta E} = c2\pi\hbar\frac{\hbar^2 n^3}{G^2M^2m^3} = c\frac{2\pi\hbar^3}{G^2M^2m^3}\left(\frac{GMm^2 r_o}{\hbar^2}\right)^{3/2} = c\left(2\pi\sqrt{\frac{r_o^3}{GM}}\right).$$

But (from (c)) $v = \sqrt{GM/r_o} = 2\pi r_o/T$, where T is the period of the orbit (in this case one year), so $T = 2\pi\sqrt{r_o^3/GM}$, and hence $\boxed{\lambda = cT}$ (one light year). [Incidentally, the same goes for hydrogen: The wavelength of the photon emitted in a transition from a highly excited state to the next lower one is equal to the distance light would travel in one orbital period.]

Problem 4.21

$$\langle f|L_\pm g\rangle = \langle f|L_x g\rangle \pm i\langle f|L_y g\rangle = \langle L_x f|g\rangle \pm i\langle L_y f|g\rangle = \langle (L_x \mp iL_y)f|g\rangle = \langle L_\mp f|g\rangle, \text{ so } (L_\pm)^\dagger = L_\mp.$$

Now, using Eq. 4.112, in the form $L_\mp L_\pm = L^2 - L_z^2 \mp \hbar L_z$:

$$\begin{aligned}\langle f_\ell^m|L_\mp L_\pm f_\ell^m\rangle &= \langle f_\ell^m|(L^2 - L_z^2 \mp \hbar L_z)f_\ell^m\rangle = \langle f_\ell^m|\left[\hbar^2\ell(\ell+1) - \hbar^2 m^2 \mp \hbar^2 m\right] f_\ell^m\rangle \\ &= \hbar^2\left[\ell(\ell+1) - m(m\pm 1)\right]\langle f_\ell^m|f_\ell^m\rangle = \hbar^2\left[\ell(\ell+1) - m(m\pm 1)\right] = \langle L_\pm f_\ell^m|L_\pm f_\ell^m\rangle\end{aligned}$$

Upper signs:

$$\hbar^2[\ell(\ell+1) - m(m+1)] = \langle L_+ f_\ell^m|L_+ f_\ell^m\rangle = \langle A_\ell^m f_\ell^{m+1}|A_\ell^m f_\ell^{m+1}\rangle = |A_\ell^m|^2 \Rightarrow \boxed{A_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m+1)}.}$$

Lower signs:

$$\hbar^2[\ell(\ell+1) - m(m-1)] = \langle L_- f_\ell^m|L_- f_\ell^m\rangle = \langle B_\ell^m f_\ell^{m-1}|B_\ell^m f_\ell^{m-1}\rangle = |B_\ell^m|^2 \Rightarrow \boxed{B_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m-1)}.}$$

At the top of the ladder ($m = \ell$) we get $A_\ell^\ell = 0$, so there is no higher rung; at the bottom of the ladder ($m = -\ell$) we get $B_\ell^{-\ell} = 0$, so there is no lower rung.

Problem 4.22

(a)

$$[L_z, x] = [xp_y - yp_x, x] = [xp_y, x] - [yp_x, x] = 0 - y[p_x, x] = i\hbar y. \checkmark$$

$$[L_z, y] = [xp_y - yp_x, y] = [xp_y, y] - [yp_x, y] = x[p_y, y] - 0 = -i\hbar x. \checkmark$$

$$[L_z, z] = [xp_y - yp_x, z] = [xp_y, z] - [yp_x, z] = 0 - 0 = 0. \checkmark$$

$$[L_z, p_x] = [xp_y - yp_x, p_x] = [xp_y, p_x] - [yp_x, p_x] = p_y[x, p_x] - 0 = i\hbar p_y. \checkmark$$

$$[L_z, p_y] = [xp_y - yp_x, p_y] = [xp_y, p_y] - [yp_x, p_y] = 0 - p_x[y, p_y] = -i\hbar p_x. \checkmark$$

$$[L_z, p_z] = [xp_y - yp_x, p_z] = [xp_y, p_z] - [yp_x, p_z] = 0 - 0 = 0. \checkmark$$

(b)

$$\begin{aligned}[L_z, L_x] &= [L_z, yp_z - zp_y] = [L_z, yp_z] - [L_z, zp_y] = [L_z, y]p_z - [L_z, p_y]z \\ &= -i\hbar x p_z + i\hbar p_x z = i\hbar(zp_x - xp_z) = i\hbar L_y.\end{aligned}$$

(So, by cyclic permutation of the indices, $[L_x, L_y] = i\hbar L_z$.)

(c)

$$[L_z, r^2] = [L_z, x^2] + [L_z, y^2] + [L_z, z^2] = [L_z, x]x + x[L_z, x] + [L_z, y]y + y[L_z, y] + 0$$
$$= i\hbar yx + xi\hbar y + (-i\hbar x)y + y(-i\hbar x) = \boxed{0.}$$

$$[L_z, p^2] = [L_z, p_x^2] + [L_z, p_y^2] + [L_z, p_z^2] = [L_z, p_x]p_x + p_x[L_z, p_x] + [L_z, p_y]p_y + p_y[L_z, p_y] + 0$$
$$= i\hbar p_y p_x + p_x i\hbar p_y + (-i\hbar p_x)p_y + p_y(-i\hbar p_x) = \boxed{0.}$$

(d) It follows from (c) that all three components of **L** commute with r^2 and p^2. L_z also commutes with r, as we can show using a test function $f(r)$:

$$[L_z, r]f = -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}, r\right]f = -i\hbar\left(x\frac{\partial(rf)}{\partial y} - y\frac{\partial(rf)}{\partial x} - rx\frac{\partial f}{\partial y} + ry\frac{\partial f}{\partial x}\right) = -i\hbar\left(x\frac{\partial r}{\partial y} - y\frac{\partial r}{\partial x}\right)f.$$

But

$$\frac{\partial r}{\partial x} = \frac{\partial}{\partial x}\sqrt{x^2+y^2+z^2} = \frac{x}{r}, \quad \text{so} \quad \left(x\frac{\partial r}{\partial y} - y\frac{\partial r}{\partial x}\right) = 0,$$

and hence $[L_z, r] = 0$ (and the same goes for the other two components). So **L** commutes with $H = p^2/2m + V(r)$. QED

Problem 4.23

(a)

$$\text{Equation 3.73} \Rightarrow \frac{d\langle L_x\rangle}{dt} = \frac{i}{\hbar}\langle[H, L_x]\rangle. \quad [H, L_x] = \frac{1}{2m}[p^2, L_x] + [V, L_x].$$

The first term is zero (Problem 4.22(c)); the second would be too if V were a function only of $r = |\mathbf{r}|$, but in general

$$[H, L_x] = [V, yp_z - zp_y] = y[V, p_z] - z[V, p_y]. \quad \text{Now (Problem 3.14(c)):}$$

$$[V, p_z] = i\hbar\frac{\partial V}{\partial z} \text{ and } [V, p_y] = i\hbar\frac{\partial V}{\partial y}. \quad \text{So } [H, L_x] = yi\hbar\frac{\partial V}{\partial z} - zi\hbar\frac{\partial V}{\partial y} = i\hbar[\mathbf{r}\times(\nabla V)]_x.$$

Thus $\frac{d\langle L_x\rangle}{dt} = -\langle[\mathbf{r}\times(\nabla V)]_x\rangle$, and the same goes for the other two components:

$$\frac{d\langle\mathbf{L}\rangle}{dt} = \langle[\mathbf{r}\times(-\nabla V)]\rangle = \langle\mathbf{N}\rangle. \quad \text{QED}$$

(b)

$$\text{If } V(\mathbf{r}) = V(r), \text{ then } \nabla V = \frac{\partial V}{\partial r}\hat{r}, \text{ and } \mathbf{r}\times\hat{r} = 0, \text{ so } \frac{d\langle\mathbf{L}\rangle}{dt} = 0. \quad \text{QED}$$

Problem 4.24

(a)

$$\begin{aligned}
L_+L_-f &= -\hbar^2 e^{i\phi}\left(\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}\right)\left[e^{-i\phi}\left(\frac{\partial f}{\partial\theta}-i\cot\theta\frac{\partial f}{\partial\phi}\right)\right] \\
&= -\hbar^2 e^{i\phi}\left\{e^{-i\phi}\left[\frac{\partial^2 f}{\partial\theta^2}-i\left(-\csc^2\theta\frac{\partial f}{\partial\phi}+\cot\theta\frac{\partial^2 f}{\partial\theta\,\partial\phi}\right)\right]\right. \\
&\quad \left. +i\cot\theta\left[-ie^{-i\phi}\left(\frac{\partial f}{\partial\theta}-i\cot\theta\frac{\partial f}{\partial\phi}\right)+e^{-i\phi}\left(\frac{\partial^2 f}{\partial\phi\,\partial\theta}-i\cot\theta\frac{\partial^2 f}{\partial\phi^2}\right)\right]\right\} \\
&= -\hbar^2\left(\frac{\partial^2 f}{\partial\theta^2}+i\csc^2\theta\frac{\partial f}{\partial\phi}-i\cot\theta\frac{\partial^2 f}{\partial\theta\,\partial\phi}+\cot\theta\frac{\partial f}{\partial\theta}-i\cot^2\theta\frac{\partial f}{\partial\phi}+i\cot\theta\frac{\partial^2 f}{\partial\phi\,\partial\theta}+\cot^2\theta\frac{\partial^2 f}{\partial\phi^2}\right) \\
&= -\hbar^2\left[\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\cot^2\theta\frac{\partial^2}{\partial\phi^2}+i(\csc^2\theta-\cot^2\theta)\frac{\partial}{\partial\phi}\right]f, \quad \text{so} \\
L_+L_- &= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\cot^2\theta\frac{\partial^2}{\partial\phi^2}+i\frac{\partial}{\partial\phi}\right). \quad \text{QED}
\end{aligned}$$

(b) Equation 4.129 $\Rightarrow L_z = -i\hbar\dfrac{\partial}{\partial\phi}$, Eq. 4.112 $\Rightarrow L^2 = L_+L_- + L_z^2 - \hbar L_z$, so, using (a):

$$\begin{aligned}
L^2 &= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\cot^2\theta\frac{\partial^2}{\partial\phi^2}+i\frac{\partial}{\partial\phi}\right)-\hbar^2\frac{\partial^2}{\partial\phi^2}-\hbar\left(\frac{\hbar}{i}\right)\frac{\partial}{\partial\phi} \\
&= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+(\cot^2\theta+1)\frac{\partial^2}{\partial\phi^2}+i\frac{\partial}{\partial\phi}-i\frac{\partial}{\partial\phi}\right) = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) \\
&= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]. \quad \text{QED}
\end{aligned}$$

Problem 4.25

(a) $\boxed{L_+Y_\ell^\ell = 0}$ (top of the ladder).

(b)

$$L_zY_\ell^\ell = \hbar\ell Y_\ell^\ell \Rightarrow \frac{\hbar}{i}\frac{\partial}{\partial\phi}Y_\ell^\ell = \hbar\ell Y_\ell^\ell, \quad \text{so } \frac{\partial Y_\ell^\ell}{\partial\phi} = i\ell Y_\ell^\ell, \text{ and hence } Y_\ell^\ell = f(\theta)e^{i\ell\phi}.$$

[*Note:* $f(\theta)$ is the "constant" here—it's constant with respect to ϕ ... but still can depend on θ.]

$$L_+Y_\ell^\ell = 0 \Rightarrow \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}\right)\left[f(\theta)e^{i\ell\phi}\right] = 0, \quad \text{or } \frac{df}{d\theta}e^{i\ell\phi}+if\cot\theta\, i\ell\, e^{i\ell\phi} = 0, \text{ so}$$

$$\frac{df}{d\theta} = \ell\cot\theta f \Rightarrow \frac{df}{f} = \ell\cot\theta d\theta \Rightarrow \int\frac{df}{f} = \ell\int\frac{\cos\theta}{\sin\theta}\,d\theta \Rightarrow \ln f = \ell\ln(\sin\theta)+\textit{constant}.$$

$$\ln f = \ln(\sin^\ell\theta)+K \Rightarrow \ln\left(\frac{f}{\sin^\ell\theta}\right) = K \Rightarrow \frac{f}{\sin^\ell\theta} = \textit{constant} \Rightarrow f(\theta) = A\sin^\ell\theta.$$

$$\boxed{Y_\ell^\ell(\theta,\phi) = A(e^{i\phi}\sin\theta)^\ell.}$$

(c)

$$1 = A^2 \int \sin^{2\ell}\theta \sin\theta \, d\theta \, d\phi = 2\pi A^2 \int_0^\pi \sin^{(2\ell+1)}\theta \, d\theta = 2\pi A^2 \, 2\frac{(2\cdot 4\cdot 6\cdot\cdots\cdot(2\ell))}{1\cdot 3\cdot 5\cdot\cdots\cdot(2\ell+1)}$$

$$= 4\pi A^2 \frac{(2\cdot 4\cdot 6\cdot\cdots\cdot 2\ell)^2}{1\cdot 2\cdot 3\cdot 4\cdot 5\cdot\cdots\cdot(2\ell+1)} = 4\pi A^2 \frac{(2^\ell \ell!)^2}{(2\ell+1)!}, \quad \text{so} \quad \boxed{A = \frac{(-1)^\ell}{2^{\ell+1}\ell!}\sqrt{\frac{(2\ell+1)!}{\pi}}.}$$

The phase factor $(-1)^\ell$ is arbitrary, of course; I have chosen it to be consistent with Problem 4.7 and Equation 4.32.

Problem 4.26

$$L_+ Y_2^1 = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\left[-\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi}\right]$$

$$= -\sqrt{\frac{15}{8\pi}}\,\hbar e^{i\phi}\left[e^{i\phi}(\cos^2\theta - \sin^2\theta) + i\frac{\cos\theta}{\sin\theta}\sin\theta\cos\theta\, ie^{i\phi}\right]$$

$$= -\sqrt{\frac{15}{8\pi}}\hbar e^{2i\phi}\left(\cos^2\theta - \sin^2\theta - \cos^2\theta\right) = \sqrt{\frac{15}{8\pi}}\hbar\left(e^{i\phi}\sin\theta\right)^2$$

$$= \hbar\sqrt{2\cdot 3 - 1\cdot 2}\,Y_2^2 = 2\hbar Y_2^2. \qquad \therefore \boxed{Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\left(e^{i\phi}\sin\theta\right)^2.}$$

Problem 4.27

(a) Classically, $H = \frac{1}{2}I\omega^2$ and $L = I\omega$; so $H = \dfrac{L^2}{2I}$. But we know the eigenvalues of $L^2 : \hbar^2\ell(\ell+1)$. Or, since we usually label energies with n:

$$\boxed{E_n = \frac{\hbar^2 n(n+1)}{2I} \quad (n = 0, 1, 2, \ldots).}$$

(b) $\boxed{\psi_{nm}(\theta,\phi) = Y_n^m(\theta,\phi),}$ the ordinary spherical harmonics. The degeneracy of the nth energy level is the number of m-values for given n: $\boxed{2n+1.}$

(c) As in Equation 4.92, the frequency of an emitted photon, in a transition from n_i to n_f, is given by

$$E_\gamma = h\nu = 2\pi\hbar\nu = E_i - E_f = \frac{\hbar^2}{2I}\left[n_i(n_i+1) - n_f(n_j+1)\right].$$

The term in square brackets is the difference of two even numbers, so it is necessary even. It cannot be zero, but it does hit every positive even integer, since if $n_i = n_f + 1$, then $[n_i(n_i+1) - n_j(n_j+1)] = 2(n_f+1) = 2, 4, 6, \ldots$. Calling this number $2j$, $\boxed{\nu_j = \dfrac{\hbar j}{2\pi I}, \; j = 1, 2, 3, \ldots.}$

(d) $\Delta\nu = \frac{68-27}{11} = 3.73\,\text{cm}^{-1} = 3.73 \times (3 \times 10^{10})\text{Hz} = 11 \times 10^{10}/\text{s}.$

$m_{\text{C}} = 12\,\text{u} = 2.00 \times 10^{-26}\,\text{kg}, \quad m_{\text{O}} = 16\,\text{u} = (4/3)\,m_{\text{C}}; \quad \dfrac{m_1 m_2}{m_1 + m_2} = 1.14 \times 10^{-26}\,\text{kg}.$

$$I = \frac{m_1 m_2}{m_1 + m_2} a^2 = \frac{\hbar}{2\pi(\Delta\nu)} \Rightarrow a = \left(\frac{1.05 \times 10^{-34}}{2\pi(11 \times 10^{10})(1.14 \times 10^{-26})}\right)^{1/2} \text{m} = \boxed{1.15 \times 10^{-10}\,\text{m.}}$$

(The accepted value is 1.128×10^{-10}).

Problem 4.28

$$r_c = \frac{(1.6 \times 10^{-19})^2}{4\pi(8.85 \times 10^{-12})(9.11 \times 10^{-31})(3.0 \times 10^8)^2} = 2.81 \times 10^{-15}\ \text{m}.$$

$$L = \frac{1}{2}\hbar = I\omega = \left(\frac{2}{5}mr^2\right)\left(\frac{v}{r}\right) = \frac{2}{5}mrv \quad \text{so}$$

$$v = \frac{5\hbar}{4mr} = \frac{(5)(1.055 \times 10^{-34})}{(4)(9.11 \times 10^{-31})(2.81 \times 10^{-15})} = \boxed{5.15 \times 10^{10}\ \text{m/s.}}$$

Since the speed of light is 3×10^8 m/s, a point on the equator would be going more than 100 times the speed of light. $\boxed{\text{Nope :}}$ This doesn't look like a very realistic model for spin.

Problem 4.29

(a)

$$[\mathsf{S}_x, \mathsf{S}_y] = \mathsf{S}_x\mathsf{S}_y - \mathsf{S}_y\mathsf{S}_x = \frac{\hbar^2}{4}\left[\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} - \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right]$$
$$= \frac{\hbar^2}{4}\left[\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix} - \begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix}\right] = \frac{\hbar^2}{4}\begin{pmatrix}2i & 0\\ 0 & -2i\end{pmatrix} = i\hbar\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = i\hbar\mathsf{S}_z. \quad \checkmark$$

(b)

$$\sigma_x\sigma_x = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = 1 = \sigma_y\sigma_y = \sigma_z\sigma_z, \quad \text{so } \sigma_j\sigma_j = 1 \text{ for } j = x, y, \text{ or } z.$$

$$\sigma_x\sigma_y = \begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix} = i\sigma_z; \quad \sigma_y\sigma_z = \begin{pmatrix}0 & i\\ i & 0\end{pmatrix} = i\sigma_x; \quad \sigma_z\sigma_x = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} = i\sigma_y;$$

$$\sigma_y\sigma_x = \begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix} = -i\sigma_z; \quad \sigma_z\sigma_y = \begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix} = -i\sigma_x; \quad \sigma_x\sigma_z = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} = -i\sigma_y.$$

Equation 4.153 packages all this in a single formula. ✓

Problem 4.30

(a)

$$\chi^\dagger\chi = |A|^2(9+16) = 25|A|^2 = 1 \Rightarrow \boxed{A = 1/5.}$$

(b)

$$\langle S_x\rangle = \chi^\dagger \mathsf{S}_x\chi = \frac{1}{25}\frac{\hbar}{2}\begin{pmatrix}-3i & 4\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}3i\\ 4\end{pmatrix} = \frac{\hbar}{50}\begin{pmatrix}-3i & 4\end{pmatrix}\begin{pmatrix}4\\ 3i\end{pmatrix} = \frac{\hbar}{50}(-12i+12i) = \boxed{0.}$$

$$\langle S_y\rangle = \chi^\dagger \mathsf{S}_y\chi = \frac{1}{25}\frac{\hbar}{2}\begin{pmatrix}-3i & 4\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}3i\\ 4\end{pmatrix} = \frac{\hbar}{50}\begin{pmatrix}-3i & 4\end{pmatrix}\begin{pmatrix}-4i\\ -3\end{pmatrix} = \frac{\hbar}{50}(-12-12) = \boxed{-\frac{12}{25}\hbar.}$$

$$\langle S_z\rangle = \chi^\dagger \mathsf{S}_z\chi = \frac{1}{25}\frac{\hbar}{2}\begin{pmatrix}-3i & 4\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}3i\\ 4\end{pmatrix} = \frac{\hbar}{50}\begin{pmatrix}-3i & 4\end{pmatrix}\begin{pmatrix}3i\\ -4\end{pmatrix} = \frac{\hbar}{50}(9-16) = \boxed{-\frac{7}{50}\hbar.}$$

(c)

$$\langle S_x^2\rangle = \langle S_y^2\rangle = \langle S_z^2\rangle = \frac{\hbar^2}{4} \text{ (always, for spin 1/2), so } \sigma_{S_x}^2 = \langle S_x^2\rangle - \langle S_x\rangle^2 = \frac{\hbar^2}{4} - 0,\ \boxed{\sigma_{S_x} = \frac{\hbar}{2}.}$$

$$\sigma_{S_y}^2 = \langle S_y^2\rangle - \langle S_y\rangle^2 = \frac{\hbar^2}{4} - \left(\frac{12}{25}\right)^2\hbar^2 = \frac{\hbar^2}{2500}(625-576) = \frac{49}{2500}\hbar^2,\ \boxed{\sigma_{S_y} = \frac{7}{50}\hbar.}$$

$$\sigma_{S_z}^2 = \langle S_z^2\rangle - \langle S_z\rangle^2 = \frac{\hbar^2}{4} - \left(\frac{7}{50}\right)^2\hbar^2 = \frac{\hbar^2}{2500}(625-49) = \frac{576}{2500}\hbar^2,\ \boxed{\sigma_{S_z} = \frac{12}{25}\hbar.}$$

(d)

$$\sigma_{S_x}\sigma_{S_y} = \frac{\hbar}{2}\cdot\frac{7}{50}\hbar \overset{?}{\geq} \frac{\hbar}{2}|\langle S_z\rangle| = \frac{\hbar}{2}\cdot\frac{7}{50}\hbar \quad \text{(right } \textit{at} \text{ the uncertainty limit).} \checkmark$$

$$\sigma_{S_y}\sigma_{S_z} = \frac{7}{50}\hbar\cdot\frac{12}{25}\hbar \overset{?}{\geq} \frac{\hbar}{2}|\langle S_x\rangle| = 0 \quad \text{(trivial).} \checkmark$$

$$\sigma_{S_z}\sigma_{S_x} = \frac{12}{25}\hbar\cdot\frac{\hbar}{2} \overset{?}{\geq} \frac{\hbar}{2}|\langle S_y\rangle| = \frac{\hbar}{2}\cdot\frac{12}{25}\hbar \quad \text{(right } \textit{at} \text{ the uncertainty limit).} \checkmark$$

Problem 4.31

$$\langle S_x\rangle = \frac{\hbar}{2}\begin{pmatrix}a^* & b^*\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}a^* & b^*\end{pmatrix}\begin{pmatrix}b\\ a\end{pmatrix} = \boxed{\frac{\hbar}{2}(a^*b+b^*a)} = \hbar\,\mathrm{Re}(ab^*).$$

$$\langle S_y\rangle = \frac{\hbar}{2}\begin{pmatrix}a^* & b^*\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}a^* & b^*\end{pmatrix}\begin{pmatrix}-ib\\ ia\end{pmatrix}$$

$$= \frac{\hbar}{2}(-ia^*b+iab^*) = \boxed{\frac{\hbar}{2}i(ab^*-a^*b)} = -\hbar\,\mathrm{Im}(ab^*).$$

$$\langle S_z\rangle = \frac{\hbar}{2}\begin{pmatrix}a^* & b^*\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}a^* & b^*\end{pmatrix}\begin{pmatrix}a\\ -b\end{pmatrix} = \frac{\hbar}{2}(a^*a - b^*b) = \boxed{\frac{\hbar}{2}(|a|^2 - |b|^2).}$$

$$\mathsf{S}_x^2 = \frac{\hbar^2}{4}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{\hbar^2}{4}; \quad \mathsf{S}_y^2 = \frac{\hbar^2}{4}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \frac{\hbar^2}{4};$$

$$\mathsf{S}_z^2 = \frac{\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar^2}{4}; \quad \text{so } \boxed{\langle S_x^2\rangle = \langle S_y^2\rangle = \langle S_z^2\rangle = \frac{\hbar^2}{4}.}$$

$$\langle S_x^2\rangle + \langle S_y^2\rangle + \langle S_z^2\rangle = \frac{3}{4}\hbar^2 \stackrel{?}{=} s(s+1)\hbar^2 = \frac{1}{2}(\frac{1}{2}+1)\hbar^2 = \frac{3}{4}\hbar^2 = \langle S^2\rangle. \checkmark$$

Problem 4.32

(a)

$$S_y = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}; \quad \begin{vmatrix}-\lambda & -i\hbar/2\\ i\hbar/2 & -\lambda\end{vmatrix} = \lambda^2 - \frac{\hbar^2}{4} \Rightarrow \boxed{\lambda = \pm\frac{\hbar}{2}} \text{ (of course).}$$

$$\frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \pm\frac{\hbar}{2}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \Rightarrow -i\beta = \pm\alpha; \quad |\alpha|^2 + |\beta|^2 = 1 \Rightarrow |\alpha|^2 + |\alpha|^2 = 1 \Rightarrow \alpha = \frac{1}{\sqrt{2}}.$$

$$\boxed{\chi_+^{(y)} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix}; \quad \chi_-^{(y)} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix}.}$$

(b)

$$c_+ = \left(\chi_+^{(y)}\right)^\dagger \chi = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \frac{1}{\sqrt{2}}(a - ib); \quad \boxed{+\frac{\hbar}{2}, \text{ with probability } \frac{1}{2}|a-ib|^2.}$$

$$c_- = \left(\chi_-^{(y)}\right)^\dagger \chi = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & i\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \frac{1}{\sqrt{2}}(a + ib); \quad \boxed{-\frac{\hbar}{2}, \text{ with probability } \frac{1}{2}|a+ib|^2.}$$

$$\begin{aligned} P_+ + P_- &= \frac{1}{2}\left[(a^* + ib^*)(a - ib) + (a^* - ib^*)(a + ib)\right] \\ &= \frac{1}{2}\left[|a|^2 - ia^*b + iab^* + |b|^2 + |a|^2 + ia^*b - iab^* + |b|^2\right] = |a|^2 + |b|^2 = 1. \checkmark \end{aligned}$$

(c) $\boxed{\frac{\hbar^2}{4}, \text{ with probability 1.}}$

Problem 4.33

$$\begin{aligned}
\mathsf{S}_r &= \mathbf{S}\cdot\hat{r} = \mathsf{S}_x \sin\theta\cos\phi + \mathsf{S}_y \sin\theta\sin\phi + \mathsf{S}_z\cos\theta \\
&= \frac{\hbar}{2}\left[\begin{pmatrix} 0 & \sin\theta\cos\phi \\ \sin\theta\cos\phi & 0\end{pmatrix} + \begin{pmatrix} 0 & -i\sin\theta\sin\phi \\ i\sin\theta\sin\phi & 0\end{pmatrix} + \begin{pmatrix}\cos\theta & 0 \\ 0 & -\cos\theta\end{pmatrix}\right] \\
&= \frac{\hbar}{2}\begin{pmatrix}\cos\theta & \sin\theta(\cos\phi - i\sin\phi) \\ \sin\theta(\cos\phi + i\sin\phi) & -\cos\theta\end{pmatrix} = \boxed{\frac{\hbar}{2}\begin{pmatrix}\cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta\end{pmatrix}.}
\end{aligned}$$

$$\begin{vmatrix} (\frac{\hbar}{2}\cos\theta - \lambda) & \frac{\hbar}{2}e^{-i\phi}\sin\theta \\ \frac{\hbar}{2}e^{i\phi}\sin\theta & (-\frac{\hbar}{2}\cos\theta - \lambda)\end{vmatrix} = -\frac{\hbar^2}{4}\cos^2\theta + \lambda^2 - \frac{\hbar^2}{4}\sin^2\theta = 0 \;\Rightarrow$$

$$\lambda^2 = \frac{\hbar^2}{4}(\sin^2\theta + \cos^2\theta) = \frac{\hbar^2}{4} \Rightarrow \boxed{\lambda = \pm\frac{\hbar}{2}} \text{ (of course).}$$

$$\frac{\hbar}{2}\begin{pmatrix}\cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta\end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = \pm\frac{\hbar}{2}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} \Rightarrow \alpha\cos\theta + \beta e^{-i\phi}\sin\theta = \pm\alpha; \quad \beta = e^{i\phi}\frac{(\pm 1 - \cos\theta)}{\sin\theta}\alpha.$$

Upper sign: Use $1 - \cos\theta = 2\sin^2\frac{\theta}{2}$, $\sin\theta = 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}$. Then $\beta = e^{i\phi}\frac{\sin(\theta/2)}{\cos(\theta/2)}\alpha$. Normalizing:

$$1 = |\alpha|^2 + |\beta|^2 = |\alpha^2| + \frac{\sin^2(\theta/2)}{\cos^2(\theta/2)}|\alpha|^2 = |\alpha|^2\frac{1}{\cos^2(\theta/2)} \Rightarrow \alpha = \cos\frac{\theta}{2},\ \beta = e^{i\phi}\sin\frac{\theta}{2},\ \boxed{\chi_+^{(r)} = \begin{pmatrix}\cos(\theta/2) \\ e^{i\phi}\sin(\theta/2)\end{pmatrix}.}$$

Lower sign: Use $1 + \cos\theta = 2\cos^2\frac{\theta}{2}$, $\beta = -e^{i\phi}\frac{\cos(\theta/2)}{\sin(\theta/2)}\alpha$; $1 = |\alpha|^2 + \frac{\cos^2(\theta/2)}{\sin^2(\theta/2)}|\alpha|^2 = |\alpha|^2\frac{1}{\sin^2(\theta/2)}$.

Pick $\alpha = e^{-i\phi}\sin(\theta/2)$; then $\beta = -\cos(\theta/2)$, and $\boxed{\chi_-^{(r)} = \begin{pmatrix}e^{-i\phi}\sin(\theta/2) \\ -\cos(\theta/2)\end{pmatrix}.}$

Problem 4.34

There are three states: $\chi_+ = \begin{pmatrix}1\\0\\0\end{pmatrix}$, $\chi_0 = \begin{pmatrix}0\\1\\0\end{pmatrix}$, $\chi_- = \begin{pmatrix}0\\0\\1\end{pmatrix}$.

$\mathsf{S}_z\chi_+ = \hbar\chi_+,\ \mathsf{S}_z\chi_0 = 0,\ \mathsf{S}_z\chi_- = -\hbar\chi_-, \quad \Rightarrow \boxed{\mathsf{S}_z = \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}.}$ From Eq. 4.136:

$$\left.\begin{matrix}\mathsf{S}_+\chi_+ = 0, & \mathsf{S}_+\chi_0 = \hbar\sqrt{2}\chi_+,\ \mathsf{S}_+\chi_- = \hbar\sqrt{2}\chi_0 \\ \mathsf{S}_-\chi_+ = \hbar\sqrt{2}\chi_0, & \mathsf{S}_-\chi_0 = \hbar\sqrt{2}\chi_-,\ \mathsf{S}_-\chi_- = 0\end{matrix}\right\} \Rightarrow \mathsf{S}_+ = \sqrt{2}\hbar\begin{pmatrix}0 & 1 & 0\\ 0 & 0 & 1\\ 0 & 0 & 0\end{pmatrix},\ \mathsf{S}_- = \sqrt{2}\hbar\begin{pmatrix}0 & 0 & 0\\ 1 & 0 & 0\\ 0 & 1 & 0\end{pmatrix}.$$

$$\mathsf{S}_x = \frac{1}{2}(\mathsf{S}_+ + \mathsf{S}_-) = \boxed{\frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}}, \quad \mathsf{S}_y = \frac{1}{2i}(\mathsf{S}_+ - \mathsf{S}_-) = \boxed{\frac{i\hbar}{\sqrt{2}}\begin{pmatrix}0 & -1 & 0\\ 1 & 0 & -1\\ 0 & 1 & 0\end{pmatrix}}.$$

Problem 4.35

(a) Using Eqs. 4.151 and 4.163:

$$c_+^{(x)} = \chi_+^{(x)\dagger}\chi = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}\cos\frac{\alpha}{2}e^{i\gamma B_0 t/2}\\ \sin\frac{\alpha}{2}e^{-i\gamma B_0 t/2}\end{pmatrix} = \frac{1}{\sqrt{2}}\left[\cos\frac{\alpha}{2}e^{i\gamma B_0 t/2} + \sin\frac{\alpha}{2}e^{-i\gamma B_0 t/2}\right].$$

$$\begin{aligned}P_+^{(x)}(t) = |c_+^{(x)}|^2 &= \frac{1}{2}\left[\cos\frac{\alpha}{2}e^{-i\gamma B_0 t/2} + \sin\frac{\alpha}{2}e^{i\gamma B_0 t/2}\right]\left[\cos\frac{\alpha}{2}e^{i\gamma B_0 t/2} + \sin\frac{\alpha}{2}e^{-i\gamma B_0 t/2}\right]\\ &= \frac{1}{2}\left[\cos^2\frac{\alpha}{2} + \sin^2\frac{\alpha}{2} + \sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\left(e^{i\gamma B_0 t} + e^{-i\gamma B_0 t}\right)\right]\\ &= \frac{1}{2}\left[1 + 2\sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\cos(\gamma B_0 t)\right] = \boxed{\frac{1}{2}\left[1 + \sin\alpha\cos(\gamma B_0 t)\right].}\end{aligned}$$

(b) From Problem 4.32(a): $\chi_+^{(y)} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix}$.

$$c_+^{(y)} = \chi_+^{(y)\dagger}\chi = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\end{pmatrix}\begin{pmatrix}\cos\frac{\alpha}{2}e^{i\gamma B_0 t/2}\\ \sin\frac{\alpha}{2}e^{-i\gamma B_0 t/2}\end{pmatrix} = \frac{1}{\sqrt{2}}\left[\cos\frac{\alpha}{2}e^{i\gamma B_0 t/2} - i\sin\frac{\alpha}{2}e^{-i\gamma B_0 t/2}\right];$$

$$\begin{aligned}P_+^{(y)}(t) = |c_+^{(y)}|^2 &= \frac{1}{2}\left[\cos\frac{\alpha}{2}e^{-i\gamma B_0 t/2} + i\sin\frac{\alpha}{2}e^{i\gamma B_0 t/2}\right]\left[\cos\frac{\alpha}{2}e^{i\gamma B_0 t/2} - i\sin\frac{\alpha}{2}e^{-i\gamma B_0 t/2}\right]\\ &= \frac{1}{2}\left[\cos^2\frac{\alpha}{2} + \sin^2\frac{\alpha}{2} + i\sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\left(e^{i\gamma B_0 t} - e^{-i\gamma B_0 t}\right)\right]\\ &= \frac{1}{2}\left[1 - 2\sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\sin(\gamma B_0 t)\right] = \boxed{\frac{1}{2}\left[1 - \sin\alpha\sin(\gamma B_0 t)\right].}\end{aligned}$$

(c)

$$\chi_+^{(z)} = \begin{pmatrix}1\\ 0\end{pmatrix};\quad c_+^{(z)} = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}\cos\frac{\alpha}{2}e^{i\gamma B_0 t/2}\\ \sin\frac{\alpha}{2}e^{-i\gamma B_0 t/2}\end{pmatrix} = \cos\frac{\alpha}{2}e^{i\gamma B_0 t/2};\quad P_+^{(z)}(t) = |c_+^{(z)}|^2 = \boxed{\cos^2\frac{\alpha}{2}.}$$

Problem 4.36

(a)

$$\mathsf{H} = -\gamma\mathbf{B}\cdot\mathsf{S} = -\gamma B_0\cos\omega t\;\mathsf{S}_z = \boxed{-\frac{\gamma B_0\hbar}{2}\cos\omega t\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.}$$

(b)

$$\chi(t) = \begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix},\ \text{ with } \alpha(0) = \beta(0) = \frac{1}{\sqrt{2}}.$$

$$i\hbar\frac{\partial\chi}{\partial t} = i\hbar\begin{pmatrix}\dot\alpha\\ \dot\beta\end{pmatrix} = \mathsf{H}\chi = -\frac{\gamma B_0\hbar}{2}\cos\omega t\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = -\frac{\gamma B_0\hbar}{2}\cos\omega t\begin{pmatrix}\alpha\\ -\beta\end{pmatrix}.$$

$$\dot{\alpha} = i\left(\frac{\gamma B_0}{2}\right)\cos\omega t\,\alpha \Rightarrow \frac{d\alpha}{\alpha} = i\left(\frac{\gamma B_0}{2}\right)\cos\omega t\,dt \Rightarrow \ln\alpha = \frac{i\gamma B_0}{2}\frac{\sin\omega t}{\omega} + constant.$$

$$\alpha(t) = Ae^{i(\gamma B_0/2\omega)\sin\omega t};\quad \alpha(0) = A = \frac{1}{\sqrt{2}},\quad \text{so } \alpha(t) = \frac{1}{\sqrt{2}}e^{i(\gamma B_0/2\omega)\sin\omega t}.$$

$$\dot{\beta} = -i\left(\frac{\gamma B_0}{2}\right)\cos\omega t\,\beta \Rightarrow \beta(t) = \frac{1}{\sqrt{2}}e^{-i(\gamma B_0/2\omega)\sin\omega t}.\quad \boxed{\chi(t) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i(\gamma B_0/2\omega)\sin\omega t} \\ e^{-i(\gamma B_0/2\omega)\sin\omega t}\end{pmatrix}.}$$

(c)

$$c_-^{(x)} = \chi_-^{(x)\dagger}\chi = \frac{1}{2}(1\ -1)\begin{pmatrix} e^{i(\gamma B_0/2\omega)\sin\omega t} \\ e^{-i(\gamma B_0/2\omega)\sin\omega t}\end{pmatrix} = \frac{1}{2}\left[e^{i(\gamma B_0/2\omega)\sin\omega t} - e^{-i(\gamma B_0/2\omega)\sin\omega t}\right]$$

$$= i\sin\left[\frac{\gamma B_0}{2\omega}\sin\omega t\right].\quad P_-^{(x)}(t) = |c_-^{(x)}|^2 = \boxed{\sin^2\left[\frac{\gamma B_0}{2\omega}\sin\omega t\right].}$$

(d) The argument of $\sin^2$ must reach $\pi/2$ (so $P = 1$) $\Rightarrow \dfrac{\gamma B_0}{2\omega} = \dfrac{\pi}{2}$, or $\boxed{B_0 = \dfrac{\pi\omega}{\gamma}.}$

Problem 4.37

(a)

$$S_-|1\ 0\rangle = (S_-^{(1)} + S_-^{(2)})\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) = \frac{1}{\sqrt{2}}\left[(S_-\uparrow)\downarrow + (S_-\downarrow)\uparrow + \uparrow(S_-\downarrow) + \downarrow(S_-\uparrow)\right].$$

But $S_-\uparrow = \hbar\downarrow$, $S_-\downarrow = 0$ (line above Eq. 4.146), so $S_-|10\rangle = \dfrac{1}{\sqrt{2}}\left[\hbar\downarrow\downarrow + 0 + 0 + \hbar\downarrow\downarrow\right] = \sqrt{2}\hbar\downarrow\downarrow = \sqrt{2}\hbar|1 -1\rangle.$ ✓

(b)

$$S_\pm|0\ 0\rangle = (S_\pm^{(1)} + S_\pm^{(2)})\frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) = \frac{1}{\sqrt{2}}\left[(S_\pm\uparrow)\downarrow - (S_\pm\downarrow)\uparrow + \uparrow(S_\pm\downarrow) - \downarrow(S_\pm\uparrow)\right].$$

$$S_+|0\ 0\rangle = \frac{1}{\sqrt{2}}(0 - \hbar\uparrow\uparrow + \hbar\uparrow\uparrow - 0) = 0;\ S_-|0\ 0\rangle = \frac{1}{\sqrt{2}}(\hbar\downarrow\downarrow - 0 + 0 - \hbar\downarrow\downarrow) = 0.\ ✓$$

(c)

$$\begin{aligned}
S^2|1\ 1\rangle &= \left[(S^{(1)})^2 + (S^{(2)})^2 + 2\mathbf{S}^{(1)}\cdot\mathbf{S}^{(2)}\right]\uparrow\uparrow \\
&= (S^2\uparrow)\uparrow + \uparrow(S^2\uparrow) + 2\left[(S_x\uparrow)(S_x\uparrow) + (S_y\uparrow)(S_y\uparrow) + (S_z\uparrow)(S_z\uparrow)\right] \\
&= \frac{3}{4}\hbar^2\uparrow\uparrow + \frac{3}{4}\hbar^2\uparrow\uparrow + 2\left[\frac{\hbar}{2}\downarrow\frac{\hbar}{2}\downarrow + \frac{i\hbar}{2}\downarrow\frac{i\hbar}{2}\downarrow + \frac{\hbar}{2}\uparrow\frac{\hbar}{2}\uparrow\right] \\
&= \frac{3}{2}\hbar^2\uparrow\uparrow + 2\left(\frac{\hbar^2}{4}\uparrow\uparrow\right) = 2\hbar^2\uparrow\uparrow = 2\hbar^2|1\ 1\rangle = (1)(1+1)\hbar^2|1\ 1\rangle,\ \text{as it } \textit{should} \text{ be.}
\end{aligned}$$

$$\begin{aligned}
S^2|1\ \ -1\rangle &= \left[(S^{(1)})^2 + (S^{(2)})^2 + 2\mathbf{S}^{(1)}\cdot\mathbf{S}^{(2)}\right]\downarrow\downarrow \\
&= \frac{3\hbar^2}{4}\downarrow\downarrow + \frac{3\hbar^2}{4}\downarrow\downarrow + 2\left[(S_x\downarrow)(S_x\downarrow) + (S_y\downarrow)(S_y\downarrow) + (S_z\downarrow)(S_z\downarrow)\right] \\
&= \frac{3}{2}\hbar^2\downarrow\downarrow + 2\left[\left(\frac{\hbar}{2}\uparrow\right)\left(\frac{\hbar}{2}\uparrow\right) + \left(-\frac{i\hbar}{2}\uparrow\right)\left(-\frac{i\hbar}{2}\uparrow\right) + \left(-\frac{\hbar}{2}\downarrow\right)\left(-\frac{\hbar}{2}\downarrow\right)\right] \\
&= \frac{3}{2}\hbar^2\downarrow\downarrow + 2\frac{\hbar^2}{4}\downarrow\downarrow = 2\hbar^2\downarrow\downarrow = 2\hbar^2|1\ \ -1\rangle.\ \checkmark
\end{aligned}$$

Problem 4.38

(a) 1/2 and 1/2 gives 1 or zero; 1/2 and 1 gives 3/2 or 1/2; 1/2 and 0 gives 1/2 only. So baryons can have $\boxed{\text{spin } 3/2 \text{ or spin } 1/2}$ (and the latter can be acheived in two distinct ways). [Incidentally, the lightest baryons *do* carry spin 1/2 (proton, neutron, etc.) or 3/2 (Δ, Ω^-, etc.); heavier baryons can have higher total spin, but this is because the quarks have orbital angular momentum as well.]

(b) 1/2 and 1/2 gives $\boxed{\text{spin 1 or spin 0.}}$ [Again, these *are* the observed spins for the lightest mesons: π's and K's have spin 0, ρ's and ω's have spin 1.]

Problem 4.39

Reading down the vertical columns of the $(1/2 \times 1/2)$ table:

$$\begin{aligned}
|11\rangle &= |\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle = |\uparrow\uparrow\rangle \quad \checkmark \\
|10\rangle &= \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{-1}{2}\rangle + \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\tfrac{-1}{2}\tfrac{1}{2}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \quad \checkmark \\
|1-1\rangle &= |\tfrac{1}{2}\tfrac{1}{2}\tfrac{-1}{2}\tfrac{-1}{2}\rangle = |\downarrow\downarrow\rangle \quad \checkmark \\
|00\rangle &= \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{-1}{2}\rangle - \frac{1}{\sqrt{2}}|\tfrac{1}{2}\tfrac{1}{2}\tfrac{-1}{2}\tfrac{1}{2}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \quad \checkmark
\end{aligned}$$

Problem 4.40

(a) From the 2×1 Clebsch-Gordan table we get

$$|3\ 1\rangle = \sqrt{\frac{1}{15}}\,|2\ 2\rangle|1\ \ -1\rangle + \sqrt{\frac{8}{15}}\,|2\ 1\rangle|1\ 0\rangle + \sqrt{\frac{6}{15}}\,|2\ 0\rangle|1\ 1\rangle,$$

so you might get $\boxed{2\hbar \text{ (probability } 1/15),\ \hbar \text{ (probability } 8/15),\ \text{or } 0 \text{ (probability } 6/15).}$

(b) From the $1\times\frac{1}{2}$ table: $|1\ 0\rangle|\frac{1}{2}\ -\frac{1}{2}\rangle = \sqrt{\frac{2}{3}}\,|\frac{3}{2}\ -\frac{1}{2}\rangle + \sqrt{\frac{1}{3}}\,|\frac{1}{2}\ -\frac{1}{2}\rangle$. So the total is 3/2 or 1/2, with $l(l+1)\hbar^2 =$ $15/4\hbar^2$ and $3/4\hbar^2$, respectively. Thus you get $\boxed{\frac{15}{4}\hbar^2 \text{ (probability } 2/3),\ \text{or } \frac{3}{4}\hbar^2 \text{ (probability } 1/3).}$

Problem 4.41

Using Eq. 4.177: $[S^2, S_z^{(1)}] = [S^{(1)^2}, S_z^{(1)}] + [S^{(2)^2}, S_z^{(1)}] + 2[\mathbf{S}^{(1)} \cdot \mathbf{S}^{(2)}, S_z^{(1)}]$. But $[S^2, S_z] = 0$ (Eq. 4.102), and anything with superscript (2) commutes with anything with superscript (1). So

$$\begin{aligned}
[S^2, S_z^{(1)}] &= 2\left\{S_x^{(2)}[S_x^{(1)}, S_z^{(1)}] + S_y^{(2)}[S_y^{(1)}, S_z^{(1)}] + S_z^{(2)}[S_z^{(1)}, S_z^{(1)}]\right\} \\
&= 2\left\{-i\hbar S_y^{(1)} S_x^{(2)} + i\hbar S_x^{(1)} S_y^{(2)}\right\} = 2i\hbar(\mathbf{S}^{(1)} \times \mathbf{S}^{(2)})z.
\end{aligned}$$

$\boxed{[S^2, S_z^{(1)}] = 2i\hbar(S_x^{(1)} S_y^{(2)} - S_y^{(1)} S_x^{(2)}),}$ and $[S^2, \mathbf{S}^{(1)}] = 2i\hbar(\mathbf{S}^{(1)} \times \mathbf{S}^{(2)})$. Note that $[S^2, \mathbf{S}^{(2)}] = 2i\hbar(\mathbf{S}^{(2)} \times \mathbf{S}^{(1)}) = -2i\hbar(\mathbf{S}^{(1)} \times \mathbf{S}^{(2)})$, so $[S^2, (\mathbf{S}^{(1)} + \mathbf{S}^{(2)})] = 0$.]

Problem 4.42

(a)

Start with Eq. 3.73: $\dfrac{d\langle \mathbf{r}\rangle}{dt} = \dfrac{i}{\hbar}\langle [H, \mathbf{r}]\rangle$.

$H = \dfrac{1}{2m}(\mathbf{p} - q\mathbf{A}) \cdot (\mathbf{p} - q\mathbf{A}) + q\varphi = \dfrac{1}{2m}\left[p^2 - q(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + q^2 A^2\right] + q\varphi.$

$[H, x] = \dfrac{1}{2m}[p^2, x] - \dfrac{q}{2m}[(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}), x].$

$[p^2, x] = [(p_x^2 + p_y^2 + p_z^2), x] = [p_x^2, x] = p_x[p_x, x] + [p_x, x]p_x = p_x(-i\hbar) + (-i\hbar)p_x = -2i\hbar p_x.$

$[\mathbf{p} \cdot \mathbf{A}, x] = [(p_x A_x + p_y A_y + p_z A_z), x] = [p_x A_x, x] = p_x[A_x, x] + [p_x, x]A_x = -i\hbar A_x.$

$[\mathbf{A} \cdot \mathbf{p}, x] = [(A_x p_x + A_y p_y + A_z p_z), x] = [A_x p_x, x] = A_x[p_x, x] + [A_x, x]p_x = -i\hbar A_x.$

$[H, x] = \dfrac{1}{2m}(-2i\hbar p_x) - \dfrac{q}{2m}(-2i\hbar A_x) = -\dfrac{i\hbar}{m}(p_x - qA_x);\quad [H, \mathbf{r}] = -\dfrac{i\hbar}{m}(\mathbf{p} - q\mathbf{A}).$

$\dfrac{d\langle \mathbf{r}\rangle}{dt} = \dfrac{1}{m}\langle(\mathbf{p} - q\mathbf{A})\rangle.$ QED

(b)

We define the operator $\mathbf{v} \equiv \dfrac{1}{m}(\mathbf{p} - q\mathbf{A});\quad \dfrac{d\langle \mathbf{v}\rangle}{dt} = \dfrac{i}{\hbar}\langle [H, \mathbf{v}]\rangle + \langle \dfrac{\partial \mathbf{v}}{\partial t}\rangle;\quad \dfrac{\partial \mathbf{v}}{\partial t} = -\dfrac{q}{m}\dfrac{\partial \mathbf{A}}{\partial t}.$

$H = \dfrac{1}{2}mv^2 + q\varphi \Rightarrow [H, \mathbf{v}] = \dfrac{m}{2}[v^2, \mathbf{v}] + q[\varphi, \mathbf{v}];\quad [\varphi, \mathbf{v}] = \dfrac{1}{m}[\varphi, \mathbf{p}].$

$[\varphi, p_x] = i\hbar\dfrac{\partial\varphi}{\partial x}$ (Eq. 3.66), so $[\varphi, \mathbf{p}] = i\hbar\nabla\varphi$, and $[\varphi, \mathbf{v}] = \dfrac{i\hbar}{m}\nabla\varphi.$

$[v^2, v_x] = [(v_x^2 + v_y^2 + v_z^2), v_x] = [v_y^2, v_x] + [v_z^2, v_x] = v_y[v_y, v_x] + [v_y, v_x]v_y + v_z[v_z, v_x] + [v_z, v_x]v_z.$

$$\begin{aligned}
[v_y, v_x] &= \frac{1}{m^2}[(p_y - qA_y), (p_x - qA_x)] = -\frac{q}{m^2}\left([A_y, p_x] + [p_y, A_x]\right) \\
&= -\frac{q}{m^2}\left(i\hbar\frac{\partial A_y}{\partial x} - i\hbar\frac{\partial A_x}{\partial y}\right) = -\frac{i\hbar q}{m^2}\left(\nabla \times \mathbf{A}\right)_z = -\frac{i\hbar q}{m^2}B_z.
\end{aligned}$$

$$\begin{aligned}
[v_z, v_x] &= \frac{1}{m^2}[(p_z - qA_z), (p_x - qA_x)] = -\frac{q}{m^2}\left([A_z, p_x] + [p_z, A_x]\right) \\
&= -\frac{q}{m^2}\left(i\hbar\frac{\partial A_z}{\partial x} - i\hbar\frac{\partial A_x}{\partial z}\right) = \frac{i\hbar q}{m^2}\left(\nabla \times \mathbf{A}\right)_y = \frac{i\hbar q}{m^2}B_y.
\end{aligned}$$

$$\therefore [v^2, v_x] = \frac{i\hbar q}{m^2}\left(-v_y B_z - B_z v_y + v_z B_y + B_y v_z\right) = \frac{i\hbar q}{m^2}\left[-(\mathbf{v}\times\mathbf{B})_x + (\mathbf{B}\times\mathbf{v})_x\right].$$

$[v^2, \mathbf{v}] = \dfrac{i\hbar q}{m^2}\left[(\mathbf{B}\times\mathbf{v}) - (\mathbf{v}\times\mathbf{B})\right]$. Putting all this together:

$$\frac{d\langle\mathbf{v}\rangle}{dt} = \frac{i}{\hbar}\left\langle\left[\frac{m}{2}\frac{i\hbar q}{m^2}\left(\mathbf{B}\times\mathbf{v} - \mathbf{v}\times\mathbf{B}\right) + \frac{qi\hbar}{m}\nabla\varphi\right]\right\rangle - \frac{q}{m}\langle\frac{\partial\mathbf{A}}{\partial t}\rangle.$$

$[\bigstar]$ $\quad m\dfrac{d\langle\mathbf{v}\rangle}{dt} = \dfrac{q}{2}\langle(\mathbf{v}\times\mathbf{B}) - (\mathbf{B}\times\mathbf{v})\rangle + q\left\langle -\nabla\varphi - \dfrac{\partial\mathbf{A}}{dt}\right\rangle = \dfrac{q}{2}\langle(\mathbf{v}\times\mathbf{B} - \mathbf{B}\times\mathbf{v})\rangle + q\langle\mathbf{E}\rangle$. Or, since

$$\mathbf{v}\times\mathbf{B} - \mathbf{B}\times\mathbf{v} = \frac{1}{m}\left[(\mathbf{p}-q\mathbf{A})\times\mathbf{B} - \mathbf{B}\times(\mathbf{p}-q\mathbf{A})\right] = \frac{1}{m}\left[\mathbf{p}\times\mathbf{B} - \mathbf{B}\times\mathbf{p}\right] - \frac{q}{m}\left[\mathbf{A}\times\mathbf{B} - \mathbf{B}\times\mathbf{A}\right].$$

$$m\frac{d\langle\mathbf{v}\rangle}{dt} = q\langle\mathbf{E}\rangle + \frac{q}{2m}\langle\mathbf{p}\times\mathbf{B} - \mathbf{B}\times\mathbf{p}\rangle - \frac{q^2}{m}\langle\mathbf{A}\times\mathbf{B}\rangle. \quad \text{QED}$$

(c) Go back to Eq. $\bigstar$, and use $\langle\mathbf{E}\rangle = \mathbf{E}$, $\langle\mathbf{v}\times\mathbf{B}\rangle = \langle\mathbf{v}\rangle\times\mathbf{B}$; $\langle\mathbf{B}\times\mathbf{v}\rangle = \mathbf{B}\times\langle\mathbf{v}\rangle = -\langle\mathbf{v}\rangle\times\mathbf{B}$. Then

$$m\frac{d\langle\mathbf{v}\rangle}{dt} = q\langle\mathbf{v}\rangle\times\mathbf{B} + q\mathbf{E}. \quad \text{QED}$$

Problem 4.43

(a)

$$\mathbf{E} = -\boldsymbol{\nabla}\varphi = \boxed{-2Kz\hat{k}.} \qquad \mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \partial/\partial x & \partial/\partial y & \partial/\partial z \\ -B_0 y/2 & B_0 x/2 & 0 \end{vmatrix} = \boxed{B_0\hat{k}.}$$

(b) For time-independent potentials Eq. 4.191 separates in the usual way:

$$\frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right)\cdot\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right)\psi + q\varphi\psi = E\psi, \quad \text{or}$$

$-\dfrac{\hbar^2}{2m}\nabla^2\psi + \dfrac{iq\hbar}{2m}\left[\boldsymbol{\nabla}\cdot(\mathbf{A}\psi) + \mathbf{A}\cdot(\boldsymbol{\nabla}\psi)\right] + \dfrac{q^2}{2m}A^2\psi + q\varphi\psi = E\psi$. But $\boldsymbol{\nabla}\cdot(\mathbf{A}\psi) = (\boldsymbol{\nabla}\cdot\mathbf{A})\psi + \mathbf{A}\cdot(\boldsymbol{\nabla}\psi)$, so

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{iq\hbar}{2m}\left[2\mathbf{A}\cdot(\boldsymbol{\nabla}\psi) + (\boldsymbol{\nabla}\cdot\mathbf{A})\psi\right] + \left(\frac{q^2}{2m}A^2 + q\varphi\right)\psi = E\psi.}$$

This is the time-independent Schrödinger equation for electrodynamics. In the present case

$$\boldsymbol{\nabla}\cdot\mathbf{A} = 0, \quad \mathbf{A}\cdot(\boldsymbol{\nabla}\psi) = \frac{B_0}{2}\left(x\frac{\partial\psi}{\partial y} - y\frac{\partial\psi}{\partial x}\right), \quad A^2 = \frac{B_0^2}{4}\left(x^2+y^2\right), \quad \varphi = Kz^2.$$

But $\quad L_z = -i\hbar\left(x\dfrac{\partial}{\partial y} - y\dfrac{\partial}{\partial x}\right)$, $\quad$ so $\quad -\dfrac{\hbar^2}{2m}\nabla^2\psi - \dfrac{qB_0}{2m}L_z\psi + \left[\dfrac{q^2B_0^2}{8m}\left(x^2+y^2\right) + qKz^2\right]\psi = E\psi.$

Since L_z commutes with H, we may as well pick simultaneous eigenfunctions of both: $L_z\psi = \bar{m}\hbar\psi$, where $\bar{m} = 0, \pm1, \pm2, \ldots$ (with the overbar to distinguish the magnetic quantum number from the mass). Then

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{(qB_0)^2}{8m}\left(x^2+y^2\right) + qKz^2\right]\psi = \left(E + \frac{qB_0\hbar}{2m}\bar{m}\right)\psi.$$

Now let $\omega_1 \equiv qB_0/m, \quad \omega_2 \equiv \sqrt{2Kq/m}$, and use cylindrical coordinates (r, ϕ, z) (you can also do it in Cartesian coordinates):

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2}+\frac{\partial^2\psi}{\partial z^2}\right]+\left[\frac{1}{8}m\omega_1^2\left(x^2+y^2\right)+\frac{1}{2}m\omega_2^2z^2\right]\psi=\left(E+\frac{1}{2}\bar{m}\hbar\omega_1\right)\psi.$$

But $L_z = -i\hbar\dfrac{\partial}{\partial\phi}$, so $\dfrac{\partial^2\psi}{\partial\phi^2} = -\dfrac{1}{\hbar^2}L_z^2\psi = -\dfrac{1}{\hbar^2}\bar{m}^2\hbar^2\psi = -\bar{m}^2\psi$. Use separation of variables: $\psi(r,\phi,z) = R(r)\Phi(\phi)Z(z)$:

$$-\frac{\hbar^2}{2m}\left[\Phi Z\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right)-\frac{\bar{m}^2}{r^2}R\Phi Z+R\Phi\frac{d^2Z}{dz^2}\right]+\left(\frac{1}{8}m\omega_1^2r^2+\frac{1}{2}m\omega_2^2z^2\right)R\Phi Z=\left(E+\frac{1}{2}\bar{m}\hbar\omega_1\right)R\Phi Z.$$

Divide by $R\Phi Z$ and collect terms:

$$\left\{-\frac{\hbar^2}{2m}\left[\frac{1}{rR}\frac{d}{dr}\left(r\frac{dR}{dr}\right)-\frac{\bar{m}^2}{r^2}\right]+\frac{1}{8}m\omega_1^2r^2\right\}+\left\{-\frac{\hbar^2}{2m}\frac{1}{Z}\frac{d^2Z}{dz^2}+\frac{1}{2}m\omega_2^2z^2\right\}=\left(E+\frac{1}{2}\bar{m}\hbar\omega_1\right).$$

The first term depends only on r, the second only on z, so they're both constants; call them E_r and E_z:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right)-\frac{\bar{m}^2}{r^2}R\right]+\frac{1}{8}m\omega_1^2r^2R=E_rR;\quad -\frac{\hbar^2}{2m}\frac{d^2Z}{dz^2}+\frac{1}{2}m\omega_2^2z^2Z=E_zZ;\quad E=E_r+E_z-\frac{1}{2}\bar{m}\hbar\omega_1.$$

The z equation is a one-dimensional harmonic oscillator, and we can read off immediately that $E_z = (n_2+1/2)\hbar\omega_2$, with $n_2 = 0, 1, 2, \ldots$. The r equation is actually a two-dimensional harmonic oscillator; to get E_r, let $u(r) \equiv \sqrt{r}\,R$, and follow the method of Sections 4.1.3 and 4.2.1:

$$R=\frac{u}{\sqrt{r}},\quad \frac{dR}{dr}=\frac{u'}{\sqrt{r}}-\frac{u}{2r^{3/2}},\quad r\frac{dR}{dr}=\sqrt{r}\,u'-\frac{u}{2\sqrt{r}},\quad \frac{d}{dr}\left(r\frac{dR}{dr}\right)=\sqrt{r}\,u''+\frac{u}{4r^{3/2}},$$

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right)=\frac{u''}{\sqrt{r}}+\frac{u}{4r^{5/2}};\quad -\frac{\hbar^2}{2m}\left(\frac{u''}{\sqrt{r}}+\frac{1}{4}\frac{u}{r^2}\frac{1}{\sqrt{r}}-\frac{\bar{m}^2}{r^2}\frac{u}{\sqrt{r}}\right)+\frac{1}{8}m\omega_1^2r^2\frac{u}{\sqrt{r}}=E_r\frac{u}{\sqrt{r}}$$

$$-\frac{\hbar^2}{2m}\left[\frac{d^2u}{dr^2}+\left(\frac{1}{4}-\bar{m}^2\right)\frac{u}{r^2}\right]+\frac{1}{8}m\omega_1^2r^2u=E_ru.$$

This is identical to the equation we shall encounter in Problem 4.47 (the three-dimentional harmonic oscillator), only with $\omega \to \omega_1/2, E \to E_r$, and $\ell(\ell+1) \to \bar{m}^2 - 1/4$, which is to say, $\ell^2+\ell+1/4 = \bar{m}^2$, or $(\ell+1/2)^2 = \bar{m}^2$, or $\ell = |\bar{m}| - 1/2$. [Our present equation depends only on $\bar{m}^2$, and hence is the same for either sign, but the solution to Problem 4.47 assumes $\ell + 1/2 \geq 0$ (else u is not normalizable), so we need $|m|$ here.] Quoting that solution:

$$E=(j_{\max}+\ell+3/2)\hbar\omega\to E_r=(j_{\max}+|\bar{m}|+1)\hbar\omega_1/2,\quad \text{where}\quad j_{\max}=0,2,4,\ldots.$$

$$E=(j_{\max}+|\bar{m}|+1)\hbar\omega_1/2+(n_2+1/2)\hbar\omega_2-\bar{m}\hbar\omega_1/2=\boxed{(n_1+\tfrac{1}{2})\hbar\omega_1+(n_2+\tfrac{1}{2})\hbar\omega_2,}$$

where $n_1 = 0, 1, 2, \ldots$ (if $\bar{m} \geq 0$, then $n_1 = j_{\max}/2$; if $\bar{m} < 0$, then $n_1 = j_{\max}/2 - \bar{m}$).

[A more elegant solution runs as follows: Let

$$P\equiv\frac{1}{\sqrt{2}}\left[(p_x+p_y)-\frac{qB_0}{2}(x-y)\right],\quad Q\equiv\frac{1}{\sqrt{2}}\left[\frac{1}{qB_0}(p_x-p_y)+\frac{1}{2}(x+y)\right].$$

Show (a) P and Q satisfy the canonical commutation relations (Eq. 2.52): $[Q, P] = i\hbar$, and (b) the Hamiltonian (square brackets in Eq. 4.191) can be written as

$$H = \left(\frac{1}{2m}P^2 + \frac{1}{2}m\omega_1^2 Q^2\right) + \left(\frac{1}{2m}p_z^2 + \frac{1}{2}m\omega_2^2 z^2\right).$$

The problem is therefore mathematically identical to two independent harmonic oscillators, with the same mass, and frequencies ω_1 and ω_2; the total energy is just the sum: $(n_1 + \frac{1}{2})\hbar\omega_1 + (n_2 + \frac{1}{2})\hbar\omega_2$.]

Problem 4.44

Assume that Ψ satisfies the Schrödinger equation (4.191):

$$i\hbar\frac{\partial \Psi}{\partial t} = \left[\frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right)^2 + q\varphi\right]\Psi.$$

Let $\Psi' = e^{iq\Lambda/\hbar}\Psi$. Then

$$i\hbar\frac{\partial \Psi'}{\partial t} = i\hbar\left[e^{iq\Lambda/\hbar}\frac{\partial \Psi}{\partial t} + \frac{iq}{\hbar}\frac{\partial \Lambda}{\partial t}e^{iq\Lambda/\hbar}\Psi\right] = e^{iq\Lambda/\hbar}\left[\frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right)^2 + q\varphi - q\frac{\partial \Lambda}{\partial t}\right]\Psi.$$

[Note that $\boldsymbol{\nabla}$ does *not* act on $e^{iq\Lambda/\hbar}$, so it's important to keep that factor on the left.] But $\varphi = \varphi' + \partial\Lambda/\partial t$ and $\mathbf{A} = \mathbf{A}' - \boldsymbol{\nabla}\Lambda$ (Equation 4.196), so

$$i\hbar\frac{\partial \Psi'}{\partial t} = e^{iq\Lambda/\hbar}\left[\frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla}\Lambda)\right)^2 + q\varphi'\right]\Psi.$$

Now we need to move $e^{iq\Lambda/\hbar}$ through to the right. First note that

$$-i\hbar\boldsymbol{\nabla}\left(e^{iq\Lambda/\hbar}f\right) = -i\hbar e^{iq\Lambda/\hbar}\boldsymbol{\nabla}f + q(\boldsymbol{\nabla}\Lambda)e^{iq\Lambda/\hbar}f = e^{iq\Lambda/\hbar}\left[-i\hbar\boldsymbol{\nabla} + q(\boldsymbol{\nabla}\Lambda)\right]f,$$

for any function $f(\mathbf{r}, t)$, so

$$e^{iq\Lambda/\hbar}\left[-i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla}\Lambda)\right]f = \left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}'\right)\left(e^{iq\Lambda/\hbar}f\right).$$

Then

$$\begin{aligned} e^{iq\Lambda/\hbar}\left[-i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla}\Lambda)\right]^2\Psi &= e^{iq\Lambda/\hbar}\left[-i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla}\Lambda)\right]\underbrace{e^{-iq\Lambda/\hbar}e^{iq\Lambda/\hbar}\left[-i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla}\Lambda)\right]\Psi}_{f} \\ &= \left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}'\right)\left[e^{iq\Lambda/\hbar}e^{-iq\Lambda/\hbar}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}'\right)\left(e^{iq\Lambda/\hbar}\Psi\right)\right] \\ &= \left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}'\right)^2\Psi'. \end{aligned}$$

Therefore,

$$i\hbar\frac{\partial \Psi'}{\partial t} = \left[\frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}'\right)^2 + q\varphi'\right]\Psi'. \quad \text{QED}$$

Problem 4.45

(a) Giving H a test function f to act upon:

$$Hf = \frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right)\cdot\left(-i\hbar\boldsymbol{\nabla}f - q\mathbf{A}f\right) + q\varphi f$$
$$= \frac{1}{2m}\Bigg[-\hbar^2\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}f) + iq\hbar\underbrace{\boldsymbol{\nabla}\cdot(\mathbf{A}f)}_{(\boldsymbol{\nabla}\cdot A)f+\mathbf{A}\cdot(\boldsymbol{\nabla}f)} + iq\hbar\mathbf{A}\cdot(\boldsymbol{\nabla}f) + q^2\mathbf{A}\cdot\mathbf{A}f\Bigg] + q\varphi f.$$

But $\boldsymbol{\nabla}\cdot\mathbf{A} = 0$ and $\varphi = 0$ (see comments after Eq. 4.198), so

$$Hf = \frac{1}{2m}\left[-\hbar^2\nabla^2 f + 2iq\hbar\mathbf{A}\cdot\boldsymbol{\nabla}f + q^2A^2 f\right], \quad \text{or} \quad H = \frac{1}{2m}\left[-\hbar^2\nabla^2 + q^2A^2 + 2iq\hbar\mathbf{A}\cdot\boldsymbol{\nabla}\right]. \quad \text{QED}$$

(b) Apply $(-i\hbar\boldsymbol{\nabla} - q\mathbf{A})\cdot$ to both sides of Eq. 4.210:

$$\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right)^2\Psi = \left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right)\cdot\left(-i\hbar e^{ig}\boldsymbol{\nabla}\Psi'\right) = -\hbar^2\boldsymbol{\nabla}\cdot(e^{ig}\boldsymbol{\nabla}\Psi') + iq\hbar e^{ig}\mathbf{A}\cdot\boldsymbol{\nabla}\Psi'.$$

But $\boldsymbol{\nabla}\cdot(e^{ig}\boldsymbol{\nabla}\Psi') = ie^{ig}(\boldsymbol{\nabla}g)\cdot(\boldsymbol{\nabla}\Psi') + e^{ig}\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\Psi')$ and $\boldsymbol{\nabla}g = \frac{q}{\hbar}\mathbf{A}$, so the right side is

$$-i\hbar^2\frac{q}{\hbar}e^{ig}\mathbf{A}\cdot\boldsymbol{\nabla}\Psi' - \hbar^2 e^{ig}\nabla^2\Psi' + iq\hbar e^{ig}\mathbf{A}\cdot\boldsymbol{\nabla}\Psi' = -\hbar^2 e^{ig}\nabla^2\Psi'. \quad \text{QED}$$

Problem 4.46

(a)

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + \frac{1}{2}m\omega^2\left(x^2+y^2+z^2\right)\psi = E\psi.$$

Let $\psi(x,y,z) = X(x)Y(y)Z(z)$; plug it in, divide by XYZ, and collect terms:

$$\left(-\frac{\hbar^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{2}m\omega^2x^2\right) + \left(-\frac{\hbar^2}{2m}\frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{2}m\omega^2y^2\right) + \left(-\frac{\hbar^2}{2m}\frac{1}{Z}\frac{d^2Z}{dz^2} + \frac{1}{2}m\omega^2z^2\right) = E.$$

The first term is a function only of x, the second only of y, and the third only of z. So each is a constant (call the constants E_x, E_y, E_z, with $E_x + E_y + E_z = E$). Thus:

$$-\frac{\hbar^2}{2m}\frac{d^2X}{dx^2} + \frac{1}{2}m\omega^2x^2X = E_xX; \; -\frac{\hbar^2}{2m}\frac{d^2Y}{dy^2} + \frac{1}{2}m\omega^2y^2Y = E_yY; \; -\frac{\hbar^2}{2m}\frac{d^2Z}{dz^2} + \frac{1}{2}m\omega^2z^2Z = E_zZ.$$

Each of these is simply the one-dimensional harmonic oscillator (Eq. 2.45). We know the allowed energies (Eq. 2.62):

$$E_x = (n_x + \tfrac{1}{2})\hbar\omega; \; E_y = (n_y + \tfrac{1}{2})\hbar\omega; \; E_z = (n_z + \tfrac{1}{2})\hbar\omega; \text{ where } n_x, n_y, n_z = 0, 1, 2, 3, \ldots.$$

So $E = (n_x + n_y + n_y + \frac{3}{2})\hbar\omega = \boxed{(n + \frac{3}{2})\hbar\omega,}$ with $n \equiv n_x + n_y + n_z$.

(b) The question is: "How many ways can we add three non-negative integers to get sum n?"

If $n_x = n$, then $n_y = n_z = 0$; *one* way.
If $n_x = n - 1$, then $n_y = 0, n_z = 1$, or else $n_y = 1, n_z = 0$; *two* ways.
If $n_x = n - 2$, then $n_y = 0, n_z = 2$, or $n_y = 1, n_z = 1$, or $n_y = 2, n_z = 0$; *three* ways.

And so on. Evidently $d(n) = 1 + 2 + 3 + \cdots + (n+1) = \boxed{\frac{(n+1)(n+2)}{2}.}$

Problem 4.47

Eq. 4.37: $-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[\frac{1}{2}m\omega^2r^2+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u=Eu.$

Following Eq. 2.72, let $\xi\equiv\sqrt{\frac{m\omega}{\hbar}}r$. Then $-\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{d^2u}{d\xi^2}+\left[\frac{1}{2}m\omega^2\frac{\hbar}{m\omega}\xi^2+\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{\ell(\ell+1)}{\xi^2}\right]u=Eu,$

or $\frac{d^2u}{d\xi^2}=\left[\xi^2+\frac{\ell(\ell+1)}{\xi^2}-K\right]u,$ where $K\equiv\frac{2E}{\hbar\omega}$ (as in Eq. 2.74).

At large ξ, $\frac{d^2u}{d\xi^2}\approx\xi^2u$, and $u\sim(\;)e^{-\xi^2/2}$ (see Eq. 2.78).

At small ξ, $\frac{d^2u}{d\xi^2}\approx\frac{\ell(\ell+1)}{\xi^2}u$, and $u\sim(\;)\xi^{\ell+1}$ (see Eq. 4.59).

So let $u(\xi)\equiv\xi^{\ell+1}e^{-\xi^2/2}v(\xi)$. [This defines the new function $v(\xi)$.]

$$\frac{du}{d\xi}=(\ell+1)\xi^\ell e^{-\xi^2/2}v-\xi^{\ell+2}e^{-\xi^2/2}v+\xi^{\ell+1}e^{-\xi^2/2}v'.$$

$$\begin{aligned}\frac{d^2u}{d\xi^2}&=\ell(\ell+1)\xi^{\ell-1}e^{-\xi^2/2}v-(\ell+1)\xi^{\ell+1}e^{-\xi^2/2}v+(\ell+1)\xi^\ell e^{-\xi^2/2}v'-(\ell+2)\xi^{\ell+1}e^{-\xi^2/2}v\\&\quad+\xi^{\ell+3}e^{-\xi^2/2}v-\xi^{\ell+2}e^{-\xi^2/2}v'+(\ell+1)\xi^\ell e^{-\xi^2/2}v'-\xi^{\ell+2}e^{-\xi^2/2}v'+\xi^{\ell+1}e^{-\xi^2/2}v''\\&=\cancel{\ell(\ell+1)\xi^{\ell-1}e^{-\xi^2/2}}v-(2\ell+3)\xi^{\ell+1}e^{-\xi^2/2}v+\cancel{\xi^{\ell+3}e^{-\xi^2/2}}v+2(\ell+1)\xi^\ell e^{-\xi^2/2}v'\\&\quad-2\xi^{\ell+2}e^{-\xi^2/2}v'+\xi^{\ell+1}e^{-\xi^2/2}v''=\cancel{\xi^{\ell+3}e^{-\xi^2/2}}v+\cancel{\ell(\ell+1)\xi^{\ell-1}e^{-\xi^2/2}}v-K\xi^{\ell+1}e^{-\xi^2/2}v.\end{aligned}$$

Cancelling the indicated terms, and dividing off $\xi^{\ell+1}e^{-\xi^2/2}$, we have:

$$v''+2v'\left(\frac{\ell+1}{\xi}-\xi\right)+(K-2\ell-3)\,v=0.$$

Let $v(\xi)\equiv\sum_{j=0}^{\infty}a_j\xi^j$, so $v'=\sum_{j=0}^{\infty}ja_j\xi^{j-1}$; $v''=\sum_{j=2}^{\infty}j(j-1)a_j\xi^{j-2}$. Then

$$\sum_{j=2}^{\infty}j(j-1)a_j\xi^{j-2}+2(\ell+1)\sum_{j=1}^{\infty}ja_j\xi^{j-2}-2\sum_{j=1}^{\infty}ja_j\xi^j+(K-2\ell-3)\sum_{j=0}^{\infty}a_j\xi^j=0.$$

In the first two sums, let $j\to j+2$ (rename the dummy index):

$$\sum_{j=0}^{\infty}(j+2)(j+1)a_{j+2}\xi^j+2(\ell+1)\sum_{j=0}^{\infty}(j+2)a_{j+2}\xi^j-2\sum_{j=0}^{\infty}ja_j\xi^j+(K-2\ell-3)\sum_{j=0}^{\infty}a_j\xi^j=0.$$

Note: the second sum should start at $j=-1$; to eliminate this term (there is no compensating one in ξ^{-1}) we must take $a_1=0$. Combining the terms:

$$\sum_{j=0}^{\infty}\left[(j+2)(j+2\ell+3)a_{j+2}+(K-2j-2\ell-3)a_j\right]=0,\ \text{so}\ \boxed{a_{j+2}=\frac{(2j+2\ell+3-K)}{(j+2)(j+2\ell+3)}a_j.}$$

Since $a_1=0$, this gives us a single sequence: $a_0,a_2,a_4,\ldots$. But the series must terminate (else we get the wrong behavior as $\xi\to\infty$), so there occurs some even number $j_{\max}$ such that $a_{j_{\max}}\neq0$ but $a_{j_{\max}+2}=0$. Thus

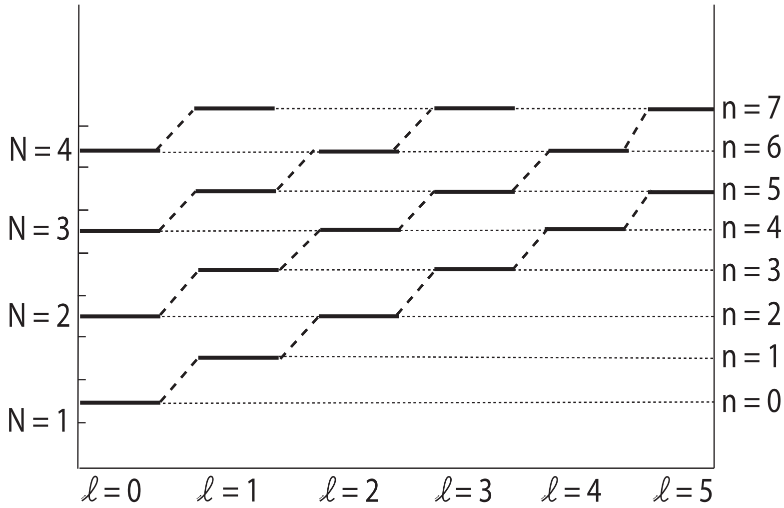
$K = 2j_{\max} + 2\ell + 3.$ But $E = \dfrac{1}{2}\hbar\omega K,$ so $E = \left(j_{\max} + \ell + \frac{3}{2}\right)\hbar\omega.$ Or, letting $j_{\max} + \ell \equiv n,$

$\boxed{E_n = (n + \frac{3}{2})\hbar\omega,}$ and n can be any nonnegative integer; this agrees with Equation 4.216.

Since $v(\xi)$ is a polynomial of degree $j_{\max}$ in ξ, or $j_{\max}/2$ in ξ^2, the number of nodes (roots of $v(\xi)$ is $j_{\max}/2 = N - 1$, so $n = j_{\max} + \ell \Rightarrow \boxed{n = 2N + \ell - 2.}$ Suppose n is *even*; then (since $j_{\max}$ is even) $\ell = 0, 2, 4, \dots, n$. For each ℓ there are $(2\ell + 1)$ values for m. So

$$d(n) = \sum_{\ell=0,2,4,\dots}^{n} (2\ell+1). \quad \text{Let } j = \ell/2; \quad \text{then } d(n) = \sum_{j=0}^{n/2}(4j+1) = 4\sum_{j=0}^{n/2} j + \sum_{j=0}^{n/2} 1$$

$$= 4\frac{(\frac{n}{2})(\frac{n}{2}+1)}{2} + (\tfrac{n}{2}+1) = (\tfrac{n}{2}+1)(n+1) = \frac{(n+1)(n+2)}{2}, \text{ as before (Problem 4.46(b)).}$$



Problem 4.48

(a)

$$\frac{d}{dt}\langle \mathbf{r}\cdot\mathbf{p}\rangle = \frac{i}{\hbar}\langle [H, \mathbf{r}\cdot\mathbf{p}]\rangle.$$

$$[H, \mathbf{r}\cdot\mathbf{p}] = \sum_{i=1}^{3}[H, r_i p_i] = \sum_{i=1}^{3}\left([H, r_i]p_i + r_i[H, p_i]\right) = \sum_{i=1}^{3}\left(\frac{1}{2m}[p^2, r_i]p_i + r_i[V, p_i]\right).$$

$$[p^2, r_i] = \sum_{j=1}^{3}[p_j p_j, r_i] = \sum_{j=1}^{3}\left(p_j[p_j, r_i] + [p_j, r_i]p_j\right) = \sum_{j=1}^{3}\left[p_j(-i\hbar\delta_{ij}) + (-i\hbar\delta_{ij})p_j\right] = -2i\hbar p_i.$$

$$[V, p_i] = i\hbar\frac{\partial V}{\partial r_i} \text{ (Problem 3.13(c)).} \quad [H, \mathbf{r}\cdot\mathbf{p}] = \sum_{i=1}^{3}\left[\frac{1}{2m}(-2i\hbar)p_i p_i + r_i\left(i\hbar\frac{\partial V}{\partial r_i}\right)\right]$$

$$= i\hbar\left(-\frac{p^2}{m} + \mathbf{r}\cdot\nabla V\right). \quad \frac{d}{dt}\langle \mathbf{r}\cdot\mathbf{p}\rangle = \langle \frac{p^2}{m} - \mathbf{r}\cdot\nabla V\rangle = 2\langle T\rangle - \langle \mathbf{r}\cdot\nabla V\rangle.$$

For stationary states $\dfrac{d}{dt}\langle \mathbf{r}\cdot\mathbf{p}\rangle = 0,$ so $2\langle T\rangle = \langle \mathbf{r}\cdot\nabla V\rangle.$ QED

(b)

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \Rightarrow \nabla V = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r^2}\hat{r} \Rightarrow \mathbf{r}\cdot\nabla V = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} = -V. \quad \text{So } 2\langle T\rangle = -\langle V\rangle.$$

But $\langle T\rangle + \langle V\rangle = E_n$, so $\langle T\rangle - 2\langle T\rangle = E_n$, or $\langle T\rangle = -E_n$; $\langle V\rangle = 2E_n$. QED

(c)

$$V = \frac{1}{2}m\omega^2 r^2 \Rightarrow \nabla V = m\omega^2 r\,\hat{r} \Rightarrow \mathbf{r}\cdot\nabla V = m\omega^2 r^2 = 2V. \quad \text{So } 2\langle T\rangle = 2\langle V\rangle, \text{ or } \langle T\rangle = \langle V\rangle.$$

But $\langle T\rangle + \langle V\rangle = E_n$, so $\langle T\rangle = \langle V\rangle = \frac{1}{2}E_n$. QED

Problem 4.49

(a) $\nabla\cdot\mathbf{J} = \frac{i\hbar}{2m}\left[\nabla\Psi\cdot\nabla\Psi^* + \Psi(\nabla^2\Psi^*) - \nabla\Psi^*\cdot\nabla\Psi - \Psi^*(\nabla^2\Psi)\right] = \frac{i\hbar}{2m}\left[\Psi(\nabla^2\Psi^*) - \Psi^*(\nabla^2\Psi)\right].$

But the Schrödinger equation says $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$, so

$\nabla^2\Psi = \frac{2m}{\hbar^2}\left(V\Psi - i\hbar\frac{\partial\Psi}{\partial t}\right)$, $\nabla^2\Psi^* = \frac{2m}{\hbar^2}\left(V\Psi^* + i\hbar\frac{\partial\Psi^*}{\partial t}\right)$. Therefore

$$\begin{aligned}\nabla\cdot\mathbf{J} &= \frac{i\hbar}{2m}\frac{2m}{\hbar^2}\left[\Psi\left(V\Psi^* + i\hbar\frac{\partial\Psi^*}{\partial t}\right) - \Psi^*\left(V\Psi - i\hbar\frac{\partial\Psi}{\partial t}\right)\right] \\ &= \frac{i}{\hbar}i\hbar\left(\Psi\frac{\partial\Psi^*}{\partial t} + \Psi^*\frac{\partial\Psi}{\partial t}\right) = -\frac{\partial}{\partial t}(\Psi^*\Psi) = -\frac{\partial}{\partial t}|\Psi|^2. \quad \checkmark\end{aligned}$$

(b) From Problem 4.13(b), $\Psi_{2\,1\,1} = -\frac{1}{\sqrt{\pi a}}\frac{1}{8a^2}re^{-r/2a}\sin\theta e^{i\phi}e^{-iE_2 t/\hbar}$. In spherical coordinates,

$\nabla\Psi = \frac{\partial\Psi}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial\Psi}{\partial\theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial\Psi}{\partial\phi}\hat{\phi}$, so

$$\begin{aligned}\nabla\Psi_{2\,1\,1} &= -\frac{1}{\sqrt{\pi a}}\frac{1}{8a^2}\left[\left(1-\frac{r}{2a}\right)e^{-r/2a}\sin\theta e^{i\phi}e^{-iE_2t/\hbar}\,\hat{r} + \frac{1}{r}re^{-r/2a}\cos\theta e^{i\phi}e^{-iE_2t/\hbar}\,\hat{\theta}\right. \\ &\quad \left. + \frac{1}{r\sin\theta}re^{-r/2a}\sin\theta\, ie^{i\phi}e^{-iE_2t/\hbar}\,\hat{\phi}\right] = \left[\left(1-\frac{r}{2a}\right)\hat{r} + \cot\theta\,\hat{\theta} + \frac{i}{\sin\theta}\hat{\phi}\right]\frac{1}{r}\Psi_{2\,1\,1}.\end{aligned}$$

Therefore

$$\begin{aligned}\mathbf{J} &= \frac{i\hbar}{2m}\left[\left(1-\frac{r}{2a}\right)\hat{r} + \cot\theta\,\hat{\theta} - \frac{i}{\sin\theta}\hat{\phi} - \left(1-\frac{r}{2a}\right)\hat{r} - \cot\theta\,\hat{\theta} - \frac{i}{\sin\theta}\hat{\phi}\right]\frac{1}{r}|\Psi_{2\,1\,1}|^2 \\ &= \frac{i\hbar}{2m}\frac{(-2i)}{r\sin\theta}|\Psi_{2\,1\,1}|^2\,\hat{\phi} = \frac{\hbar}{m}\frac{1}{\pi a}\frac{1}{64a^4}\frac{r^2e^{-r/a}\sin^2\theta}{r\sin\theta}\,\hat{\phi} = \boxed{\frac{\hbar}{64\pi m a^5}re^{-r/a}\sin\theta\,\hat{\phi}.}\end{aligned}$$

(c) Now $\mathbf{r}\times\mathbf{J} = \dfrac{\hbar}{64\pi m a^5} r^2 e^{-r/a}\sin\theta\left(\hat{r}\times\hat{\phi}\right)$, while $\left(\hat{r}\times\hat{\phi}\right) = -\hat{\theta}$ and $\hat{z}\cdot\hat{\theta} = -\sin\theta$, so $\mathbf{r}\times\mathbf{J}_z = \dfrac{\hbar}{64\pi m a^5} r^2 e^{-r/a}\sin^2\theta$, and hence

$$\begin{aligned} L_z &= m\frac{\hbar}{64\pi m a^5}\int\left(r^2 e^{-r/a}\sin^2\theta\right) r^2\sin\theta\,dr\,d\theta\,d\phi \\ &= \frac{\hbar}{64\pi a^5}\int_0^\infty r^4 e^{-r/a}\,dr\int_0^\pi \sin^3\theta\,d\theta\int_0^{2\pi} d\phi = \frac{\hbar}{64\pi a^5}\left(4!a^5\right)\left(\frac{4}{3}\right)(2\pi) = \boxed{\hbar,} \end{aligned}$$

as it *should* be, since (Eq. 4.133) $L_z = \hbar m$, and $m = 1$ for this state.

Problem 4.50

(a)

$$\psi = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \Rightarrow \phi(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}}\frac{1}{\sqrt{\pi a^3}}\int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} e^{-r/a} r^2\sin\theta\,dr\,d\theta\,d\phi.$$

With axes as suggested, $\mathbf{p}\cdot\mathbf{r} = pr\cos\theta$. Doing the (trivial) ϕ integral:

$$\phi(\mathbf{p}) = \frac{2\pi}{(2\pi a\hbar)^{3/2}}\frac{1}{\sqrt{\pi}}\int_0^\infty r^2 e^{-r/a}\left[\int_0^\pi e^{-ipr\cos\theta/\hbar}\sin\theta\,d\theta\right] dr.$$

$$\int_0^\pi e^{-ipr\cos\theta/\hbar}\sin\theta\,d\theta = \frac{\hbar}{ipr}\left. e^{-ipr\cos\theta/\hbar}\right|_0^\pi = \frac{\hbar}{ipr}\left(e^{ipr/\hbar} - e^{-ipr/\hbar}\right) = \frac{2\hbar}{pr}\sin\left(\frac{pr}{\hbar}\right).$$

$$\phi(\mathbf{p}) = \frac{1}{\pi\sqrt{2}}\frac{1}{(a\hbar)^{3/2}}\frac{2\hbar}{p}\int_0^\infty r e^{-r/a}\sin\left(\frac{pr}{\hbar}\right) dr.$$

$$\begin{aligned} \int_0^\infty r e^{-r/a}\sin\left(\frac{pr}{\hbar}\right) dr &= \frac{1}{2i}\left[\int_0^\infty r e^{-r/a} e^{ipr/\hbar} dr - \int_0^\infty r e^{-r/a} e^{-ipr/\hbar} dr\right] \\ &= \frac{1}{2i}\left[\frac{1}{(1/a - ip/\hbar)^2} - \frac{1}{(1/a + ip/\hbar)^2}\right] = \frac{1}{2i}\frac{(2ip/a\hbar)2}{\left[(1/a)^2 + (p/\hbar)^2\right]^2} \\ &= \frac{(2p/\hbar)a^3}{\left[1 + (ap/\hbar)^2\right]^2}. \end{aligned}$$

$$\phi(\mathbf{p}) = \sqrt{\frac{2}{\hbar}}\frac{1}{a^{3/2}}\frac{1}{\pi p}\frac{2pa^3}{\hbar}\frac{1}{\left[1 + (ap/\hbar)^2\right]^2} = \boxed{\frac{1}{\pi}\left(\frac{2a}{\hbar}\right)^{3/2}\frac{1}{\left[1 + (ap/\hbar)^2\right]^2}.}$$

(b)

$$\int |\phi|^2\,d^3\mathbf{p} = 4\pi\int_0^\infty p^2|\phi|^2 dp = 4\pi\frac{1}{\pi^2}\left(\frac{2a}{\hbar}\right)^3\int_0^\infty \frac{p^2}{\left[1 + (ap/\hbar)^2\right]^4} dp.$$

From math tables: $\displaystyle\int_0^\infty \frac{x^2}{(m + x^2)^4}\,dx = \frac{\pi}{32} m^{-5/2}$, so

$$\int_0^\infty \frac{p^2}{\left[1 + (ap/\hbar)^2\right]^4} dp = \left(\frac{\hbar}{a}\right)^8\frac{\pi}{32}\left(\frac{\hbar}{a}\right)^{-5} = \frac{\pi}{32}\left(\frac{\hbar}{a}\right)^3;\quad \int |\phi|^2 d^3\mathbf{p} = \frac{32}{\pi}\left(\frac{a}{\hbar}\right)^3\frac{\pi}{32}\left(\frac{\hbar}{a}\right)^3 = 1.\ \checkmark$$

(c)

$$\langle p^2\rangle = \int p^2|\phi|^2\, d^3\mathbf{p} = \frac{1}{\pi^2}\left(\frac{2a}{\hbar}\right)^3 4\pi\int_0^\infty \frac{p^4}{[1+(ap/\hbar)^2]^4}dp. \quad \text{From math tables:}$$

$$\int_0^\infty \frac{x^4}{[m+x^2]^4}dx = \left(\frac{\pi}{32}\right)m^{-3/2}. \quad \text{So} \quad \langle p^2\rangle = \frac{4}{\pi}\left(\frac{2a}{\hbar}\right)^3\left(\frac{\hbar}{a}\right)^8\frac{\pi}{32}\left(\frac{\hbar}{a}\right)^{-3} = \boxed{\frac{\hbar^2}{a^2}.}$$

(d)

$$\langle T\rangle = \frac{1}{2m}\langle p^2\rangle = \frac{1}{2m}\frac{\hbar^2}{a^2} = \frac{\hbar^2}{2m}\frac{m^2}{\hbar^4}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = \frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = \boxed{-E_1,}$$

which *is* consistent with Eq. 4.218.

Problem 4.51

$$V(r) = \begin{cases} -V_0 & (r \le a), \\ 0 & (r > a). \end{cases}$$

The Laplacian in polar coordinates (r,θ) is

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}.$$

The Schrödinger equation says

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}\right] + V\psi = E\psi.$$

Solve by separation of variables, $\psi(r,\theta) = R(r)\,\Theta(\theta)$:

$$-\frac{\hbar^2}{2m}\left[\frac{\Theta}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{R}{r^2}\frac{d^2\Theta}{d\theta^2}\right] + VR\Theta = ER\Theta \quad\Rightarrow\quad -\frac{\hbar^2}{2m}\left[\frac{r}{R}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2}\right] + r^2V(r) = r^2E.$$

$\dfrac{1}{\Theta}\dfrac{d^2\Theta}{d\theta^2} = -\ell^2$ (a constant) $\Rightarrow \Theta = e^{i\ell\theta}$, $\ell = 0, \pm1, \pm2, \dots$. But for the ground state we want $\ell = 0$ (circular symmetry). This leaves the radial equation:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right)\right] + VR = ER; \quad \frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} = -\frac{2m}{\hbar^2}(E-V)R = \begin{cases} \kappa^2 R & (r > a), \\ -l^2 R & (r \le a), \end{cases}$$

where $\kappa \equiv \sqrt{-2mE}/\hbar$ and $l \equiv \sqrt{2m(E+V_0)}/\hbar$. The solutions are Bessel functions: $R(r) = AJ_0(lr)$, for $r \le a$ (the other solution blows up at the origin) and $R(r) = BK_0(\kappa r)$ for $r > a$ (the other solution blows up as $r \to \infty$).

The boundary conditions are $AJ_0(la) = BK_0(\kappa a)$ and $AlJ_0'(la) = B\kappa K_0'(\kappa a)$; dividing,

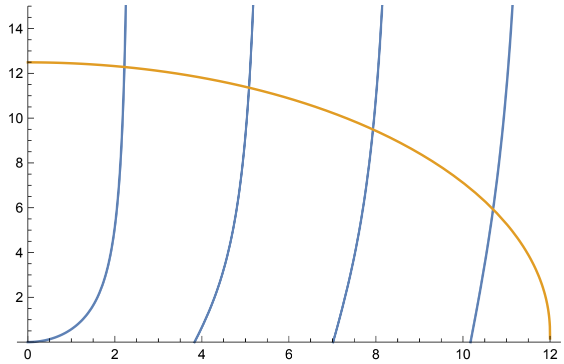
$$l\frac{J_0'(la)}{J_0(la)} = \kappa\frac{K_0'(\kappa a)}{K_0(\kappa a)}.$$

This determines the allowed energies. Borrowing the notation of Equation 2.158, $z \equiv la$, $z_0 \equiv a\sqrt{2mV_0}/\hbar$, $\kappa a = \sqrt{z_0^2 - z^2}$, and using the fact that $J_0'(x) = -J_1(x)$ and $K_0'(x) = -K_1(x)$:

$$z\frac{J_1(z)}{J_0(z)} = \sqrt{z_0^2 - z^2}\,\frac{K_1(\sqrt{z_0^2 - z^2})}{K_0(\sqrt{z_0^2 - z^2})}. \qquad [\bigstar]$$

Plotting both sides (as in Figure 2.17), we look for intersections:

```
Plot[{x BesselJ[1, x] / BesselJ[0, x],
  √(144 - x²) BesselK[1, √(144 - x²)] / BesselK[0, √(144 - x²)]},
 {x, 0, 12}, PlotRange -> {0, 15}]
```



The graph is for $z_0 = 12$; as z_0 (the "strength" of the potential well) decreases, the left side of Equation ★ (the rising vertical curves, on the graph) does not change, but the right side (the falling curve) shrinks down as the zero crossing moves left along the horizontal axis. There always remains one intersection, however, so like the one-dimensional case (but unlike the 3-dimensional case) there is always (at least) one bound state for the circular well.

Problem 4.52

(a) From Tables 4.3 and 4.7,

$$\psi_{321} = R_{32}Y_2^1 = \frac{4}{81\sqrt{30}}\frac{1}{a^{3/2}}\left(\frac{r}{a}\right)^2 e^{-r/3a}\left[-\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi}\right] = \boxed{-\frac{1}{\sqrt{\pi}}\frac{1}{81a^{7/2}}r^2 e^{-r/3a}\sin\theta\cos\theta e^{i\phi}.}$$

(b)

$$\begin{aligned}
\int |\psi|^2 d^3\mathbf{r} &= \frac{1}{\pi}\frac{1}{(81)^2a^7}\int\left(r^4 e^{-2r/3a}\sin^2\theta\cos^2\theta\right) r^2\sin\theta\,dr\,d\theta\,d\phi \\
&= \frac{1}{\pi(81)^2a^7}2\pi\int_0^\infty r^6 e^{-2r/3a}\,dr\int_0^\pi(1-\cos^2\theta)\cos^2\theta\sin\theta\,d\theta \\
&= \frac{2}{(81)^2a^7}\left[6!\left(\frac{3a}{2}\right)^7\right]\left[-\frac{\cos^3\theta}{3}+\frac{\cos^5\theta}{5}\right]\Bigg|_0^\pi \\
&= \frac{2}{3^8a^7}6\cdot5\cdot4\cdot3\cdot2\frac{3^7a^7}{2^7}\left[\frac{2}{3}-\frac{2}{5}\right] = \frac{3\cdot5}{4}\cdot\frac{4}{15} = 1. \quad \checkmark
\end{aligned}$$

(c)

$$\langle r^s \rangle = \int_0^\infty r^s |R_{32}|^2 r^2 dr = \left(\frac{4}{81}\right)^2 \frac{1}{30}\frac{1}{a^7}\int_0^\infty r^{s+6} e^{-2r/3a} dr$$
$$= \frac{8}{15(81)^2 a^7}(s+6)!\left(\frac{3a}{2}\right)^{s+7} = \boxed{(s+6)!\left(\frac{3a}{2}\right)^s \frac{1}{720}} = \frac{(s+6)!}{6!}\left(\frac{3a}{2}\right)^s.$$

Finite for $\boxed{s > -7}$.

Problem 4.53

(a) From Tables 4.3 and 4.7,

$$\psi_{433} = R_{43} Y_3^3 = \frac{1}{768\sqrt{35}}\frac{1}{a^{3/2}}\left(\frac{r}{a}\right)^3 e^{-r/4a}\left(-\sqrt{\frac{35}{64\pi}}\sin^3\theta e^{3i\phi}\right) = \boxed{-\frac{1}{6144\sqrt{\pi}a^{9/2}} r^3 e^{-r/4a}\sin^3\theta e^{3i\phi}.}$$

(b)

$$\langle r \rangle = \int r|\psi|^2 d^3\mathbf{r} = \frac{1}{(6144)^2\pi a^9}\int r\left(r^6 e^{-r/2a}\sin^6\theta\right) r^2 \sin\theta\, dr\, d\theta\, d\phi$$
$$= \frac{1}{(6144)^2\pi a^9}\int_0^\infty r^9 e^{-r/2a}\, dr \int_0^\pi \sin^7\theta\, d\theta \int_0^{2\pi} d\phi$$
$$= \frac{1}{(6144)^2\pi a^9}\left[9!(2a)^{10}\right]\left(2\frac{2\cdot 4\cdot 6}{3\cdot 5\cdot 7}\right)(2\pi) = \boxed{18a.}$$

(c) Using Eq. 4.133: $L_x^2 + L_y^2 = L^2 - L_z^2 = 3(4)\hbar^2 - (3\hbar)^2 = \boxed{3\hbar^2,\ \text{with probability 1.}}$

Problem 4.54

(a)

$$P = \int |\psi|^2\, d^3\mathbf{r} = \frac{4\pi}{\pi a^3}\int_0^b e^{-2r/a} r^2 dr = \frac{4}{a^3}\left[-\frac{a}{2}r^2 e^{-2r/a} + \frac{a^3}{4}e^{-2r/a}\left(-\frac{2r}{a} - 1\right)\right]\Bigg|_0^b$$
$$= -\left(1 + \frac{2r}{a} + \frac{2r^2}{a^2}\right)e^{-2r/a}\Bigg|_0^b = \boxed{1 - \left(1 + \frac{2b}{a} + 2\frac{b^2}{a^2}\right)e^{-2b/a}.}$$

(b)

$$P = 1 - \left(1 + \epsilon + \frac{1}{2}\epsilon^2\right)e^{-\epsilon} \approx 1 - \left(1 + \epsilon + \frac{1}{2}\epsilon^2\right)\left(1 - \epsilon + \frac{\epsilon^2}{2} - \frac{\epsilon^3}{3!}\right)$$
$$\approx 1 - 1 + \epsilon - \frac{\epsilon^2}{2} + \frac{\epsilon^3}{6} - \epsilon + \epsilon^2 - \frac{\epsilon^3}{2} - \frac{\epsilon^2}{2} + \frac{\epsilon^3}{2} = \epsilon^3\left(\frac{1}{6} - \frac{1}{2} + \frac{1}{2}\right)$$
$$= \frac{1}{6}\left(\frac{2b}{a}\right)^3 = \boxed{\frac{4}{3}\left(\frac{b}{a}\right)^3.}$$

(c)

$$|\psi(0)|^2 = \frac{1}{\pi a^3} \Rightarrow P \approx \frac{4}{3}\pi b^3 \frac{1}{\pi a^3} = \frac{4}{3}\left(\frac{b}{a}\right)^3. \quad \checkmark$$

(d)

$$P = \frac{4}{3}\left(\frac{10^{-15}}{0.5\times 10^{-10}}\right)^3 = \frac{4}{3}\left(2\times 10^{-5}\right)^3 = \frac{4}{3}\cdot 8\times 10^{-15} = \frac{32}{3}\times 10^{-15} = \boxed{1.07\times 10^{-14}.}$$

Problem 4.55

(a) Equation 4.75 $\Rightarrow R_{n(n-1)} = \frac{1}{r}\rho^n e^{-\rho}v(\rho)$, where $\rho \equiv \frac{r}{na}$; Eq. 4.76 $\Rightarrow c_1 = \frac{2(n-n)}{(1)(2n)}c_0 = 0.$

So $v(\rho) = c_0$, and hence $R_{n(n-1)} = N_n r^{n-1}e^{-r/na}$, where $N_n \equiv \frac{c_0}{(na)^n}$.

$$1 = \int_0^\infty |R|^2 r^2 dr = (N_n)^2\int_0^\infty r^{2n}e^{-2r/na}dr = (N_n)^2(2n)!\left(\frac{na}{2}\right)^{2n+1}; \quad \boxed{N_n = \left(\frac{2}{na}\right)^n\sqrt{\frac{2}{na(2n)!}}.}$$

(b)

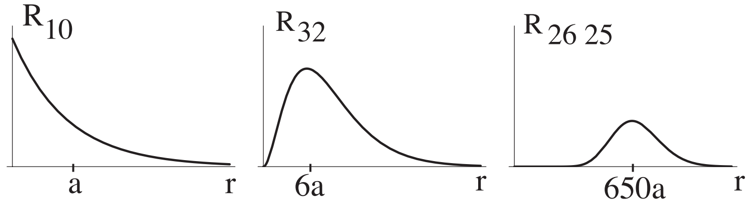
$$\langle r^l\rangle = \int_0^\infty |R|^2 r^{l+2}dr = N_n^2\int_0^\infty r^{2n+l}e^{-2r/na}dr.$$

$$\langle r\rangle = \left(\frac{2}{na}\right)^{2n+1}\frac{1}{(2n)!}(2n+1)!\left(\frac{na}{2}\right)^{2n+2} = \boxed{\left(n+\frac{1}{2}\right)na.}$$

$$\langle r^2\rangle = \left(\frac{2}{na}\right)^{2n+1}\frac{1}{(2n)!}(2n+2)!\left(\frac{na}{2}\right)^{2n+3} = (2n+2)(2n+1)\left(\frac{na}{2}\right)^2 = \boxed{\left(n+\frac{1}{2}\right)(n+1)(na)^2.}$$

(c)

$$\sigma_r^2 = \langle r^2\rangle - \langle r\rangle^2 = \left[\left(n+\frac{1}{2}\right)(n+1)(na)^2 - \left(n+\frac{1}{2}\right)^2(na)^2\right]$$
$$= \frac{1}{2}\left(n+\frac{1}{2}\right)(na)^2 = \frac{1}{2(n+1/2)}\langle r\rangle^2; \quad \boxed{\sigma_r = \frac{\langle r\rangle}{\sqrt{2n+1}}.}$$



Maxima occur at: $\frac{dR_{n,n-1}}{dr} = 0 \Rightarrow (n-1)r^{n-2}e^{-r/na} - \frac{1}{na}r^{n-1}e^{-r/na} = 0 \Rightarrow r = na(n-1).$

Problem 4.56

Here are a couple of examples: {32, 28} and {224,56}; {221, 119} and {119, 91}. For further discussion see D. Wyss and W. Wyss, *Foundations of Physics* **23**, 465 (1993).

Problem 4.57

(a) Using Eqs. 3.64 and 4.122: $[A, B] = [x^2, L_z] = x[x, L_z] + [x, L_z]x = x(-i\hbar y) + (-i\hbar y)x = -2i\hbar xy.$

Equation 3.62 $\Rightarrow \sigma_A^2 \sigma_B^2 \geq \left[\frac{1}{2i}(-2i\hbar)\langle xy\rangle\right]^2 = \hbar^2\langle xy\rangle^2 \Rightarrow \boxed{\sigma_A \sigma_B \geq \hbar|\langle xy\rangle|.}$

(b) Equation 4.118 $\Rightarrow \langle B\rangle = \langle L_z\rangle = m\hbar;\quad \langle B^2\rangle = \langle L_z^2\rangle = m^2\hbar^2;\quad$ so $\quad \sigma_B = m^2\hbar^2 - m^2\hbar^2 = \boxed{0.}$

(c) Since the left side of the uncertainty principle is zero, the right side must also be: $\boxed{\langle xy\rangle = 0,}$ for eigenstates of L_z.

Problem 4.58

(a) $1 = |A|^2(1 + 4 + 4) = 9|A|^2;\quad \boxed{A = 1/3.}$

(b) $\boxed{\frac{\hbar}{2},\text{ with probability } \frac{5}{9};\ -\frac{\hbar}{2},\text{ with probability } \frac{4}{9}.}\ \langle S_z\rangle = \frac{5}{9}\frac{\hbar}{2} + \frac{4}{9}\left(-\frac{\hbar}{2}\right) = \boxed{\frac{\hbar}{18}.}$

(c) From Eq. 4.151,

$$c_+^{(x)} = \left(\chi_+^{(x)}\right)^\dagger \chi = \frac{1}{3}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}1-2i\\2\end{pmatrix} = \frac{1}{3\sqrt{2}}(1-2i+2) = \frac{3-2i}{3\sqrt{2}};\quad |c_+^{(x)}|^2 = \frac{9+4}{9\cdot 2} = \frac{13}{18}.$$
$$c_-^{(x)} = \left(\chi_-^{(x)}\right)^\dagger \chi = \frac{1}{3}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\end{pmatrix}\begin{pmatrix}1-2i\\2\end{pmatrix} = \frac{1}{3\sqrt{2}}(1-2i-2) = -\frac{1+2i}{3\sqrt{2}};\quad |c_-^{(x)}|^2 = \frac{1+4}{9\cdot 2} = \frac{5}{18}.$$

$\boxed{\frac{\hbar}{2},\text{ with probability } \frac{13}{18};\ -\frac{\hbar}{2},\text{ with probability } \frac{5}{18}.}\quad \langle S_x\rangle = \frac{13}{18}\frac{\hbar}{2} + \frac{5}{18}\left(-\frac{\hbar}{2}\right) = \boxed{\frac{2\hbar}{9}.}$

(d) From Problem 4.32(a),

$$c_+^{(y)} = \left(\chi_+^{(y)}\right)^\dagger \chi = \frac{1}{3}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\end{pmatrix}\begin{pmatrix}1-2i\\2\end{pmatrix} = \frac{1}{3\sqrt{2}}(1-2i-2i) = \frac{1-4i}{3\sqrt{2}};\quad |c_+^{(y)}|^2 = \frac{1+16}{9\cdot 2} = \frac{17}{18}.$$
$$c_-^{(y)} = \left(\chi_-^{(y)}\right)^\dagger \chi = \frac{1}{3}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & i\end{pmatrix}\begin{pmatrix}1-2i\\2\end{pmatrix} = \frac{1}{3\sqrt{2}}(1-2i+2i) = \frac{1}{3\sqrt{2}};\quad |c_-^{(y)}|^2 = \frac{1}{9\cdot 2} = \frac{1}{18}.$$

$\boxed{\frac{\hbar}{2},\text{ with probability } \frac{17}{18};\ -\frac{\hbar}{2},\text{ with probability } \frac{1}{18}.}\quad \langle S_y\rangle = \frac{17}{18}\frac{\hbar}{2} + \frac{1}{18}\left(-\frac{\hbar}{2}\right) = \boxed{\frac{4\hbar}{9}.}$

Problem 4.59

We may as well choose axes so that $\hat{a}$ lies along the z axis and $\hat{b}$ is in the xz plane. Then $S_a^{(1)} = S_z^{(1)}$, and $S_b^{(2)} = \cos\theta\, S_z^{(2)} + \sin\theta\, S_x^{(2)}$. $\langle 0\ 0|S_a^{(1)}S_b^{(2)}|0\ 0\rangle$ is to be calculated.

$$S_a^{(1)}S_b^{(2)}|0\ 0\rangle = \frac{1}{\sqrt{2}}\left[S_z^{(1)}(\cos\theta\, S_z^{(2)} + \sin\theta\, S_x^{(2)})\right](|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$= \frac{1}{\sqrt{2}}\left[(S_z|\uparrow\rangle)(\cos\theta\, S_z|\downarrow\rangle + \sin\theta\, S_x|\downarrow\rangle) - (S_z|\downarrow\rangle)(\cos\theta\, S_z|\uparrow\rangle + \sin\theta\, S_x|\uparrow\rangle)\right]$$

$$= \frac{1}{\sqrt{2}}\left\{\left(\frac{\hbar}{2}|\uparrow\rangle\right)\left[\cos\theta\left(-\frac{\hbar}{2}|\downarrow\rangle\right) + \sin\theta\left(\frac{\hbar}{2}|\uparrow\rangle\right)\right] - \left(-\frac{\hbar}{2}|\downarrow\rangle\right)\left[\cos\theta\left(\frac{\hbar}{2}|\uparrow\rangle\right) + \sin\theta\left(\frac{\hbar}{2}|\downarrow\rangle\right)\right]\right\} \text{ (using Eq. 4.145)}$$

$$= \frac{\hbar^2}{4}\left[\cos\theta\frac{1}{\sqrt{2}}(-|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) + \sin\theta\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)\right] = \frac{\hbar^2}{4}\left[-\cos\theta|0\ 0\rangle + \sin\theta\frac{1}{\sqrt{2}}(|1\ 1\rangle + |1\ -1\rangle)\right].$$

so $\langle S_a^{(1)}S_b^{(2)}\rangle = \langle 0\ 0|S_a^{(1)}S_b^{(2)}|0\ 0\rangle = \frac{\hbar^2}{4}\langle 0\ 0|\left[-\cos\theta|0\ 0\rangle + \sin\theta\frac{1}{\sqrt{2}}(|1\ 1\rangle + |1\ -1\rangle)\right] = -\frac{\hbar^2}{4}\cos\theta\langle 0\ 0|0\ 0\rangle$

(by orthogonality), and hence $\langle S_a^{(1)}S_b^{(2)}\rangle = -\frac{\hbar^2}{4}\cos\theta$. QED

Problem 4.60

(a) First note from Eq. 4.136 and line after Eq. 4.146 that

$$\begin{aligned}S_x|s\ m\rangle &= \frac{1}{2}\left[S_+|s\ m\rangle + S_-|s\ m\rangle\right]\\ &= \frac{\hbar}{2}\left[\sqrt{s(s+1)-m(m+1)}|s\ m+1\rangle + \sqrt{s(s+1)-m(m-1)}|s\ m-1\rangle\right]\end{aligned}$$

$$\begin{aligned}S_y|s\ m\rangle &= \frac{1}{2i}\left[S_+|s\ m\rangle - S_-|s\ m\rangle\right]\\ &= \frac{\hbar}{2i}\left[\sqrt{s(s+1)-m(m+1)}|s\ m+1\rangle - \sqrt{s(s+1)-m(m-1)}|s\ m-1\rangle\right]\end{aligned}$$

Now, using Eqs. 4.177 and 4.147:

$$S^2|s\ m\rangle = \left[(S^{(1)})^2 + (S^{(2)})^2 + 2(S_x^{(1)}S_x^{(2)} + S_y^{(1)}S_y^{(2)} + S_z^{(1)}S_z^{(2)})\right]\left[A|\tfrac{1}{2}\ \tfrac{1}{2}\rangle|s_2\ m-\tfrac{1}{2}\rangle + B|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|s_2\ m+\tfrac{1}{2}\rangle\right]$$

$$\begin{aligned}&= A\Big\{\left(S^2|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\right)|s_2\ m-\tfrac{1}{2}\rangle + |\tfrac{1}{2}\ \tfrac{1}{2}\rangle\left(S^2|s_2\ m-\tfrac{1}{2}\rangle\right)\\
&\quad +2\Big[\left(S_x|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\right)\left(S_x|s_2\ m-\tfrac{1}{2}\rangle\right) + \left(S_y|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\right)\left(S_y|s_2\ m-\tfrac{1}{2}\rangle\right) + \left(S_z|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\right)\left(S_z|s_2\ m-\tfrac{1}{2}\rangle\right)\Big]\Big\}\\
&\quad +B\Big\{\left(S^2|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle\right)|s_2\ m+\tfrac{1}{2}\rangle + |\tfrac{1}{2}\ -\tfrac{1}{2}\rangle\left(S^2|s_2\ m+\tfrac{1}{2}\rangle\right)\\
&\quad +2\Big[\left(S_x|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle\right)\left(S_x|s_2\ m+\tfrac{1}{2}\rangle\right) + \left(S_y|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle\right)\left(S_y|s_2\ m+\tfrac{1}{2}\rangle\right) + \left(S_z|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle\right)\left(S_z|s_2\ m+\tfrac{1}{2}\rangle\right)\Big]\Big\}\\
&= A\Big\{\tfrac{3}{4}\hbar^2|\tfrac{1}{2}\ \tfrac{1}{2}\rangle|s_2\ m-\tfrac{1}{2}\rangle + \hbar^2 s_2(s_2+1)|\tfrac{1}{2}\ \tfrac{1}{2}\rangle|s_2\ m-\tfrac{1}{2}\rangle\end{aligned}$$

$$+2\Bigg[\tfrac{\hbar}{2}|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle\tfrac{\hbar}{2}\Bigg(\sqrt{s_2(s_2+1)-(m-\tfrac{1}{2})(m+\tfrac{1}{2})}|s_2\ m+\tfrac{1}{2}\rangle$$
$$+\sqrt{s_2(s_2+1)-(m-\tfrac{1}{2})(m-\tfrac{3}{2})}|s_2\ m-\tfrac{3}{2}\rangle\Bigg)$$
$$+\left(\frac{i\hbar}{2}\right)|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle\tfrac{\hbar}{2i}\Bigg(\sqrt{s_2(s_2+1)-(m-\tfrac{1}{2})(m+\tfrac{1}{2})}|s_2\ m+\tfrac{1}{2}\rangle$$
$$-\sqrt{s_2(s_2+1)-(m-\tfrac{1}{2})(m-\tfrac{3}{2})}|s_2\ m-\tfrac{3}{2}\rangle\Bigg)+\tfrac{\hbar}{2}|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\hbar(m-\tfrac{1}{2})|s_2\ m-\tfrac{1}{2}\rangle\Bigg]\Bigg\}$$
$$+B\Bigg\{\tfrac{3}{4}\hbar^2|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|s_2\ m+\tfrac{1}{2}\rangle+\hbar^2 s_2(s_2+1)|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|s_2\ m+\tfrac{1}{2}\rangle$$
$$+2\Bigg[\tfrac{\hbar}{2}|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\tfrac{\hbar}{2}\Bigg(\sqrt{s_2(s_2+1)-(m+\tfrac{1}{2})(m+\tfrac{3}{2})}|s_2\ m+\tfrac{3}{2}\rangle+\sqrt{s_2(s_2+1)-(m+\tfrac{1}{2})(m-\tfrac{1}{2})}|s_2\ m-\tfrac{1}{2}\rangle\Bigg)$$
$$+\left(\frac{-i\hbar}{2}\right)|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\tfrac{\hbar}{2i}\Bigg(\sqrt{s_2(s_2+1)-(m+\tfrac{1}{2})(m+\tfrac{3}{2})}|s_2\ m+\tfrac{3}{2}\rangle$$
$$-\sqrt{s_2(s_2+1)-(m+\tfrac{1}{2})(m-\tfrac{1}{2})}|s_2\ m-\tfrac{1}{2}\rangle\Bigg)+\left(\tfrac{-\hbar}{2}\right)|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle\hbar(m+\tfrac{1}{2})|s_2\ m+\tfrac{1}{2}\rangle\Bigg]\Bigg\}$$
$$=\hbar^2\left\{A\left[\tfrac{3}{4}+s_2(s_2+1)+m-\tfrac{1}{2}\right]+B\sqrt{s_2(s_2+1)-m^2+\tfrac{1}{4}}\right\}|\tfrac{1}{2}\ \tfrac{1}{2}\rangle|s_2\ m-\tfrac{1}{2}\rangle$$
$$+\hbar^2\left\{B\left[\tfrac{3}{4}+s_2(s_2+1)-m-\tfrac{1}{2}\right]+A\sqrt{s_2(s_2+1)-m^2+\tfrac{1}{4}}\right\}|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|s_2\ m+\tfrac{1}{2}\rangle$$
$$=\hbar^2 s(s+1)|s\ m\rangle=\hbar^2 s(s+1)\Big[A|\tfrac{1}{2}\ \tfrac{1}{2}\rangle|s_2\ m-\tfrac{1}{2}\rangle+B|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|s_2\ m+\tfrac{1}{2}\rangle\Big].$$

$$\left\{\begin{array}{ll} A\left[s_2(s_2+1)+\tfrac{1}{4}+m\right] & +B\sqrt{s_2(s_2+1)-m^2+\tfrac{1}{4}}=s(s+1)A, \\ B\left[s_2(s_2+1)+\tfrac{1}{4}-m\right] & +A\sqrt{s_2(s_2+1)-m^2+\tfrac{1}{4}}=s(s+1)B, \end{array}\right\}\quad\text{or}$$

$$\left\{\begin{array}{ll} A\left[s_2(s_2+1)-s(s+1)+\tfrac{1}{4}+m\right] & +B\sqrt{s_2(s_2+1)-m^2+\tfrac{1}{4}}=0, \\ B\left[s_2(s_2+1)-s(s+1)+\tfrac{1}{4}-m\right] & +A\sqrt{s_2(s_2+1)-m^2+\tfrac{1}{4}}=0, \end{array}\right\}\quad\text{or}\quad\left\{\begin{array}{ll} A(a+m) & +Bb=0 \\ B(a-m) & +Ab=0 \end{array}\right\},$$

where $a\equiv s_2(s_2+1)-s(s+1)+\frac{1}{4},\ b\equiv\sqrt{s_2(s_2+1)-m^2+\frac{1}{4}}$. Multiply by $(a-m)$ and b, then subtract:
$A(a^2-m^2)+Bb(a-m)=0;\ Bb(a-m)+Ab^2=0\Rightarrow A(a^2-m^2-b^2)=0\Rightarrow a^2-b^2=m^2,$ or:
$\left[s_2(s_2+1)-s(s+1)+\frac{1}{4}\right]^2-s_2(s_2+1)+m^2-\frac{1}{4}=m^2,$
$\left[s_2(s_2+1)-s(s+1)+\frac{1}{4}\right]^2=s_2^2+s_2+\frac{1}{4}=\left(s_2+\frac{1}{2}\right)^2$, so
$s_2(s_2+1)-s(s+1)+\frac{1}{4}=\pm\left(s_2+\frac{1}{2}\right);\quad s(s+1)=s_2(s_2+1)\mp\left(s_2+\frac{1}{2}\right)+\frac{1}{4}.$
Add $\frac{1}{4}$ to both sides:

$$s^2+s+\tfrac{1}{4}=\left(s+\tfrac{1}{2}\right)^2=s_2(s_2+1)\mp\left(s_2+\tfrac{1}{2}\right)+\tfrac{1}{2}=\left\{\begin{array}{l} s_2^2+s_2-s_2-\tfrac{1}{2}+\tfrac{1}{2}=s_2^2 \\ \\ s_2^2+s_2+s_2+\tfrac{1}{2}+\tfrac{1}{2}=(s_2+1)^2 \end{array}\right\}.$$

So $\left\{\begin{array}{ll} s+\frac{1}{2}=\pm s_2 & \Rightarrow s=\pm s_2-\frac{1}{2}=\left\{\begin{array}{l} s_2-\frac{1}{2} \\ -s_2-\frac{1}{2} \end{array}\right. \\ s+\frac{1}{2}=\pm(s_2+1) & \Rightarrow s=\pm(s_2+1)-\frac{1}{2}=\left\{\begin{array}{l} s_2+\frac{1}{2} \\ -s_2-\frac{3}{2} \end{array}\right. \end{array}\right\}.$

But $s \geq 0$, so the possibilities are $\boxed{s = s_2 \pm 1/2.}$ Then:

$$a = s_2^2 + s_2 - \left(s_2 \pm \frac{1}{2}\right)\left(s_2 \pm \frac{1}{2} + 1\right) + \frac{1}{4}$$
$$= s_2^2 + s_2 - s_2^2 \mp \frac{1}{2}s_2 - s_2 \mp \frac{1}{2}s_2 - \frac{1}{4} \mp \frac{1}{2} + \frac{1}{4} = \mp s_2 \mp \frac{1}{2} = \mp\left(s_2 + \frac{1}{2}\right).$$
$$b = \sqrt{\left(s_2^2 + s_2 + \frac{1}{4}\right) - m^2} = \sqrt{\left(s_2 + \frac{1}{2}\right)^2 - m^2} = \sqrt{\left(s_2 + \frac{1}{2} + m\right)\left(s_2 + \frac{1}{2} - m\right)}.$$

$$\therefore A\left[\mp\left(s_2 + \tfrac{1}{2}\right) + m\right] = \mp A\left(s_2 + \tfrac{1}{2} \mp m\right) = -Bb = -B\sqrt{\left(s_2 + \tfrac{1}{2} + m\right)\left(s_2 + \tfrac{1}{2} - m\right)}$$
$$\Rightarrow A\sqrt{s_2 + \tfrac{1}{2} \mp m} = \pm B\sqrt{s_2 + \tfrac{1}{2} \pm m}. \quad \text{But } |A|^2 + |B|^2 = 1, \quad \text{so}$$

$$|A|^2 + |A|^2\left(\frac{s_2 + \frac{1}{2} \mp m}{s_2 + \frac{1}{2} \pm m}\right) = \frac{|A|^2}{(s_2 + \frac{1}{2} \pm m)}\left[s_2 + \frac{1}{2} \pm m + s_2 + \frac{1}{2} \mp m\right] = \frac{(2s_2 + 1)}{(s_2 + \frac{1}{2} \pm m)}|A|^2 = 1.$$

$$\Rightarrow \boxed{A = \sqrt{\frac{s_2 \pm m + \frac{1}{2}}{2s_2 + 1}}.} \quad B = \pm A\frac{\sqrt{s_2 + \frac{1}{2} \mp m}}{\sqrt{s_2 + \frac{1}{2} \pm m}} = \boxed{\pm\sqrt{\frac{s_2 \mp m + \frac{1}{2}}{2s_2 + 1}}.}$$

(b) Here are four examples:

(i) From the $1/2 \times 1/2$ table ($s_2 = 1/2$), pick $s = 1$ (upper signs), $m = 0$. Then
$A = \sqrt{\frac{\frac{1}{2}+0+\frac{1}{2}}{1+1}} = \frac{1}{\sqrt{2}}$; $\quad B = \sqrt{\frac{\frac{1}{2}-0+\frac{1}{2}}{1+1}} = \frac{1}{\sqrt{2}}$.

(ii) From the $1 \times 1/2$ table ($s_2 = 1$), pick $s = 3/2$ (upper signs), $m = 1/2$. Then
$A = \sqrt{\frac{1+\frac{1}{2}+\frac{1}{2}}{2+1}} = \sqrt{\frac{2}{3}}$; $\quad B = \sqrt{\frac{1-\frac{1}{2}+\frac{1}{2}}{2+1}} = \frac{1}{\sqrt{3}}$.

(iii) From the $3/2 \times 1/2$ table ($s_2 = 3/2$), pick $s = 1$ (lower signs), $m = -1$. Then
$A = \sqrt{\frac{\frac{3}{2}+1+\frac{1}{2}}{3+1}} = \frac{\sqrt{3}}{2}$; $\quad B = -\sqrt{\frac{\frac{3}{2}-1+\frac{1}{2}}{3+1}} = -\frac{1}{2}$.

(iv) From the $2 \times 1/2$ table ($s_2 = 2$), pick $s = 3/2$ (lower signs), $m = 1/2$. Then
$A = \sqrt{\frac{2-\frac{1}{2}+\frac{1}{2}}{4+1}} = \sqrt{\frac{2}{5}}$; $\quad B = -\sqrt{\frac{2+\frac{1}{2}+\frac{1}{2}}{4+1}} = -\sqrt{\frac{3}{5}}$.

These all check with the values on Table 4.8, except that the signs (which are conventional) are reversed in (iii) and (iv). Normalization does not determine the sign of A (nor, therefore, of B).

Problem 4.61

$$|\tfrac{3}{2}\ \tfrac{3}{2}\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}; \quad |\tfrac{3}{2}\ \tfrac{1}{2}\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}; \quad |\tfrac{3}{2}\ \tfrac{-1}{2}\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}; \quad |\tfrac{3}{2}\ \tfrac{-3}{2}\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}. \quad \text{Equation 4.136} \Rightarrow$$

$$\begin{cases} S_+|\tfrac{3}{2}\ \tfrac{3}{2}\rangle = 0, \quad S_+|\tfrac{3}{2}\ \tfrac{1}{2}\rangle = \sqrt{3}\hbar|\tfrac{3}{2}\ \tfrac{3}{2}\rangle, \quad S_+|\tfrac{3}{2}\ \tfrac{-1}{2}\rangle = 2\hbar|\tfrac{3}{2}\ \tfrac{1}{2}\rangle, \quad S_+|\tfrac{3}{2}\ \tfrac{-3}{2}\rangle = \sqrt{3}\hbar|\tfrac{3}{2}\ \tfrac{-1}{2}\rangle; \\ S_-|\tfrac{3}{2}\ \tfrac{3}{2}\rangle = \sqrt{3}\hbar|\tfrac{3}{2}\ \tfrac{1}{2}\rangle, \quad S_-|\tfrac{3}{2}\ \tfrac{1}{2}\rangle = 2\hbar|\tfrac{3}{2}\ \tfrac{-1}{2}\rangle, \quad S_-|\tfrac{3}{2}\ \tfrac{-1}{2}\rangle = \sqrt{3}\hbar|\tfrac{3}{2}\ \tfrac{-3}{2}\rangle, \quad S_-|\tfrac{3}{2}\ \tfrac{-3}{2}\rangle = 0. \end{cases}$$

$$\text{So:}\quad S_+ = \hbar\begin{pmatrix}0 & \sqrt{3} & 0 & 0\\ 0 & 0 & 2 & 0\\ 0 & 0 & 0 & \sqrt{3}\\ 0 & 0 & 0 & 0\end{pmatrix};\quad S_- = \hbar\begin{pmatrix}0 & 0 & 0 & 0\\ \sqrt{3} & 0 & 0 & 0\\ 0 & 2 & 0 & 0\\ 0 & 0 & \sqrt{3} & 0\end{pmatrix};\quad S_x = \frac{1}{2}(S_+ + S_-) = \boxed{\frac{\hbar}{2}\begin{pmatrix}0 & \sqrt{3} & 0 & 0\\ \sqrt{3} & 0 & 2 & 0\\ 0 & 2 & 0 & \sqrt{3}\\ 0 & 0 & \sqrt{3} & 0\end{pmatrix}}.$$

$$\begin{vmatrix}-\lambda & \sqrt{3} & 0 & 0\\ \sqrt{3} & -\lambda & 2 & 0\\ 0 & 2 & -\lambda & \sqrt{3}\\ 0 & 0 & \sqrt{3} & -\lambda\end{vmatrix} = -\lambda\begin{vmatrix}-\lambda & 2 & 0\\ 2 & -\lambda & \sqrt{3}\\ 0 & \sqrt{3} & -\lambda\end{vmatrix} - \sqrt{3}\begin{vmatrix}\sqrt{3} & 2 & 0\\ 0 & -\lambda & \sqrt{3}\\ 0 & \sqrt{3} & -\lambda\end{vmatrix}$$

$$= -\lambda\left[-\lambda^3 + 3\lambda + 4\lambda\right] - \sqrt{3}\left[\sqrt{3}\lambda^2 - 3\sqrt{3}\right] = \lambda^4 - 7\lambda^2 - 3\lambda^2 + 9 = 0,$$

or $\lambda^4 - 10\lambda^2 + 9 = 0$; $\quad (\lambda^2 - 9)(\lambda^2 - 1) = 0$; $\quad \lambda = \pm 3, \pm 1$. So the eigenvalues of S_x are $\boxed{\frac{3}{2}\hbar,\ \frac{1}{2}\hbar,\ -\frac{1}{2}\hbar,\ -\frac{3}{2}\hbar.}$

Problem 4.62

From Eq. 4.135, $S_z|s\,m\rangle = \hbar m|s\,m\rangle$. Since s is fixed, here, let's just identify the states by the value of m (which runs from $-s$ to $+s$). The matrix elements of S_z are

$$\mathsf{S}_{nm} = \langle n|S_z|m\rangle = \hbar m\langle n|m\rangle = \hbar m\delta_{n\,m}.$$

It's a *diagonal* matrix, with elements $m\hbar$, ranging from $m = s$ in the upper left corner to $m = -s$ in the lower right corner:

$$\mathsf{S}_z = \hbar\begin{pmatrix}s & 0 & 0 & \cdots & 0\\ 0 & s-1 & 0 & \cdots & 0\\ 0 & 0 & s-2 & \cdots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & \cdots & -s\end{pmatrix}.$$

From Eq. 4.136,

$$S_\pm|s\,m\rangle = \hbar\sqrt{s(s+1) - m(m\pm 1)}\,|s\,(m\pm 1)\rangle = \hbar\sqrt{(s\mp m)(s\pm m+1)}\,|s\,(m\pm 1)\rangle.$$

$$(\mathsf{S}_+)_{nm} = \langle n|S_+|m\rangle = \hbar\sqrt{(s-m)(s+m+1)}\,\langle n|m+1\rangle = \hbar b_{m+1}\delta_{n\,(m+1)} = \hbar b_n\delta_{n\,(m+1)}.$$

All nonzero elements have row index (n) one greater than the column index (m), so they are on the diagonal just *above* the main diagonal (note that the indices go *down*, here: s, $s-1$, $s-2\ldots$, $-s$):

$$\mathsf{S}_+ = \hbar\begin{pmatrix}0 & b_s & 0 & 0 & \cdots & 0\\ 0 & 0 & b_{s-1} & 0 & \cdots & 0\\ 0 & 0 & 0 & b_{s-2} & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & 0 & \cdots & b_{-s+1}\\ 0 & 0 & 0 & 0 & \cdots & 0\end{pmatrix}.$$

Similarly

$$(\mathsf{S}_-)_{nm} = \langle n|S_-|m\rangle = \hbar\sqrt{(s+m)(s-m+1)}\,\langle n|m-1\rangle = \hbar b_m\delta_{n\,(m-1)}.$$

This time the nonzero elements are on the diagonal just *below* the main diagonal:

$$\mathsf{S}_- = \hbar \begin{pmatrix} 0 & 0 & 0 \cdots & 0 & 0 \\ b_s & 0 & 0 \cdots & 0 & 0 \\ 0 & b_{s-1} & 0 \cdots & 0 & 0 \\ \vdots & \vdots & \vdots \ddots & \vdots & \vdots \\ 0 & 0 & 0 \cdots & b_{-s+1} & 0 \end{pmatrix}.$$

To construct $\mathsf{S}_x = \frac{1}{2}(\mathsf{S}_+ + \mathsf{S}_-)$ and $\mathsf{S}_y = \frac{1}{2i}(\mathsf{S}_+ - \mathsf{S}_-)$, simply add and subtract the matrices S_+ and S_-:

$$\mathsf{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & b_s & 0 & 0 & \cdots & 0 & 0 \\ b_s & 0 & b_{s-1} & 0 & \cdots & 0 & 0 \\ 0 & b_{s-1} & 0 & b_{s-2} & \cdots & 0 & 0 \\ 0 & 0 & b_{s-2} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & b_{-s+1} \\ 0 & 0 & 0 & 0 & \cdots & b_{-s+1} & 0 \end{pmatrix}; \quad \mathsf{S}_y = \frac{\hbar}{2i}\begin{pmatrix} 0 & b_s & 0 & 0 & \cdots & 0 & 0 \\ -b_s & 0 & b_{s-1} & 0 & \cdots & 0 & 0 \\ 0 & -b_{s-1} & 0 & b_{s-2} & \cdots & 0 & 0 \\ 0 & 0 & -b_{s-2} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & b_{-s+1} \\ 0 & 0 & 0 & 0 & \cdots & -b_{-s+1} & 0 \end{pmatrix}.$$

Problem 4.63

$L_+ Y_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m+1)}\,Y_\ell^{m+1}$ (Eqs. 4.120 and 121). Equation 4.130 $\Rightarrow$

$$\hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right) K_\ell^m e^{im\phi} P_\ell^m(\cos\theta) = \hbar\sqrt{\ell(\ell+1) - m(m+1)}\,K_\ell^{m+1} e^{i(m+1)\phi} P_\ell^{m+1}(\cos\theta).$$

$$K_\ell^m\left(\frac{d}{d\theta} - m\cot\theta\right) P_\ell^m(\cos\theta) = \sqrt{\ell(\ell+1) - m(m+1)}\,K_\ell^{m+1} P_\ell^{m+1}(\cos\theta).$$

Let $x \equiv \cos\theta$; $\cot\theta = \dfrac{\cos\theta}{\sin\theta} = \dfrac{x}{\sqrt{1-x^2}}$; $\dfrac{d}{d\theta} = \dfrac{dx}{d\theta}\dfrac{d}{dx} = -\sin\theta\dfrac{d}{dx} = -\sqrt{1-x^2}\dfrac{d}{dx}$. So, using 4.226:

$$K_\ell^m\left[-\sqrt{1-x^2}\frac{d}{dx} - m\frac{x}{\sqrt{1-x^2}}\right] P_\ell^m(x) = -K_\ell^m\frac{1}{\sqrt{1-x^2}}\left[(1-x^2)\frac{dP_\ell^m}{dx} + mxP_\ell^m\right] = K_\ell^m\,P_\ell^{m+1}$$

$$= \sqrt{\ell(\ell+1) - m(m+1)}\,K_\ell^{m+1} P_\ell^{m+1}(x). \quad \Rightarrow \quad \boxed{K_\ell^{m+1} = \frac{1}{\sqrt{\ell(\ell+1) - m(m+1)}}K_\ell^m.}$$

Now $\ell(\ell+1) - m(m+1) = (\ell-m)(\ell+m+1)$, so (assuming m is non-negative)

$$K_\ell^{m+1} = \frac{1}{\sqrt{\ell-m}\sqrt{\ell+1+m}}K_\ell^m \Rightarrow K_\ell^1 = \frac{1}{\sqrt{\ell}\sqrt{\ell+1}}K_\ell^0; \quad K_\ell^2 = \frac{1}{\sqrt{\ell-1}\sqrt{\ell+2}}K_\ell^1 = \frac{1}{\sqrt{\ell(\ell-1)}\sqrt{(\ell+1)(\ell+2)}}K_\ell^0;$$

$$K_\ell^3 = \frac{1}{\sqrt{\ell-2}\sqrt{\ell+3}}K_\ell^2 = \frac{1}{\sqrt{(\ell+3)(\ell+2)(\ell+1)\ell(\ell-1)(\ell-2)}}K_\ell^0, \quad \text{etc.}$$

The quantity inside the square root is $[(\ell+m)!/(\ell-m)!]$, so $\boxed{K_\ell^m = \sqrt{\dfrac{(\ell-m)!}{(\ell+m)!}}C(\ell)}$ (where $C(\ell) \equiv K_\ell^0$).

If m is negative, either run the same argument using L_-, or else rewrite the recursion formula as

$$K_\ell^m = \sqrt{\ell(\ell+1) - m(m+1)}\,K_\ell^{m+1}, \text{ so } K_\ell^{-1} = \sqrt{(\ell+1)\ell}\,K_\ell^0,$$

$$K_\ell^{-2} = \sqrt{(\ell+2)(\ell-1)}K_\ell^{-1} = \sqrt{(\ell+1)(\ell+2)\ell(\ell-1)}K_\ell^0,$$

$$K_\ell^{-3} = \sqrt{(\ell+3)(\ell-2)}K_\ell^{-2} = \sqrt{(\ell+3)(\ell+2)(\ell+1)\ell(\ell-1)(\ell-2)}K_\ell^0, \ldots$$

which leads to $K_\ell^{-m} = \sqrt{(\ell+m)!/(\ell-m)!}\,K_\ell^0$, so in fact the same formula holds regardless of the sign of m.

Now, Problem 4.25 says:

$$Y_\ell^\ell = \frac{(-1)^\ell}{2^\ell \ell!}\sqrt{\frac{(2\ell+1)!}{4\pi}}(e^{i\phi}\sin\theta)^\ell = K_\ell^\ell e^{i\ell\phi}P_\ell^\ell(\cos\theta). \quad \text{But (Equation 4.27)}$$

$$P_\ell^\ell(x) = (-1)^\ell(1-x^2)^{\ell/2}\left(\frac{d}{dx}\right)^\ell \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell = (-1)^\ell\frac{(1-x^2)^{\ell/2}}{2^\ell \ell!}\underbrace{\left(\frac{d}{dx}\right)^{2\ell}(x^{2\ell}-\ldots)}_{(2\ell)!}$$

$$= (-1)^\ell\frac{(2\ell)!}{2^\ell \ell!}(1-x^2)^{\ell/2}, \text{ so } P_\ell^\ell(\cos\theta) = (-1)^\ell\frac{(2\ell)!}{2^\ell \ell!}(\sin\theta)^\ell. \quad \text{Therefore}$$

$$\frac{(-1)^\ell}{2^\ell \ell!}\sqrt{\frac{(2\ell+1)!}{4\pi}}(e^{i\phi}\sin\theta)^\ell = K_\ell^\ell e^{i\ell\phi}(-1)^\ell\frac{(2\ell)!}{2^\ell \ell!}(\sin\theta)^\ell \Rightarrow K_\ell^\ell = \frac{1}{(2\ell)!}\sqrt{\frac{(2\ell+1)!}{4\pi}} = \sqrt{\frac{(2\ell+1)}{4\pi(2\ell)!}}.$$

But $K_\ell^\ell = \sqrt{\frac{1}{(2\ell)!}}C(\ell)$, so $\boxed{C(\ell) = \sqrt{\frac{2\ell+1}{4\pi}},}$ and hence $\boxed{K_\ell^m = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}},}$ in agreement with Equation 4.32.

Problem 4.64

(a) For both terms, $\ell = 1$, so $\hbar^2(1)(2) = \boxed{2\hbar^2,\ P = 1.}$

(b) $\boxed{0,\ P = \frac{1}{3},}$ or $\boxed{\hbar,\ P = \frac{2}{3}.}$

(c) $\boxed{\frac{3}{4}\hbar^2,\ P = 1.}$

(d) $\boxed{\frac{\hbar}{2},\ P = \frac{1}{3}}$, or $\boxed{-\frac{\hbar}{2},\ P = \frac{2}{3}.}$

(e) From the $1 \times \frac{1}{2}$ Clebsch-Gordan table (or Problem 4.60):

$\frac{1}{\sqrt{3}}|\frac{1}{2}\ \frac{1}{2}\rangle|1\ 0\rangle + \sqrt{\frac{2}{3}}|\frac{1}{2}\ \frac{-1}{2}\rangle|1\ 1\rangle = \frac{1}{\sqrt{3}}\left[\sqrt{\frac{2}{3}}|\frac{3}{2}\ \frac{1}{2}\rangle - \frac{1}{\sqrt{3}}|\frac{1}{2}\ \frac{1}{2}\rangle\right] + \sqrt{\frac{2}{3}}\left[\frac{1}{\sqrt{3}}|\frac{3}{2}\ \frac{1}{2}\rangle + \sqrt{\frac{2}{3}}|\frac{1}{2}\ \frac{1}{2}\rangle\right]$

$= \left(2\frac{\sqrt{2}}{3}\right)|\frac{3}{2}\ \frac{1}{2}\rangle + \left(\frac{1}{3}\right)|\frac{1}{2}\ \frac{1}{2}\rangle$. So $j = \frac{3}{2}$ or $\frac{1}{2}$. $\boxed{\frac{15}{4}\hbar^2,\ P = \frac{8}{9},}$ or $\boxed{\frac{3}{4}\hbar^2,\ P = \frac{1}{9}.}$

(f) $\boxed{\frac{1}{2}\hbar,\ P = 1.}$

(g)

$$|\psi|^2 = |R_{21}|^2\left\{\frac{1}{3}|Y_1^0|^2\underbrace{(\chi_+^\dagger\chi_+)}_{1}+\frac{\sqrt{2}}{3}\left[Y_1^{0*}Y_1^1\underbrace{(\chi_+^\dagger\chi_-)}_{0}+Y_1^{1*}Y_1^0\underbrace{(\chi_-^\dagger\chi_+)}_{0}\right]+\frac{2}{3}|Y_1^1|^2\underbrace{(\chi_-^\dagger\chi_-)}_{1}\right\}$$

$$= \frac{1}{3}|R_{21}|^2\left(|Y_1^0|^2+2|Y_1^1|^2\right) = \frac{1}{3}\cdot\frac{1}{24}\cdot\frac{1}{a^3}\cdot\frac{r^2}{a^2}e^{-r/a}\left[\frac{3}{4\pi}\cos^2\theta+2\frac{3}{8\pi}\sin^2\theta\right] \quad \text{[Tables 4.3, 4.7]}$$

$$= \frac{1}{3\cdot 24\cdot a^5}r^2e^{-r/a}\cdot\frac{3}{4\pi}(\cos^2\theta+\sin^2\theta) = \boxed{\frac{1}{96\pi a^5}r^2e^{-r/a}.}$$

(h)

$$r^2\frac{1}{3}|R_{21}|^2\int|Y_1^0|^2\sin\theta\,d\theta\,d\phi = \frac{r^2}{3}|R_{21}|^2 = \frac{1}{3}\cdot\frac{1}{24a^3}r^4e^{-r/a} = \boxed{\frac{1}{72a^5}r^4e^{-r/a}.}$$

Problem 4.65

Quartet. $\boxed{|\frac{3}{2}\frac{3}{2}\rangle = |\uparrow\uparrow\uparrow\rangle.}$ For one particle (Equation 4.146), $S_-|\uparrow\rangle = \hbar|\downarrow\rangle$, $S_-|\downarrow\rangle = 0$. For all three, $\mathbf{S} = \mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3 \Rightarrow S_- = S_{1-}+S_{2-}+S_{3-}$. So (using Equations 4.120 and 4.121):

$$S_-|\tfrac{3}{2}\tfrac{3}{2}\rangle = S_-|\uparrow\uparrow\uparrow\rangle = \hbar\left(|\downarrow\uparrow\uparrow\rangle+|\uparrow\downarrow\uparrow\rangle+|\uparrow\uparrow\downarrow\rangle\right) = B_{3/2}^{3/2}|\tfrac{3}{2}\tfrac{1}{2}\rangle = \sqrt{3}\hbar|\tfrac{3}{2}\tfrac{1}{2}\rangle$$

$$\Rightarrow \boxed{|\tfrac{3}{2}\tfrac{1}{2}\rangle = \frac{1}{\sqrt{3}}\left(|\downarrow\uparrow\uparrow\rangle+|\uparrow\downarrow\uparrow\rangle+|\uparrow\uparrow\downarrow\rangle\right).}$$

$$S_-|\tfrac{3}{2}\tfrac{1}{2}\rangle = \frac{\hbar}{\sqrt{3}}\left(|\downarrow\downarrow\uparrow\rangle+|\downarrow\uparrow\downarrow\rangle+|\downarrow\downarrow\uparrow\rangle+|\uparrow\downarrow\downarrow\rangle+|\downarrow\uparrow\downarrow\rangle+|\uparrow\downarrow\downarrow\rangle\right) = \frac{2\hbar}{\sqrt{3}}\left(|\downarrow\downarrow\uparrow\rangle+|\downarrow\uparrow\downarrow\rangle+|\uparrow\downarrow\downarrow\rangle\right)$$

$$= B_{3/2}^{1/2}|\tfrac{3}{2}\tfrac{-1}{2}\rangle = 2\hbar|\tfrac{3}{2}\tfrac{-1}{2}\rangle \Rightarrow \boxed{|\tfrac{3}{2}\tfrac{-1}{2}\rangle = \frac{1}{\sqrt{3}}\left(|\downarrow\downarrow\uparrow\rangle+|\downarrow\uparrow\downarrow\rangle+|\uparrow\downarrow\downarrow\rangle\right).}$$

$$S_-|\tfrac{3}{2}\tfrac{-1}{2}\rangle = \frac{\hbar}{\sqrt{3}}\left(|\downarrow\downarrow\downarrow\rangle+|\downarrow\downarrow\downarrow\rangle+|\downarrow\downarrow\downarrow\rangle\right) = \sqrt{3}\hbar|\downarrow\downarrow\downarrow\rangle = B_{3/2}^{-1/2}|\tfrac{3}{2}\tfrac{-3}{2}\rangle = \sqrt{3}\hbar|\tfrac{3}{2}\tfrac{-3}{2}\rangle$$

$$\Rightarrow \boxed{|\tfrac{3}{2}\tfrac{-3}{2}\rangle = |\downarrow\downarrow\downarrow\rangle.}$$

Doublet 1. $\boxed{|\frac{1}{2}\frac{1}{2}\rangle_1 = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\rangle\right).}$

$$S_-|\tfrac{1}{2}\tfrac{1}{2}\rangle_1 = \frac{\hbar}{\sqrt{2}}\left(|\downarrow\downarrow\uparrow\rangle+|\uparrow\downarrow\downarrow\rangle-|\downarrow\downarrow\uparrow\rangle-|\downarrow\uparrow\downarrow\rangle\right) = \frac{\hbar}{\sqrt{2}}\left(|\uparrow\downarrow\downarrow\rangle-|\downarrow\uparrow\downarrow\rangle\right)$$

$$= B_{1/2}^{1/2}|\tfrac{1}{2}\tfrac{-1}{2}\rangle_1 = \hbar|\tfrac{1}{2}\tfrac{-1}{2}\rangle_1 \Rightarrow \boxed{|\tfrac{1}{2}\tfrac{-1}{2}\rangle_1 = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\downarrow\rangle-|\downarrow\uparrow\downarrow\rangle\right).}$$

Doublet 2. $|\frac{1}{2}\frac{1}{2}\rangle_2 = a|\uparrow\uparrow\downarrow\rangle+b|\uparrow\downarrow\uparrow\rangle+c|\downarrow\uparrow\uparrow\rangle$. Make it orthogonal to $|\frac{1}{2}\frac{1}{2}\rangle_1$ and $|\frac{3}{2}\frac{1}{2}\rangle$:

$${}_1\langle\tfrac{1}{2}\tfrac{1}{2}|\tfrac{1}{2}\tfrac{1}{2}\rangle_2 = \frac{1}{\sqrt{2}}(\langle\uparrow\downarrow\uparrow|-\langle\downarrow\uparrow\uparrow|)(a|\uparrow\uparrow\downarrow\rangle+b|\uparrow\downarrow\uparrow\rangle+c|\downarrow\uparrow\uparrow\rangle) = \frac{1}{\sqrt{2}}(b-c) = 0 \;\Rightarrow\; c = b.$$

$$\langle \tfrac{3}{2}\tfrac{1}{2}|\tfrac{1}{2}\tfrac{1}{2}\rangle_2 = \frac{1}{\sqrt{3}}(\langle\downarrow\uparrow\uparrow| + \langle\uparrow\downarrow\uparrow| + \langle\uparrow\uparrow\downarrow|)(a|\uparrow\uparrow\downarrow\rangle + b|\uparrow\downarrow\uparrow\rangle + c|\downarrow\uparrow\uparrow\rangle) = \frac{1}{\sqrt{3}}(a+b+c) = 0 \;\Rightarrow\; a = -2b.$$

Normalization: $|a|^2 + |b|^2 + |c|^2 = 1 \Rightarrow 4|b|^2 + |b|^2 + |b|^2 = 6|b|^2 = 1 \;\Rightarrow\; b = \frac{1}{\sqrt{6}},\ c = \frac{1}{\sqrt{6}},\ a = -\frac{2}{\sqrt{6}}.$

$$\boxed{|\tfrac{1}{2}\tfrac{1}{2}\rangle_2 = \frac{1}{\sqrt{6}}(-2|\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle).}$$

$$\begin{aligned} S_-|\tfrac{1}{2}\tfrac{1}{2}\rangle_2 &= \frac{\hbar}{\sqrt{6}}\left(-2|\downarrow\uparrow\downarrow\rangle - 2|\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\downarrow\rangle\right) \\ &= \frac{\hbar}{\sqrt{6}}\left(-|\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\rangle + 2|\downarrow\downarrow\uparrow\rangle\right) = B^{1/2}_{1/2}|\tfrac{1}{2}\tfrac{-1}{2}\rangle_2 = \hbar|\tfrac{1}{2}\tfrac{-1}{2}\rangle_2. \end{aligned}$$

$$\boxed{|\tfrac{1}{2}\tfrac{-1}{2}\rangle_2 = \frac{1}{\sqrt{6}}\left(-|\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\rangle + 2|\downarrow\downarrow\uparrow\rangle\right).}$$

Problem 4.66

From Problem 4.31 we know that in the generic state $\chi = \begin{pmatrix} a \\ b \end{pmatrix}$ (with $|a|^2 + |b|^2 = 1$),

$$\langle S_z\rangle = \frac{\hbar}{2}\left(|a|^2 - |b|^2\right), \quad \langle S_x\rangle = \hbar\mathrm{Re}(ab^*), \quad \langle S_y\rangle = -\hbar\mathrm{Im}(ab^*); \quad \langle S_x^2\rangle = \langle S_y^2\rangle = \frac{\hbar^2}{4}.$$

Writing $a = |a|e^{i\phi_a}$, $b = |b|e^{i\phi_b}$, we have $ab^* = |a||b|e^{i(\phi_a-\phi_b)} = |a||b|e^{i\theta}$, where $\theta \equiv \phi_a - \phi_b$ is the phase difference between a and b. Then

$$\langle S_x\rangle = \hbar\mathrm{Re}(|a||b|e^{i\theta}) = \hbar|a||b|\cos\theta, \quad \langle S_y\rangle = -\hbar\mathrm{Im}(|a||b|e^{i\theta}) = -\hbar|a||b|\sin\theta.$$

$$\sigma^2_{S_x} = \langle S_x^2\rangle - \langle S_x\rangle^2 = \frac{\hbar^2}{4} - \hbar^2|a|^2|b|^2\cos^2\theta; \quad \sigma^2_{S_y} = \langle S_y^2\rangle - \langle S_y\rangle^2 = \frac{\hbar^2}{4} - \hbar^2|a|^2|b|^2\sin^2\theta.$$

We want $\sigma^2_{S_x}\sigma^2_{S_y} = \frac{\hbar^2}{4}\langle S_z\rangle^2$, or

$$\frac{\hbar^2}{4}\left(1 - 4|a|^2|b|^2\cos^2\theta\right)\frac{\hbar^2}{4}\left(1 - 4|a|^2|b|^2\sin^2\theta\right) = \frac{\hbar^2}{4}\frac{\hbar^2}{4}\left(|a|^2 - |b|^2\right)^2.$$

$$1 - 4|a|^2|b|^2\left(\cos^2\theta + \sin^2\theta\right) + 16|a|^4|b|^4\sin^2\theta\cos^2\theta = |a|^4 - 2|a|^2|b|^2 + |b|^4.$$

$$1 + 16|a|^4|b|^4\sin^2\theta\cos^2\theta = |a|^4 + 2|a|^2|b|^2 + |b|^4 = \left(|a|^2 + |b|^2\right)^2 = 1 \quad \Rightarrow |a|^2|b|^2\sin\theta\cos\theta = 0.$$

So either $\theta = 0$ or π, in which case a and b are relatively real, or else $\theta = \pm\pi/2$, in which case a and b are relatively imaginary (these two options subsume trivially the solutions $a = 0$ and $b = 0$).

Problem 4.67

(a) $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 \Rightarrow S^2 = S_1^2 + S_2^2 + S_3^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 + 2\mathbf{S}_1 \cdot \mathbf{S}_3 + 2\mathbf{S}_2 \cdot \mathbf{S}_3$, so $H = \frac{1}{2}J(S^2 - S_1^2 - S_2^2 - S_3^2)$.

But $S_i^2 = \hbar^2 s(s+1) = \frac{3}{4}\hbar^2$ (because they all have spin 1/2), so $\boxed{H = \frac{1}{2}J\left(S^2 - \frac{9}{4}\hbar^2\right).}$

(b) $S^2 = s(s+1)\hbar^2$, where s is the total spin. Combine two spin 1/2 states and you get spin 1 or spin 0; add spin 1/2 to spin 1 and you get $1 + \frac{1}{2} = \frac{3}{2}$ or $1 - \frac{1}{2} = \frac{1}{2}$; add $\frac{1}{2}$ to 0 and you get $\frac{1}{2}$. So the total spin is 3/2 (four states) or 1/2 (two states)—and the latter occurs in two different ways. There are $2^3 = 8$ states in all (each of the three could be spin up or spin down), 4 of which carry spin 1/2 (the ground state). The degeneracy of the ground state is $\boxed{4,}$ and its energy is $\frac{1}{2}J\left(\frac{1}{2}\left(\frac{3}{2}\right)\hbar^2 - \frac{9}{4}\hbar^2\right) = \boxed{-\frac{3}{4}\hbar^2 J.}$ (c) $S^2 = S_1^2 + S_2^2 + S_3^2 + S_4^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 + 2\mathbf{S}_1 \cdot \mathbf{S}_3 + 2\mathbf{S}_1 \cdot \mathbf{S}_4 + 2\mathbf{S}_2 \cdot \mathbf{S}_3 + 2\mathbf{S}_2 \cdot \mathbf{S}_4 + 2\mathbf{S}_3 \cdot \mathbf{S}_4$.

$S^2 - (\mathbf{S}_1 + \mathbf{S}_3)^2 - (\mathbf{S}_2 + \mathbf{S}_4)^2 = \cancel{S_1^2} + \cancel{S_2^2} + \cancel{S_3^2} + \cancel{S_4^2} + 2\mathbf{S}_1 \cdot \mathbf{S}_2 + \cancel{2\mathbf{S}_1 \cdot \mathbf{S}_3} + 2\mathbf{S}_1 \cdot \mathbf{S}_4 + 2\mathbf{S}_2 \cdot \mathbf{S}_3 + \cancel{2\mathbf{S}_2 \cdot \mathbf{S}_4} + 2\mathbf{S}_3 \cdot \mathbf{S}_4 - \cancel{S_1^2} - \cancel{S_3^2} - \cancel{2\mathbf{S}_1 \cdot \mathbf{S}_3} - \cancel{S_2^2} - \cancel{S_4^2} - \cancel{2\mathbf{S}_2 \cdot \mathbf{S}_4} = 2\left(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_1 \cdot \mathbf{S}_4 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4\right) = 2H/J$,
so $H = \frac{1}{2}J\left[S^2 - (\mathbf{S}_1 + \mathbf{S}_3)^2 - (\mathbf{S}_2 + \mathbf{S}_4)^2\right]$. QED

Write $H = \frac{1}{2}\hbar^2 J\left[s(s+1) - s_{13}(s_{13}+1) - s_{24}(s_{24}+1)\right]$, where s is the total spin, s_{13} is the spin of the 1,3 combination, and s_{24} that of the 2,4 combination. For the ground state we want s as *small* as possible, and s_{13}, s_{24} as *large* as possible: $s = 0$, $s_{13} = s_{24} = 1$ (the triplet combinations). Then $E = \frac{1}{2}\hbar^2 J(0 - 2 - 2) = \boxed{-2\hbar^2 J.}$

[Are we sure we can construct such a state? From 1 and 3 we can make singlet or triplet combinations; likewise 2 and 4: $\frac{1}{2} \otimes \frac{1}{2} = 1, 0$. If both are in the triplet state we can get a total spin of 2, 1, or 0: $1 \otimes 1 = 2, 1, 0$. So yes: here is the total spin 0 with each pair having total spin 1. By the way, the other possibilities are $1 \otimes 0 = 1$, $0 \otimes 1 = 1$, and $0 \otimes 0 = 0$. Thus the total spin could be

$$\begin{array}{ll} s = 2 & (2s+1) = 5 \text{ states,} \\ s = 1 \text{ (three ways)} & 3 \times 3 = 9 \text{ states,} \\ s = 0 \text{ (two ways)} & 2 \times 1 = 2 \text{ states,} \end{array}$$

a total of $5 + 9 + 2 = 16$ states, which is just right: $2^4 = 16$. But the ground state is unique—there's exactly *one* combination that puts 1,3 and 2,4 in the triplet configuration *and* gets a total spin of 0.]

Problem 4.68

(a) The effective potential is (Equation 4.53): $V(r) = -\dfrac{e^2}{4\pi\epsilon_0}\dfrac{1}{r} + \dfrac{\hbar^2}{2m_e}\dfrac{\ell(\ell+1)}{r^2}$.

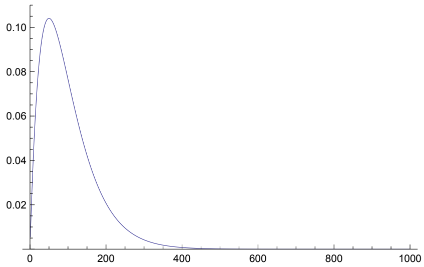
Now $V_j = V(r_j)$, $r_j = j\Delta r$, $\Delta r = \dfrac{b}{N+1}$, $\lambda = \dfrac{\hbar^2}{2m_e(\Delta r)^2}$, so

$$v_j \equiv \frac{V_j}{\lambda} = \frac{2m_e}{\hbar^2}\frac{b^2}{(N+1)^2}\left[-\frac{e^2}{4\pi\epsilon_0}\frac{(N+1)}{jb} + \frac{\hbar^2}{2m_e}\frac{\ell(\ell+1)(N+1)^2}{j^2 b^2}\right]$$
$$= -\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2}\frac{b}{(N+1)}\frac{1}{j} + \frac{\ell(\ell+1)}{j^2} = -\frac{2b}{a(N+1)}\frac{1}{j} + \frac{\ell(\ell+1)}{j^2} = -\frac{2\beta}{j} + \frac{\ell(\ell+1)}{j^2}. \quad \checkmark$$

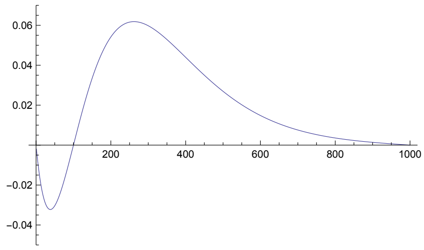
(b) $\Delta r \ll a \ll b \Rightarrow \dfrac{b}{N+1} \ll \dfrac{b}{(N+1)\beta} \ll b \Rightarrow 1 \ll (1/\beta) \ll N+1 \sim N$. ✓ Note that $u(0) = 0$ (Equation 4.59), and $u(b) = 0$, so we have the same boundary conditions as Problem 2.61.

$\underline{\ell = 0}$

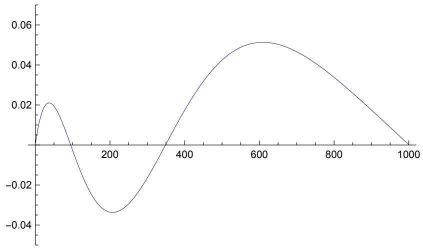
```
h = Table[If[i == j, 2 - (1/(25 j)), 0], {i, 1000}, {j, 1000}]
k = Table[If[i == j + 1, -1, 0], {i, 1000}, {j, 1000}]
m = Table[If[i == j - 1, -1, 0], {i, 1000}, {j, 1000}]
p = Table[h[[i, j]] + k[[i, j]] + m[[i, j]], {i, 1000}, {j, 1000}]
EIG = Eigenvalues[N[p]]
EVE = Eigenvectors[N[p]]
ListLinePlot[EVE[[994]], PlotRange -> {0, 0.11}]
```




```
ListLinePlot[EVE[[997]], PlotRange -> {-0.05, 0.07}]
```




```
ListLinePlot[EVE[[999]], PlotRange -> {-0.05, 0.07}]
```




```
EIG[[994]]
-0.00039996
EIG[[997]]
-0.0000999873
EIG[[999]]
-0.0000399639
```

To get the actual energy (see Equation 2.199), multiply by $\lambda = \frac{\hbar^2(N+1)^2}{2m_e b^2} = \frac{\hbar^2}{2m_e a^2}\frac{1}{\beta^2} = -E_1/\beta^2$; in other words, we must multiply by $1/\beta^2 = 2500$, and the result will be the energy in units of 13.6 eV (the exact answer, of course, would be $-1/n^2 = -1, -0.25, -0.1111$):

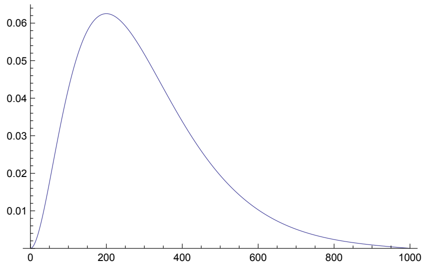
$$-0.00039996\times(2500) = \boxed{0.9999E_1,}\ -0.000099987\times(2500) = \boxed{0.24997E_1,}\ -0.000039964\times(2500) = \boxed{0.09991E_1.}$$

The first two are pretty good; the third is a bit off (but notice from the graph that the wave function has *not* dropped to zero well before $r = b$).

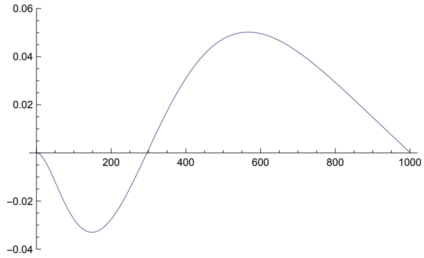
$\ell = 1$

```
h = Table[If[i == j, 2 - (1/(25 j)) + (2/(j^2)), 0], {i, 1000}, {j, 1000}]

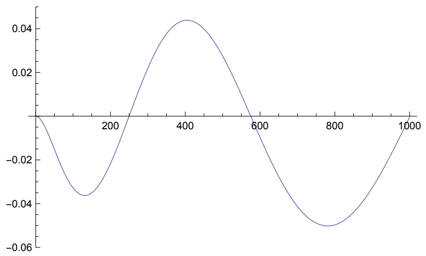
k = Table[If[i == j + 1, -1, 0], {i, 1000}, {j, 1000}]
m = Table[If[i == j - 1, -1, 0], {i, 1000}, {j, 1000}]
p = Table[h[[i, j]] + k[[i, j]] + m[[i, j]], {i, 1000}, {j, 1000}]
EIG = Eigenvalues[N[p]]
EVE = Eigenvectors[N[p]]
ListLinePlot[EVE[[997]], PlotRange -> {0, 0.065}]
```



```
ListLinePlot[EVE[[999]], PlotRange -> {-0.04, 0.06}]
```



```
ListLinePlot[EVE[[1000]], PlotRange -> {-0.06, 0.05}]
```



```
EIG[[997]] * 2500
-0.249991
EIG[[999]] * 2500
-0.103278
EIG[[1000]] * 2500
0.0158618
```

For $\ell = 1$ the lowest state is $n = 2$, so the exact energies (in units of E_1) are 0.25, 0.1111, and 0.0625

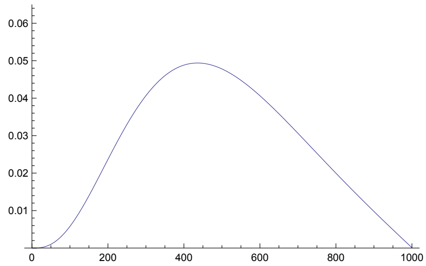
$$\boxed{0.24999E_1,}\ \boxed{0.10328E_1,}\ \boxed{-0.015862E_1.}$$

The first is good; the second is a bit off (but notice from the graph that the wave function has *not* dropped to zero well before $r = b$), and the third is terrible (wrong sign).

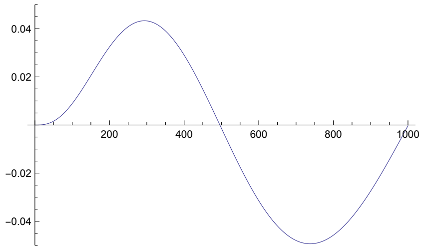
$\underline{\ell = 2}$

```
h = Table[If[i == j, 2 - (1/(25 j)) + (6/(j^2)), 0], {i, 1000}, {j, 1000}]

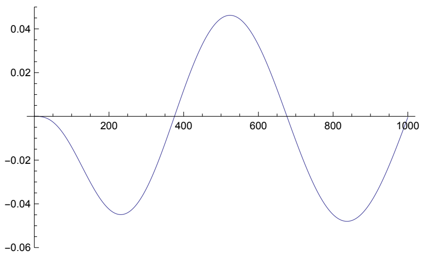
k = Table[If[i == j + 1, -1, 0], {i, 1000}, {j, 1000}]
m = Table[If[i == j - 1, -1, 0], {i, 1000}, {j, 1000}]
p = Table[h[[i, j]] + k[[i, j]] + m[[i, j]], {i, 1000}, {j, 1000}]
EIG = Eigenvalues[N[p]]
EVE = Eigenvectors[N[p]]
ListLinePlot[EVE[[999]], PlotRange -> {0, 0.065}]
```




```
ListLinePlot[EVE[[1000]], PlotRange -> {-0.05, 0.05}]
```




```
ListLinePlot[EVE[[998]], PlotRange -> {-0.06, 0.05}]
```




```
EIG[[999]] * 2500
-0.107958

EIG[[1000]] * 2500
-0.0112765

EIG[[998]] * 2500
0.135962
```

For $\ell = 2$ the lowest state is $n = 3$, so the exact energies (in units of E_1) are 0.1111, 0.0625, and 0.04.

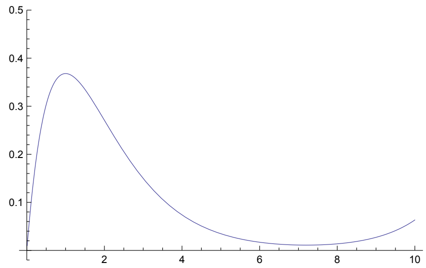
$$\boxed{0.10796E_1,}\ \boxed{0.011277E_1,}\ \boxed{-0.13596E_1.}$$

The first is OK; the second is a way off, and the third is terrible (wrong sign). But in all three cases the wave function has not dropped to zero well before $r = b$. To improve the results we would a substantially larger b.

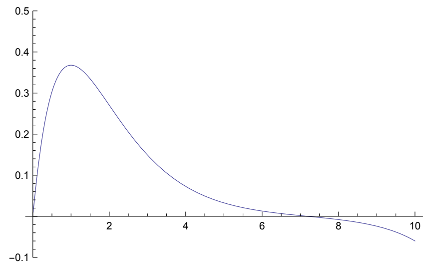
Problem 4.69

$\underline{\ell = 0}$

```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - (2 * 0.9999
        ) / (x + 0.000001)) u[x] == 0, u[0] == 0, u'[0] == 1}, u[x], {x, 10^(-8), 10},
    MaxSteps → 10000]], {x, 0.01, 10}, PlotRange → {-0.02, 0.5}]
```

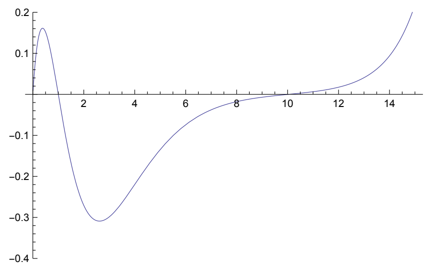



```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - (2 * 1.0001
        ) / (x + 0.000001)) u[x] == 0, u[0] == 0, u'[0] == 1}, u[x], {x, 10^(-8), 10},
    MaxSteps → 10000]], {x, 0.01, 10}, PlotRange → {-0.1, 0.5}]
```

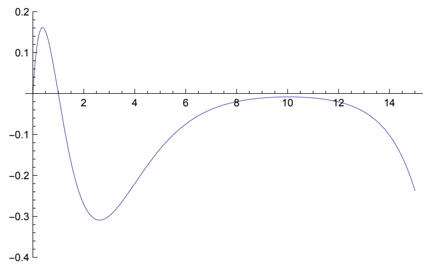


So the lowest n is between 0.9999 and 1.0001.

```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - (2 * 2.0001
        ) / (x + 0.000001)) u[x] == 0, u[0] == 0, u'[0] == 1}, u[x], {x, 10^(-8), 15},
    MaxSteps → 10000]], {x, 0.01, 15}, PlotRange → {-0.4, 0.2}]
```

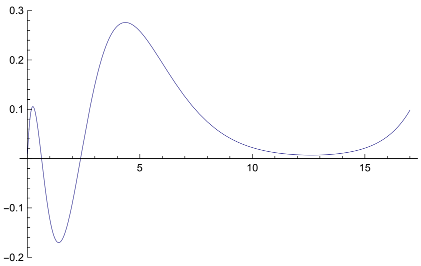



```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - (2 * 1.9999
        ) / (x + 0.000001)) u[x] == 0, u[0] == 0, u'[0] == 1}, u[x], {x, 10^(-8), 15},
    MaxSteps → 10000]], {x, 0.01, 15}, PlotRange → {-0.4, 0.2}]
```

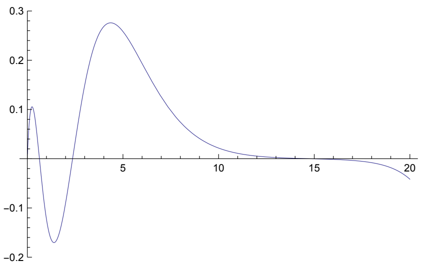


So the next n is between 1.9999 and 2.0001.

```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - (2 * 2.9999
      ) / (x + 0.000001)) u[x] == 0, u[0] == 0, u'[0] == 1}, u[x], {x, 10^(-8), 17},
   MaxSteps → 10 000]], {x, 0.01, 17}, PlotRange → {-0.2, 0.3}]
```



```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - (2 * 3.00001
      ) / (x + 0.000001)) u[x] == 0, u[0] == 0, u'[0] == 1}, u[x], {x, 10^(-8), 20},
   MaxSteps → 10 000]], {x, 0.01, 20}, PlotRange → {-0.2, 0.3}]
```

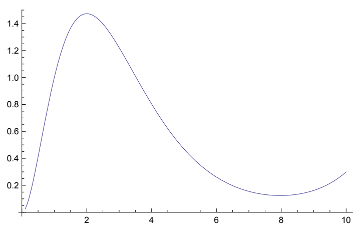


So the third n is between 2.9999 and 3.00001.

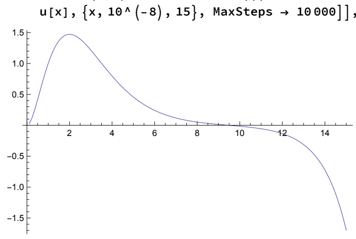
$\underline{\ell = 1}$

This time there is no solution for $n = 1$; the lowest state (no nodes) is around $n = 2$:

```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 1.999) / (x + 0.000001)) +
      (2 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
   u[x], {x, 10^(-8), 10}, MaxSteps → 10 000]], {x, 0.1, 10}]
```

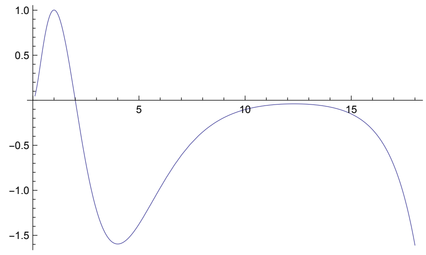


```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 2.0001) / (x + 0.000001)) +
      (2 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
   u[x], {x, 10^(-8), 15}, MaxSteps → 10 000]], {x, 0.1, 15}]
```

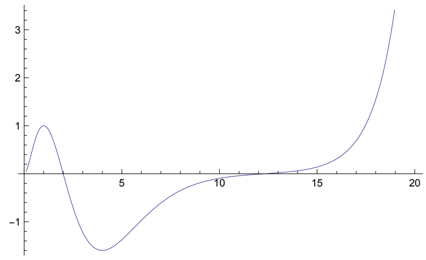


So the lowest n is between 1.999 and 2.0001.

```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 2.9999) / (x + 0.000001)) +
          (2 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
     u[x], {x, 10^(-8), 18}, MaxSteps → 10000]], {x, 0.1, 18}]
```

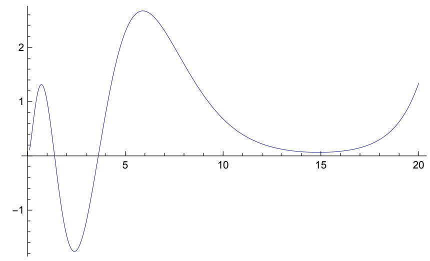


```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 3.0001) / (x + 0.000001)) +
          (2 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
     u[x], {x, 10^(-8), 20}, MaxSteps → 10000]], {x, 0.1, 20}]
```

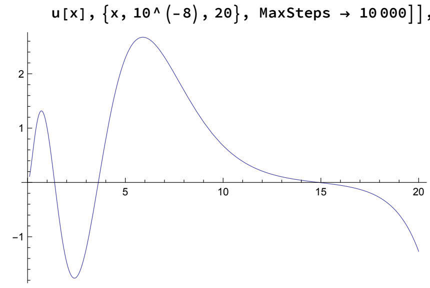


So the next n is between 2.9999 and 3.0001.

```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 3.9999) / (x + 0.000001)) +
          (2 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
     u[x], {x, 10^(-8), 20}, MaxSteps → 10000]], {x, 0.1, 20}]
```



```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 4.0001) / (x + 0.000001)) +
          (2 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
     u[x], {x, 10^(-8), 20}, MaxSteps → 10000]], {x, 0.1, 20}]
```



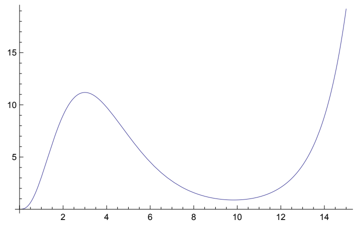
So the third n is between 3.9999 and 4.0001.

$\underline{\ell = 2}$

This time there is no solution for $n = 1$ or $n = 2$; the lowest state (no nodes) is around $n = 3$:

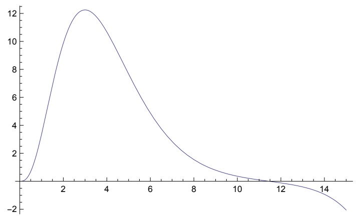
```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 2.999) / (x + 0.000001)) +
        (6 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
    u[x], {x, 10^(-8), 15}, MaxSteps → 10000]], {x, 0.1, 15}]
```

NDSolve::bvluc: The equations derived from the boundary conditions are numerically ill-conditioned. The boundary conditions may not be sufficient to uniquely define a solution. The computed solution may match the boundary conditions poorly. ≫



```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 3.0001) / (x + 0.000001)) +
        (6 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
    u[x], {x, 10^(-8), 15}, MaxSteps → 10000]], {x, 0.1, 15}]
```

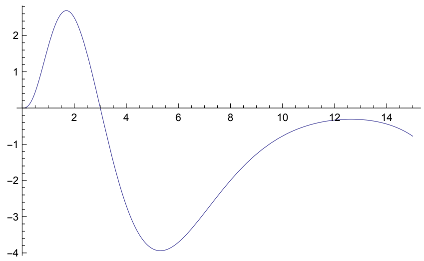
NDSolve::bvluc: The equations derived from the boundary conditions are numerically ill-conditioned. The boundary conditions may not be sufficient to uniquely define a solution. The computed solution may match the boundary conditions poorly. ≫



So the lowest n is between 2.999 and 3.0001.

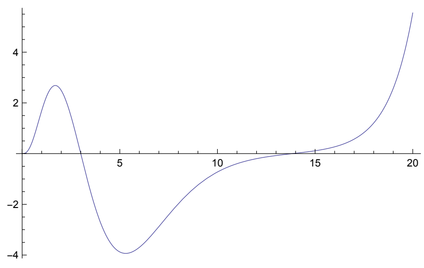
```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 3.999) / (x + 0.000001)) +
        (6 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
    u[x], {x, 10^(-8), 15}, MaxSteps → 10000]], {x, 0.1, 15}]
```

NDSolve::bvluc: The equations derived from the boundary conditions are numerically ill-conditioned. The boundary conditions may not be sufficient to uniquely define a solution. The computed solution may match the boundary conditions poorly. ≫



```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 4.0001
            ) / (x + 0.000001)) +
        (6 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
    u[x], {x, 10^(-8), 20}, MaxSteps → 10000]], {x, 0.1, 20}]
```

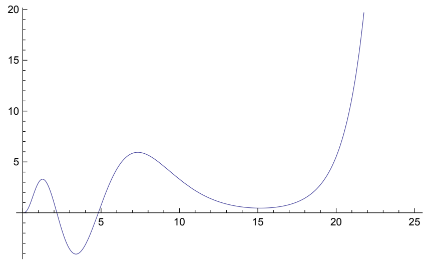
NDSolve::bvluc: The equations derived from the boundary conditions are numerically ill-conditioned. The boundary conditions may not be sufficient to uniquely define a solution. The computed solution may match the boundary conditions poorly. ≫



So the next n is between 3.9999 and 4.0001.

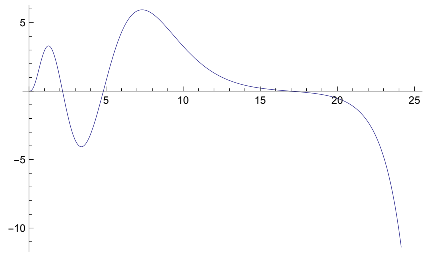
```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 4.999) / (x + 0.000001)) +
        (6 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
     u[x], {x, 10^(-8), 25}, MaxSteps → 10000]], {x, 0.1, 25}]
```

NDSolve::bvluc : The equations derived from the boundary conditions are numerically ill-conditioned. The boundary conditions may not be sufficient to uniquely define a solution. The computed solution may match the boundary conditions poorly. ≫




```
Plot[Evaluate[u[x] /. NDSolve[{u''[x] - (1 - ((2 * 5.0001) / (x + 0.000001)) +
        (6 / (x^2 + 0.000000001))) u[x] == 0, u[1] == 1, u'[0] == 0},
     u[x], {x, 10^(-8), 25}, MaxSteps → 10000]], {x, 0.1, 25}]
```

NDSolve::bvluc : The equations derived from the boundary conditions are numerically ill-conditioned. The boundary conditions may not be sufficient to uniquely define a solution. The computed solution may match the boundary conditions poorly. ≫



So the third n is between 4.9999 and 5.0001.

Problem 4.70

(a) $\boxed{\text{All of them.}}$ (If S_z was measured at t_1, everything was spin up; if S_x was measured, half of them were spin down, but the second measurement did nothing, and these were thrown away.)

(b)

$$P_{++} = \cos^2(\theta_{ab}/2)\cos^2(\theta_{bc}/2), \quad P_{+-} = \cos^2(\theta_{ab}/2)\sin^2(\theta_{bc}/2),$$
$$P_{-+} = \sin^2(\theta_{ab}/2)\cos^2(\bar{\theta}_{bc}/2), \quad P_{--} = \sin^2(\theta_{ab}/2)\sin^2(\bar{\theta}_{bc}/2),$$

where $\bar{\theta} = \pi - \theta$, so $\cos(\bar{\theta}_{bc}/2) = \cos((\pi/2) - \theta_{bc}/2) = \sin(\theta_{bc}/2)$; $\sin(\bar{\theta}_{bc}/2) = \sin((\pi/2) - \theta_{bc}/2) = \cos(\theta_{bc}/2)$. Therefore

$$P_{-+} = \sin^2(\theta_{ab}/2)\sin^2(\theta_{bc}/2), \quad P_{--} = \sin^2(\theta_{ab}/2)\cos^2(\theta_{bc}/2).$$

$$f = \frac{P_{++}}{P_{++} + P_{-+}}, \text{ or } f^{-1} = \frac{\cos^2(\theta_{ab}/2)\cos^2(\theta_{bc}/2) + \sin^2(\theta_{ab}/2)\sin^2(\theta_{bc}/2)}{\cos^2(\theta_{ab}/2)\cos^2(\theta_{bc}/2)} = \boxed{1 + \tan^2(\theta_{ab}/2)\tan^2(\theta_{bc}/2).}$$

Problem 4.71

(a)

$$\psi_{2p_x} = \frac{1}{\sqrt{32\,\pi\,a^3}}\,\frac{r\,\sin\theta\,\cos\phi}{a}\,e^{-r/2a} = \frac{1}{\sqrt{24\,a^3}}\,\frac{r}{a}\,e^{-r/2a}\sqrt{\frac{3}{4\,\pi}}\,\sin\theta\,\frac{e^{i\,\phi}+e^{-i\,\phi}}{2}$$
$$= R_{21}(r)\,\frac{-Y_1^1(\theta,\phi)+Y_1^{-1}(\theta,\phi)}{\sqrt{2}} = \boxed{\frac{1}{\sqrt{2}}\left(-\psi_{211}+\psi_{21-1}\right).}$$

A similar calculation gives

$$\psi_{2p_y} = \boxed{\frac{i}{\sqrt{2}}\left(\psi_{211}+\psi_{21-1}\right).}$$
$$\psi_{2p_z} = \frac{1}{\sqrt{32\pi a^3}}\,\frac{r\cos\theta}{a}e^{-r/2a} = \frac{1}{\sqrt{24a^3}}\,\frac{r}{a}e^{-r/2a}\sqrt{\frac{3}{4\pi}}\cos\theta = R_{21}(r)Y_1^0(\theta,\phi) = \boxed{\psi_{210}.}$$

(b) $\hat{L}_z\,\psi_{2p_z} = \hat{L}_z\,\psi_{210} = 0$, since $m = 0$. By cyclic permutation $(z \to x \to y)$ the same goes for the other two; all three wave functions are eigenstates of the respective components of angular momentum, and the eigenvalue in each case is $\boxed{0.}$

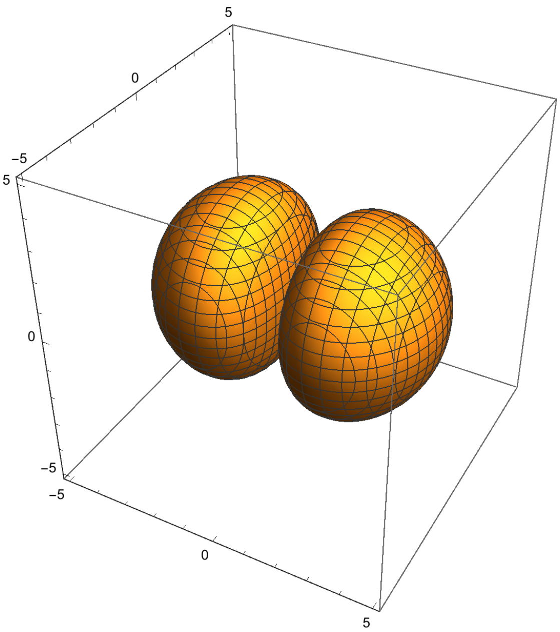
(c) Setting $a = 1/2$, define the three functions:

```
psiX[x_, y_, z_] := x e^(-Sqrt[x^2 + y^2 + z^2]) / Sqrt[π]

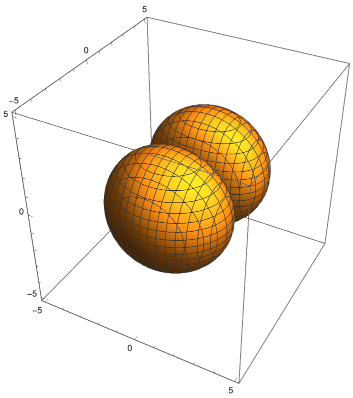
psiY[x_, y_, z_] := y e^(-Sqrt[x^2 + y^2 + z^2]) / Sqrt[π]

psiZ[x_, y_, z_] := z e^(-Sqrt[x^2 + y^2 + z^2]) / Sqrt[π]

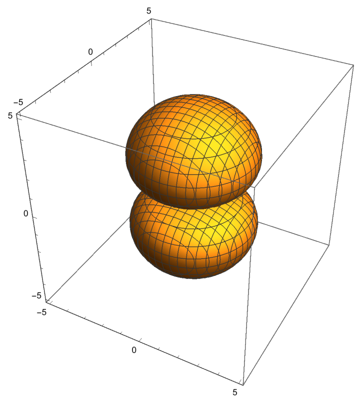
ContourPlot3D[(psiX[x, y, z])^2 == (.03)^2, {x, -5, 5}, {y, -5, 5}, {z, -5, 5}]
```



```
ContourPlot3D[(psiY[x, y, z])^2 == (.03)^2, {x, -5, 5}, {y, -5, 5}, {z, -5, 5}]
```



```
ContourPlot3D[(psiZ[x, y, z])^2 == (.03)^2, {x, -5, 5}, {y, -5, 5}, {z, -5, 5}]
```



Problem 4.72

(a)

$$\mathbf{B} = \nabla \times \mathbf{A} = -\frac{1}{2}\,\nabla \times (\mathbf{r} \times \mathbf{B}_0)$$
$$= -\frac{1}{2}\,[(\mathbf{B}_0 \cdot \nabla)\,\mathbf{r} - (\mathbf{r} \cdot \nabla)\,\mathbf{B}_0 + \mathbf{r}\,(\nabla \cdot \mathbf{B}_0) - \mathbf{B}_0\,(\nabla \cdot \mathbf{r})] = -\frac{1}{2}\,[\mathbf{B}_0 + 0 + 0 - 3\,\mathbf{B}_0] = \mathbf{B}_0. \quad \checkmark$$

(b) The Hamiltonian (Equations 4.188 and 4.158) is

$$H = \frac{1}{2\,m}(\mathbf{p} - q\,\mathbf{A})^2 + q\,\varphi - \gamma\,\mathbf{S} \cdot \mathbf{B}_0 = \frac{p^2}{2\,m} - \frac{q}{2\,m}\,(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + \frac{q^2}{2\,m}\,A^2 + q\,\varphi - \gamma\,\mathbf{S} \cdot \mathbf{B}_0\,.$$

Now

$$A^2 = \frac{1}{4}\,(\mathbf{r} \times \mathbf{B}_0) \cdot (\mathbf{r} \times \mathbf{B}_0) = \frac{1}{4}\,[\mathbf{r} \cdot (\mathbf{B}_0 \times (\mathbf{r} \times \mathbf{B}_0))] = \frac{1}{4}\mathbf{r} \cdot \left[\mathbf{r}B_0^2 - \mathbf{B}_0(\mathbf{r} \cdot \mathbf{B}_0)\right] = \frac{1}{4}\left[r^2\,B_0^2 - (\mathbf{r} \cdot \mathbf{B}_0)^2\right].$$

To evaluate the middle term we use a test function $f(\mathbf{r})$:

$$\mathbf{p} \cdot (\mathbf{A}\,f) + \mathbf{A} \cdot \mathbf{p}\,f = -i\hbar\,[(\nabla \cdot \mathbf{A})\,f + 2\,\mathbf{A} \cdot \nabla f] = \frac{1}{2}\,i\hbar\,[\nabla \cdot (\mathbf{r} \times \mathbf{B}_0)\,f + 2\,(\mathbf{r} \times \mathbf{B}_0) \cdot \nabla f]$$
$$= \frac{1}{2}\,i\hbar\,[\mathbf{B}_0 \cdot \cancel{(\nabla \times \mathbf{r})}\,f - \mathbf{r} \cdot \cancel{(\nabla \times \mathbf{B}_0)}\,f - 2\,\mathbf{B}_0 \cdot (\mathbf{r} \times \nabla\,f)] = \mathbf{B}_0 \cdot \mathbf{L}\,f\,.$$

Combining these expressions gives the desired result.

Problem 4.73

First we compute the velocity

$$\frac{d}{dt}\,\langle z \rangle = \frac{i}{\hbar}\,\langle [H, z] \rangle = \frac{1}{m}\,\langle p_z \rangle\,.$$

Then

$$\frac{d^2}{dt^2}\,\langle z \rangle = \frac{1}{m}\,\frac{d}{dt}\,\langle p_z \rangle = \frac{1}{m}\,\frac{i}{\hbar}\,\langle [H, p_z] \rangle = \frac{1}{m}\,\frac{i}{\hbar}\,\langle [-\gamma\,\mathbf{B} \cdot \mathbf{S}, p_z] \rangle = -\frac{\gamma}{m}\,\frac{i}{\hbar}\,\langle [\mathbf{B}, p_z] \rangle \cdot \mathbf{S}$$
$$= -\frac{\gamma}{m}\,\frac{i}{\hbar}\,\left\langle \left[-\alpha\,x\,\hat{\imath} + (B_0 + \alpha\,z)\,\hat{k}, p_z\right] \right\rangle \cdot \mathbf{S} = -\frac{\gamma}{m}\,\frac{i}{\hbar}\,\alpha\,\langle [z, p_z] \rangle\,\hat{k} \cdot \mathbf{S} = \frac{\gamma}{m}\alpha\,S_z\,.$$

Problem 4.74

(a) Write $\mathbf{S}$ in terms of raising and lowering operators:

$$H = \frac{p^2}{2\,m} - \gamma\left[B_x\,\frac{S_+ + S_-}{2} + B_y\,\frac{S_+ - S_-}{2\,i} + B_z\,S_z\right] = \frac{p^2}{2\,m} + \frac{1}{2}\,\gamma\,\alpha\,x\,(S_+ + S_-) - \gamma(B_0 + \alpha\,z)\;S_z.$$

Then

$$\begin{aligned}H\,\mathbf{\Psi} =& \frac{p^2}{2\,m}\,\Psi_+(\mathbf{r},t)\;\chi_+ + \frac{p^2}{2\,m}\,\Psi_-(\mathbf{r},t)\;\chi_- + \frac{1}{2}\,\gamma\,\alpha\,x\,\Psi_+(\mathbf{r},t)\;\hbar\,\chi_- + \frac{1}{2}\,\gamma\,\alpha\,x\,\Psi_-(\mathbf{r},t)\;\hbar\,\chi_+ \\ & - \gamma(B_0 + \alpha\,z)\;\Psi_+(\mathbf{r},t)\;\frac{\hbar}{2}\,\chi_+ - \gamma(B_0 + \alpha\,z)\;\Psi_-(\mathbf{r},t)\left(-\frac{\hbar}{2}\,\chi_-\right) \\ =& \left[\frac{p^2}{2\,m}\,\Psi_+ + \frac{\hbar}{2}\,\gamma\,\alpha\,x\,\Psi_- - \frac{\hbar}{2}\,\gamma(B_0 + \alpha\,z)\;\Psi_+\right]\chi_+ + \left[\frac{p^2}{2\,m}\,\Psi_- + \frac{\hbar}{2}\,\gamma\,\alpha\,x\,\Psi_+ + \frac{\hbar}{2}\,\gamma(B_0 + \alpha\,z)\;\Psi_-\right]\chi_-\,,\end{aligned}$$

while

$$i\,\hbar\,\frac{\partial}{\partial t}\mathbf{\Psi} = i\,\hbar\,\frac{\partial\Psi_+}{\partial t}\,\chi_+ + i\,\hbar\,\frac{\partial\Psi_-}{\partial t}\,\chi_-\,.$$

Since χ_+ and χ_- are orthogonal, the coefficients on either side of Schrödinger's equation must match and we have

$$\begin{aligned}&\frac{p^2}{2\,m}\,\Psi_+ + \frac{\hbar}{2}\,\gamma\,\alpha\,x\,\Psi_- - \frac{\hbar}{2}\,\gamma\,(B_0 + \alpha\,z)\;\Psi_+ = i\,\hbar\,\frac{\partial\Psi_+}{\partial t} \\ &\frac{p^2}{2\,m}\,\Psi_- + \frac{\hbar}{2}\,\gamma\,\alpha\,x\,\Psi_+ + \frac{\hbar}{2}\,\gamma\,(B_0 + \alpha\,z)\;\Psi_- = i\,\hbar\,\frac{\partial\Psi_-}{\partial t}\,.\end{aligned}$$

(b)

$$\frac{\partial\Psi_\pm}{\partial t} = \pm\frac{i}{2}\,\gamma\,B_0\,\Psi_\pm + e^{\pm i\,\gamma\,B_0\,t/2}\,\frac{\partial}{\partial t}\,\tilde{\Psi}_\pm\,.$$

Plugging into the results from (a), and cancelling the exponential factor:

$$\begin{aligned}&\frac{p^2}{2\,m}\,\tilde{\Psi}_+ + \frac{\hbar}{2}\,\gamma\,\alpha\,x\,e^{-i\,\gamma\,B_0\,t}\tilde{\Psi}_- - \frac{\hbar}{2}\,\gamma\,\alpha\,z\,\tilde{\Psi}_+ = i\,\hbar\,\frac{\partial\tilde{\Psi}_+}{\partial t} \\ &\frac{p^2}{2\,m}\,\tilde{\Psi}_- + \frac{\hbar}{2}\,\gamma\,\alpha\,x\,e^{i\,\gamma\,B_0\,t}\tilde{\Psi}_+ + \frac{\hbar}{2}\,\gamma\,\alpha\,z\,\tilde{\Psi}_- = i\,\hbar\,\frac{\partial\tilde{\Psi}_-}{\partial t}\,.\end{aligned}$$

(c) The potential $V_\pm = \mp\gamma\alpha\,\hbar z/2$ is a linear potential that decreases in the positive-z direction for spin up states, and in the negative-z direction for spin down. Therefore if the particle starts in a state where $\Psi_+ = \Psi_-$, once it enters the magnet Ψ_+ will propagate in the positive-z direction and Ψ_- will propagate in the negative-z direction.

Problem 4.75

We simply need to plug into the Schrödinger equation. Taking the time derivative

$$i\,\hbar\,\frac{\partial\Psi}{\partial t} = \hbar\,f'(t)\;\Psi(t) = \frac{\hbar^2}{2\,m\,b^2}\left(n - \frac{q\,\Phi(t)}{2\,\pi\,\hbar}\right)^2\,\Psi$$

and then evaluating the right side of Schrödinger's equation

$$H\,\Psi = \frac{1}{2\,m}\left[-\frac{\hbar^2}{b^2}\frac{\partial^2}{\partial\phi^2} + \left(\frac{q\,\Phi(t)}{2\,\pi\,b}\right)^2 + i\,\frac{\hbar\,q\,\Phi(t)}{\pi\,b^2}\frac{\partial}{\partial\phi}\right]\Psi$$

$$= \frac{1}{2\,m}\left[\frac{\hbar^2}{b^2}\,n^2 + \left(\frac{q\,\Phi(t)}{2\,\pi\,b}\right)^2 - \frac{\hbar\,q\,\Phi(t)}{\pi\,b^2}\,n\right]\Psi = \frac{\hbar^2}{2\,m\,b^2}\left(n - \frac{q\,\Phi(t)}{2\,\pi\,\hbar}\right)^2\Psi\,,$$

we see that these are equal.

Problem 4.76

(a) A changing flux introduces an EMF given by Faraday's law:

$$\mathcal{E} = \oint \mathbf{E}\cdot dl = -\frac{d\Phi}{dt} \quad\Rightarrow\quad E\,2\,\pi\,b = -\frac{d\Phi}{dt} \quad\Rightarrow\quad \mathbf{E} = -\frac{1}{2\pi b}\frac{d\Phi}{dt}\,\hat{\phi}.$$

The work done when the charge moves a distance $dl = v\,dt$ around the ring is

$$dW = qE\,dl = -\frac{q}{2\,\pi\,b}\frac{d\Phi}{dt}v\,dt = -\frac{qv}{2\pi b}\,d\Phi.$$

But v/b is the angular velocity ω, so $\dfrac{dW}{d\Phi} = -\dfrac{q\omega}{2\pi}$. ✓

(b) The mechanical angular momentum is (Equation 4.192 and foonote 62)

$$\mathbf{L}_{\text{mechanical}} = (\mathbf{r}\times\mathbf{p}) - q\,(\mathbf{r}\times\mathbf{A}) = \mathbf{L} - q\left(r\frac{\Phi}{2\pi r}\right)(\hat{r}\times\hat{\phi}) = \mathbf{L} - q\,\frac{\Phi}{2\,\pi}\,\hat{k}\,.$$

Therefore the z component of the mechanical angular momentum is

$$\left[\mathbf{L}_{\text{mechanical}}\right]_z = L_z - \frac{q\,\Phi}{2\,\pi} = -i\hbar\,\frac{d}{d\phi} - \frac{q\,\Phi}{2\,\pi}\,.$$

Acting on $\psi_n = Ae^{in\phi}$ (Equation 4.203),

$$\mathbf{L}_{[\text{mechanical}]_z}\,\psi_n = \left(-i\hbar\frac{d}{d\phi} - \frac{q\Phi}{2\pi}\right)\psi_n = \left(\hbar n - \frac{q\Phi}{2\pi}\right)\psi_n,$$

we see that ψ_n is an eigenstate with eigenvalue

$$\hbar\left(n - \frac{q\,\Phi}{2\,\pi\,\hbar}\right)\,.$$

(c) Taking the derivative of E_n (Equation 4.206), we get

$$\frac{dE_n}{d\Phi} = \frac{\hbar^2}{2\,m\,b^2}\,2\left(n - \frac{q\,\Phi}{2\,\pi\,\hbar}\right)\left(-\frac{q}{2\,\pi\,\hbar}\right) = -\frac{L_{\text{mechanical}}}{I}\,\frac{q}{2\,\pi},$$

where $I = mb^2$ is the moment of inertia, and since $L = I\,\omega$ we have

$$\frac{dE_n}{d\Phi} = -q\,\frac{\omega}{2\,\pi}\,. \quad ✓$$

Chapter 5

Identical Particles

Problem 5.1

(a)

$$(m_1+m_2)\mathbf{R} = m_1\mathbf{r}_1 + m_2\mathbf{r}_2 = m_1\mathbf{r}_1 + m_2(\mathbf{r}_1 - \mathbf{r}) = (m_1+m_2)\mathbf{r}_1 - m_2\mathbf{r} \quad \Rightarrow$$

$$\mathbf{r}_1 = \mathbf{R} + \frac{m_2}{m_1+m_2}\mathbf{r} = \mathbf{R} + \frac{\mu}{m_1}\mathbf{r}. \checkmark$$

$$(m_1+m_2)\mathbf{R} = m_1(\mathbf{r}_2+\mathbf{r}) + m_2\mathbf{r}_2 = (m_1+m_2)\mathbf{r}_2 + m_1\mathbf{r} \Rightarrow \mathbf{r}_2 = \mathbf{R} - \frac{m_1}{m_1+m_2}\mathbf{r} = \mathbf{R} - \frac{\mu}{m_2}\mathbf{r}. \checkmark$$

Let $\mathbf{R} = (X, Y, Z),\ \mathbf{r} = (x, y, z)$.

$$\begin{aligned}
(\nabla_1)_x &= \frac{\partial}{\partial x_1} = \frac{\partial X}{\partial x_1}\frac{\partial}{\partial X} + \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x} \\
&= \left(\frac{m_1}{m_1+m_2}\right)\frac{\partial}{\partial X} + (1)\frac{\partial}{\partial x} = \frac{\mu}{m_2}(\nabla_R)_x + (\nabla_r)_x, \quad \text{so} \quad \nabla_1 = \frac{\mu}{m_2}\nabla_R + \nabla_r. \quad \checkmark \\
(\nabla_2)_x &= \frac{\partial}{\partial x_2} = \frac{\partial X}{\partial x_2}\frac{\partial}{\partial X} + \frac{\partial x}{\partial x_2}\frac{\partial}{\partial x} \\
&= \left(\frac{m_2}{m_1+m_2}\right)\frac{\partial}{\partial X} - (1)\frac{\partial}{\partial x} = \frac{\mu}{m_1}(\nabla_R)_x - (\nabla_r)_x, \quad \text{so} \quad \nabla_2 = \frac{\mu}{m_1}\nabla_R - \nabla_r. \checkmark
\end{aligned}$$

(b)

$$\begin{aligned}
\nabla_1^2\psi &= \nabla_1\cdot(\nabla_1\psi) = \nabla_1\cdot\left[\frac{\mu}{m_2}\nabla_R\psi + \nabla_r\psi\right] \\
&= \frac{\mu}{m_2}\nabla_R\cdot\left(\frac{\mu}{m_2}\nabla_R\psi + \nabla_r\psi\right) + \nabla_r\cdot\left(\frac{\mu}{m_2}\nabla_R\psi + \nabla_r\psi\right) \\
&= \left(\frac{\mu}{m_2}\right)^2\nabla_R^2\psi + 2\frac{\mu}{m_2}(\nabla_r\cdot\nabla_R)\psi + \nabla_r^2\psi.
\end{aligned}$$

Likewise, $\quad \nabla_2^2\psi = \left(\dfrac{\mu}{m_1}\right)^2\nabla_R^2\psi - 2\dfrac{\mu}{m_1}(\nabla_r\cdot\nabla_R) + \nabla_r^2\psi.$

$$\therefore H\psi = -\frac{\hbar^2}{2m_1}\nabla_1^2\psi - \frac{\hbar^2}{2m_2}\nabla_2^2\psi + V(\mathbf{r}_1,\mathbf{r}_2)\psi$$
$$= -\frac{\hbar^2}{2}\left(\frac{\mu^2}{m_1 m_2^2}\nabla_R^2 + \frac{2\mu}{m_1 m_2}\nabla_r\cdot\nabla_R + \frac{1}{m_1}\nabla_r^2 + \frac{\mu^2}{m_2 m_1^2}\nabla_R^2 - \frac{2\mu}{m_2 m_1}\nabla_r\cdot\nabla_R + \frac{1}{m_2}\nabla_r^2\right)\psi$$
$$+ V(\mathbf{r})\psi = -\frac{\hbar^2}{2}\left[\frac{\mu^2}{m_1 m_2}\left(\frac{1}{m_2}+\frac{1}{m_1}\right)\nabla_R^2 + \left(\frac{1}{m_1}+\frac{1}{m_2}\right)\nabla_r^2\right]\psi + V(\mathbf{r})\psi = E\psi.$$

But $\left(\frac{1}{m_1}+\frac{1}{m_2}\right) = \frac{m_1+m_2}{m_1 m_2} = \frac{1}{\mu}$, so $\frac{\mu^2}{m_1 m_2}\left(\frac{1}{m_2}+\frac{1}{m_1}\right) = \frac{\mu}{m_1 m_2} = \frac{m_1 m_2}{m_1 m_2(m_1+m_2)} = \frac{1}{m_1+m_2}$.

$$-\frac{\hbar^2}{2(m_1+m_2)}\nabla_R^2\psi - \frac{\hbar^2}{2\mu}\nabla_r^2\psi + V(\mathbf{r})\psi = E\psi. \quad \checkmark$$

(c) Put in $\psi = \psi_r(\mathbf{r})\psi_R(\mathbf{R})$, and divide by $\psi_r\psi_R$:

$$\left[-\frac{\hbar^2}{2(m_1+m_2)}\frac{1}{\psi_R}\nabla_R^2\psi_R\right] + \left[-\frac{\hbar^2}{2\mu}\frac{1}{\psi_r}\nabla_r^2\psi_r + V(\mathbf{r})\right] = E.$$

The first term depends only on $\mathbf{R}$, the second only on $\mathbf{r}$, so each must be a constant; call them E_R and E_r, respectively. Then:

$$\boxed{-\frac{\hbar^2}{2(m_1+m_2)}\nabla^2\psi_R = E_R\psi_R;} \quad \boxed{-\frac{\hbar^2}{2\mu}\nabla^2\psi_r + V(\mathbf{r})\psi_r = E_r\psi_r,} \quad \text{with} \quad \boxed{E_R + E_r = E.}$$

Problem 5.2

(a) From Eq. 4.77, E_1 is proportional to mass, so $\frac{\Delta E_1}{E_1} = \frac{\Delta m}{\mu} = \frac{m-\mu}{\mu} = \frac{m(m+M)}{mM} - \frac{M}{M} = \frac{m}{M}$.

The fractional error is the ratio of the electron mass to the proton mass:
$\frac{9.109\times10^{-31}\,\text{kg}}{1.673\times10^{-27}\,\text{kg}} = 5.44\times10^{-4}$. The *percent* error is $\boxed{0.054\%}$ (pretty small).

(b) From Eq. 4.94, $\mathcal{R}$ is proportional to m, so $\frac{\Delta(1/\lambda)}{(1/\lambda)} = \frac{\Delta\mathcal{R}}{\mathcal{R}} = \frac{\Delta\mu}{\mu} = -\frac{(1/\lambda^2)\Delta\lambda}{(1/\lambda)} = -\frac{\Delta\lambda}{\lambda}$.

So (in magnitude) $\Delta\lambda/\lambda = \Delta\mu/\mu$. But $\mu = mM/(m+M)$, where m = electron mass, and M = nuclear mass.

$$\Delta\mu = \frac{m(2m_p)}{m+2m_p} - \frac{mm_p}{m+m_p} = \frac{mm_p}{(m+m_p)(m+2m_p)}(2m+2m_p-m-2m_p)$$
$$= \frac{m^2 m_p}{(m+m_p)(m+2m_p)} = \frac{m\mu}{m+2m_p}.$$

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta\mu}{\mu} = \frac{m}{m+2m_p} \approx \frac{m}{2m_p}, \text{ so } \boxed{\Delta\lambda = \frac{m}{2m_p}\lambda_h}, \text{ where } \lambda_h \text{ is the hydrogen wavelength.}$$

$$\frac{1}{\lambda} = R\left(\frac{1}{4} - \frac{1}{9}\right) = \frac{5}{36}R \Rightarrow \lambda = \frac{36}{5R} = \frac{36}{5(1.097 \times 10^7)}\,\text{m} = 6.563 \times 10^{-7}\,\text{m}.$$

$$\therefore \Delta\lambda = \frac{9.109 \times 10^{-31}}{2(1.673 \times 10^{-27})}(6.563 \times 10^{-7})\text{m} = \boxed{1.79 \times 10^{-10}\,\text{m.}}$$

(c) $\mu = \dfrac{mm}{m+m} = \dfrac{m}{2}$, so the energy is *half* what it would be for hydrogen: $(13.6/2)\text{eV} = \boxed{6.8\,\text{eV.}}$

(d) $\mu = \dfrac{m_p m_\mu}{m_p + m_\mu}$; $R \propto \mu$, so R is changed by a factor $\dfrac{m_p m_\mu}{m_p + m_\mu} \cdot \dfrac{m_p + m_e}{m_p m_e} = \dfrac{m_\mu(m_p + m_e)}{m_e(m_p + m_\mu)}$, as compared with hydrogen. For hydrogen, $1/\lambda = R(1 - 1/4) = \frac{3}{4}R \Rightarrow \lambda = 4/(3R) = 4/[3(1.097 \times 10^7)]\,\text{m} = 1.215 \times 10^{-7}\,\text{m}$, and $\lambda \propto 1/R$, so for muonic hydrogen the Lyman-alpha line is at

$$\lambda = \frac{m_e(m_p + m_\mu)}{m_\mu(m_p + m_e)}(1.215 \times 10^{-7}\text{m}) = \frac{1}{206.77}\frac{(1.673 \times 10^{-27} + 206.77 \times 9.109 \times 10^{-31})}{(1.673 \times 10^{-27} + 9.109 \times 10^{-31})}(1.215 \times 10^{-7}\text{m})$$
$$= \boxed{6.54 \times 10^{-10}\,\text{m.}}$$

Problem 5.3

The energy of the emitted photon, in a transition from vibrational state n_i to state n_f, is $E_p = (n_i + \frac{1}{2})\hbar\omega - (n_f + \frac{1}{2})\hbar\omega = n\hbar\omega$, (where $n \equiv n_i - n_f$). The frequency of the photon is $\nu = \dfrac{E_p}{h} = \dfrac{n\omega}{2\pi} = \dfrac{n}{2\pi}\sqrt{\dfrac{k}{\mu}}$. The splitting of this line is given by

$$\Delta\nu = \left|\frac{n}{2\pi}\sqrt{k}\left(-\frac{1}{2\mu^{3/2}}\Delta\mu\right)\right| = \frac{1}{2}\frac{n}{2\pi}\sqrt{\frac{k}{\mu}}\frac{\Delta\mu}{\mu} = \frac{1}{2}\nu\frac{\Delta\mu}{\mu}.$$

Now

$$\mu = \frac{m_h m_c}{m_h + m_c} = \frac{1}{\frac{1}{m_c} + \frac{1}{m_h}} \Rightarrow \Delta\mu = \frac{-1}{\left(\frac{1}{m_c} + \frac{1}{m_h}\right)^2}\left(-\frac{1}{m_c^2}\Delta m_c\right) = \frac{\mu^2}{m_c^2}\Delta m_c.$$

$$\Delta\nu = \frac{1}{2}\nu\frac{\mu\Delta m_c}{m_c^2} = \frac{1}{2}\nu\frac{(\Delta m_c/m_c)}{\left(1 + \frac{m_c}{m_h}\right)}.$$

Using the average value (36) for m_c, we have $\Delta m_c/m_c = 2/36$, and $m_c/m_h = 36/1$, so

$$\Delta\nu = \frac{1}{2}\frac{(1/18)}{(1+36)}\nu = \frac{1}{(36)(37)}\nu = \boxed{7.51 \times 10^{-4}\,\nu.}$$

Problem 5.4

(a)

$$1 = \int |\psi_\pm|^2 d^3\mathrm{r}_1 d^3\mathrm{r}_2$$

$$= |A|^2 \int [\psi_a(\mathrm{r}_1)\psi_b(\mathrm{r}_2) \pm \psi_b(\mathrm{r}_1)\psi_a(\mathrm{r}_2)]^* [\psi_a(\mathrm{r}_1)\psi_b(\mathrm{r}_2) \pm \psi_b(\mathrm{r}_1)\psi_a(\mathrm{r}_2)]\, d^3\mathrm{r}_1 d^3\mathrm{r}_2$$

$$= |A|^2 \left[\int |\psi_a(\mathrm{r}_1)|^2 d^3\mathrm{r}_1 \int |\psi_b(\mathrm{r}_2)|^2 d^3\mathrm{r}_2 \pm \int \psi_a(\mathrm{r}_1)^*\psi_b(\mathrm{r}_1) d^3\mathrm{r}_1 \int \psi_b(\mathrm{r}_2)^*\psi_a(\mathrm{r}_2) d^3\mathrm{r}_2 \right.$$

$$\left. \pm \int \psi_b(\mathrm{r}_1)^*\psi_a(\mathrm{r}_1) d^3\mathrm{r}_1 \int \psi_a(\mathrm{r}_2)^*\psi_b(\mathrm{r}_2) d^3\mathrm{r}_2 + \int |\psi_b(\mathrm{r}_1)|^2 d^3\mathrm{r}_1 \int |\psi_a(\mathrm{r}_2)|^2 d^3\mathrm{r}_2 \right]$$

$$= |A|^2 (1\cdot 1 \pm 0\cdot 0 \pm 0 \cdot 0 + 1 \cdot 1) = 2|A|^2 \Longrightarrow \boxed{A = 1/\sqrt{2}.}$$

(b)

$$1 = |A|^2 \int [2\psi_a(\mathrm{r}_1)\psi_a(\mathrm{r}_2)]^* [2\psi_a(\mathrm{r}_1)\psi_a(\mathrm{r}_2)]\, d^3\mathrm{r}_1 d^3\mathrm{r}_2$$

$$= 4|A|^2 \int |\psi_a(\mathrm{r}_1)|^2 d^3\mathrm{r}_1 \int |\psi_a(\mathrm{r}_2)|^2 d^3\mathrm{r}_2 = 4|A|^2. \qquad \boxed{A = 1/2.}$$

Problem 5.5

(a)

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x_2^2} = E\psi} \quad \text{(for } 0 \le x_1, x_2 \le a, \text{ otherwise } \psi = 0).$$

$$\psi = \frac{\sqrt{2}}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) - \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$$

$$\frac{d^2\psi}{dx_1^2} = \frac{\sqrt{2}}{a}\left[-\left(\frac{\pi}{a}\right)^2\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) + \left(\frac{2\pi}{a}\right)^2\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$$

$$\frac{d^2\psi}{dx_2^2} = \frac{\sqrt{2}}{a}\left[-\left(\frac{2\pi}{a}\right)^2\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) + \left(\frac{\pi}{a}\right)^2\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$$

$$\left(\frac{d^2\psi}{dx_1^2} + \frac{d^2\psi}{dx_2^2}\right) = -\left[\left(\frac{\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2\right]\psi = -5\frac{\pi^2}{a^2}\psi,$$

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx_1^2} + \frac{d^2\psi}{dx_2^2}\right) = \frac{5\pi^2\hbar^2}{2ma^2}\psi = E\psi, \quad \text{with} \quad E = \frac{5\pi^2\hbar^2}{2ma^2} = 5K. \quad \checkmark$$

(b) Distinguishable:

$$\boxed{\psi_{22} = (2/a)\sin(2\pi x_1/a)\sin(2\pi x_2/a)\,,\ \text{with } E_{22} = 8K} \quad \text{(nondegenerate).}$$

$$\boxed{\left.\begin{array}{l}\psi_{13} = (2/a)\sin(\pi x_1/a)\sin(3\pi x_2/a)\\ \psi_{31} = (2/a)\sin(3\pi x_1/a)\sin(\pi x_2/a)\end{array}\right\},\ \text{with } E_{13} = E_{31} = 10K} \quad \text{(doubly degenerate).}$$

Identical Bosons:

$$\boxed{\psi_{22} = (2/a)\sin(2\pi x_1/a)\sin(2\pi x_2/a),\ E_{22} = 8K} \quad \text{(nondegenerate).}$$

$$\boxed{\psi_{13} = (\sqrt{2}/a)\left[\sin(\pi x_1/a)\sin(3\pi x_2/a) + \sin(3\pi x_1/a)\sin(\pi x_2/a)\right],\ E_{13} = 10K} \quad \text{(nondegenerate).}$$

Identical Fermions:

$$\boxed{\psi_{13} = (\sqrt{2}/a)\left[\sin\left(\tfrac{\pi x_1}{a}\right)\sin\left(\tfrac{3\pi x_2}{a}\right) - \sin\left(\tfrac{3\pi x_1}{a}\right)\sin\left(\tfrac{\pi x_2}{a}\right)\right],\ E_{13} = 10K} \quad \text{(nondegenerate).}$$

$$\boxed{\psi_{23} = (\sqrt{2}/a)\left[\sin\left(\tfrac{2\pi x_1}{a}\right)\sin\left(\tfrac{3\pi x_2}{a}\right) - \sin\left(\tfrac{3\pi x_1}{a}\right)\sin\left(\tfrac{2\pi x_2}{a}\right)\right],\ E_{23} = 13K} \quad \text{(nondegenerate).}$$

Problem 5.6

(a) Use Eq. 5.23 and Problem 2.4, with $\langle x\rangle_n = a/2$ and $\langle x^2\rangle_n = a^2\left(\frac{1}{3} - \frac{1}{2(n\pi)^2}\right)$.

$$\langle (x_1 - x_2)^2\rangle = a^2\left(\tfrac{1}{3} - \tfrac{1}{2(n\pi)^2}\right) + a^2\left(\tfrac{1}{3} - \tfrac{1}{2(m\pi)^2}\right) - 2\cdot\tfrac{a}{2}\cdot\tfrac{a}{2} = \boxed{a^2\left[\frac{1}{6} - \frac{1}{2\pi^2}\left(\frac{1}{n^2} + \frac{1}{m^2}\right)\right]}.$$

(b)
$$\langle x\rangle_{mn} = \tfrac{2}{a}\int_0^a x\sin\left(\tfrac{m\pi}{a}x\right)\sin\left(\tfrac{n\pi}{a}x\right)dx = \tfrac{1}{a}\int_0^a x\left[\cos\left(\tfrac{(m-n)\pi}{a}x\right) - \cos\left(\tfrac{(m+n)\pi}{a}x\right)\right]dx$$

$$= \tfrac{1}{a}\left[\left(\tfrac{a}{(m-n)\pi}\right)^2\cos\left(\tfrac{(m-n)\pi}{a}x\right) + \left(\tfrac{ax}{(m-n)\pi}\right)\sin\left(\tfrac{(m-n)\pi}{a}x\right)\right.$$
$$\left.\left. - \left(\tfrac{a}{(m+n)\pi}\right)^2\cos\left(\tfrac{(m+n)\pi}{a}x\right) - \left(\tfrac{ax}{(m+n)\pi}\right)\sin\left(\tfrac{(m+n)\pi}{a}x\right)\right]\right|_0^a$$

$$= \tfrac{1}{a}\left[\left(\tfrac{a}{(m-n)\pi}\right)^2(\cos[(m-n)\pi] - 1) - \left(\tfrac{a}{(m+n)\pi}\right)^2(\cos[(m+n)\pi] - 1)\right].$$

But $\cos[(m\pm n)\pi] = (-1)^{m+n}$, so

$$\langle x\rangle_{mn} = \frac{a}{\pi^2}\left[(-1)^{m+n} - 1\right]\left(\frac{1}{(m-n)^2} - \frac{1}{(m+n)^2}\right) = \begin{cases}\frac{a(-8mn)}{\pi^2(m^2-n^2)^2}, & \text{if } m \text{ and } n \text{ have opposite parity,}\\ 0, & \text{if } m \text{ and } n \text{ have same parity.}\end{cases}$$

So Eq. 5.25 $\Rightarrow \langle (x_1 - x_2)^2\rangle = \boxed{a^2\left[\frac{1}{6} - \frac{1}{2\pi^2}\left(\frac{1}{n^2} + \frac{1}{m^2}\right)\right] - \frac{128a^2m^2n^2}{\pi^4(m^2-n^2)^4}}.$

(The last term is present only when m, n have opposite parity.)

(c) Here Eq. 5.25 $\Rightarrow \langle (x_1 - x_2)^2\rangle = \boxed{a^2\left[\frac{1}{6} - \frac{1}{2\pi^2}\left(\frac{1}{n^2} + \frac{1}{m^2}\right)\right] + \frac{128a^2m^2n^2}{\pi^4(m^2-n^2)^4}}.$

(Again, the last term is present only when m, n have opposite parity.)

Problem 5.7

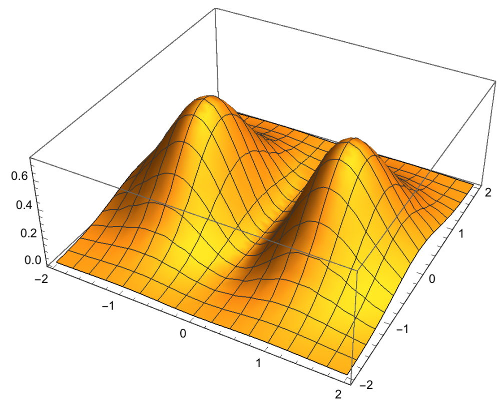
(a) From Equations 2.60 and 2.63:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}, \quad \psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}}\, x\, e^{-\frac{m\omega}{2\hbar}x^2}.$$

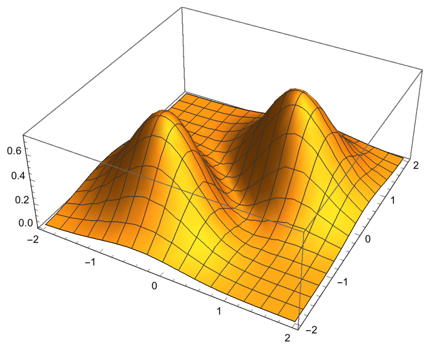
(i) $\psi_d(x_1, x_2) = \psi_0(x_1)\,\psi_1(x_2) = \boxed{\sqrt{\frac{2}{\pi}}\,\frac{m\omega}{\hbar}\,x_1\, e^{-\frac{m\omega}{2\hbar}(x_1^2+x_2^2)}}.$

(ii) and (iii) $\psi_\pm(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\psi_0(x_1)\,\psi_1(x_2) \pm \psi_1(x_1)\,\psi_0(x_2)\right] = \boxed{\sqrt{\frac{1}{\pi}}\,\frac{m\omega}{\hbar}\,(x_1 \pm x_2)\, e^{-\frac{m\omega}{2\hbar}(x_1^2+x_2^2)}}.$

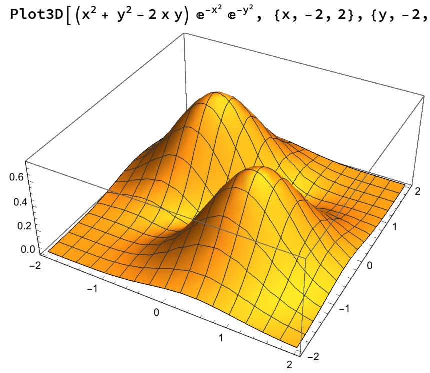
```
Plot3D[2 x^2 e^(-x^2) e^(-y^2), {x, -2, 2}, {y, -2, 2}]
```



```
Plot3D[(x^2 + y^2 + 2 x y) e^(-x^2) e^(-y^2), {x, -2, 2}, {y, -2, 2}]
```



```
Plot3D[(x^2 + y^2 - 2 x y) e^(-x^2) e^(-y^2), {x, -2, 2}, {y, -2, 2}]
```



(b) From Problem 2.11:

$$\langle x\rangle_0 = 0, \quad \langle x\rangle_1 = 0, \quad \langle x^2\rangle_0 = \frac{\hbar}{2m\omega}, \quad \langle x^2\rangle_1 = \frac{3\hbar}{2m\omega}.$$

From Equation (5.24):

$$\langle x\rangle_{01} = \int x\,\psi_0(x)\psi_1(x)\,dx = \sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{2m\omega}{\hbar}}\int_{-\infty}^{\infty} x^2\, e^{-\frac{m\omega}{\hbar}x^2}\,dx = \sqrt{\frac{2}{\pi}}\left(\frac{m\omega}{\hbar}\right) 4\sqrt{\pi}\left(\frac{1}{2}\sqrt{\frac{\hbar}{m\omega}}\right)^3 = \sqrt{\frac{\hbar}{2m\omega}}.$$

(i) $\langle (x_1 - x_2)^2 \rangle_d = \langle x^2 \rangle_0 + \langle x^2 \rangle_1 - 2\langle x \rangle_0 \langle x \rangle_1 = \boxed{\dfrac{2\hbar}{m\omega}.}$

(ii) and (iii) $\langle (x_1 - x_2)^2 \rangle_\pm = \dfrac{2\hbar}{m\omega} \mp 2\dfrac{\hbar}{2m\omega} = \boxed{\dfrac{\hbar}{m\omega}\text{ (bosons)}, \dfrac{3\hbar}{m\omega}\text{ (fermions)}.}$

(c)

$$x_1 = R + \frac{r}{2}, \quad x_2 = R - \frac{r}{2}, \quad x_1^2 + x_2^2 = 2R^2 + \frac{r^2}{2}.$$

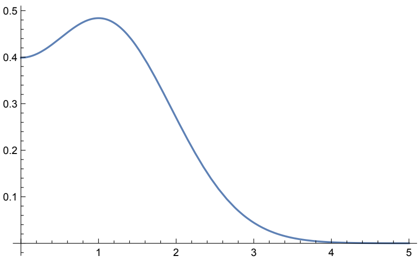
$$\boxed{\psi_d(R, r) = \sqrt{\frac{2}{\pi}\frac{m\omega}{\hbar}} \left(R + \frac{r}{2}\right) e^{-\frac{m\omega}{\hbar}\left(R^2 + \frac{r^2}{4}\right)}.} \quad \boxed{\psi_+(R, r) = \sqrt{\frac{1}{\pi}\frac{2m\omega}{\hbar}}\, R\, e^{-\frac{m\omega}{\hbar}\left(R^2 + \frac{r^2}{4}\right)}.}$$

$$\boxed{\psi_-(R, r) = \sqrt{\frac{1}{\pi}\frac{m\omega}{\hbar}}\, r\, e^{-\frac{m\omega}{\hbar}\left(R^2 + \frac{r^2}{4}\right)}.}$$

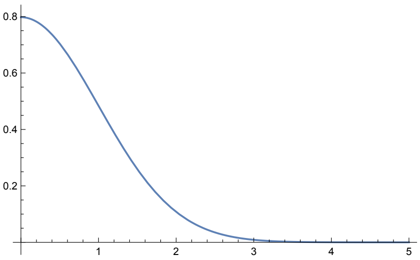
$$\begin{aligned}
P_d &= \frac{4}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 e^{-\frac{m\omega}{2\hbar}r^2} \int_{-\infty}^{\infty} \left(R^2 + Rr + \frac{r^2}{4}\right) e^{-\frac{2m\omega}{\hbar}R^2}\, dR \\
&= \frac{4}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 e^{-\frac{m\omega}{2\hbar}r^2} 2\left[\int_0^{\infty} R^2 e^{-\frac{2m\omega}{\hbar}R^2}\, dR + 0 + \frac{r^2}{4}\int_0^{\infty} e^{-\frac{2m\omega}{\hbar}R^2}\, dR\right] \\
&= \frac{8}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 e^{-\frac{m\omega}{2\hbar}r^2} \left[2\sqrt{\pi}\left(\frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\right)^3 + \frac{r^2}{4}\sqrt{\pi}\left(\frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\right)\right] \\
&= \boxed{\frac{1}{\sqrt{2\pi}}\left(\frac{m\omega}{\hbar}\right)^{3/2}\left(r^2 + \frac{\hbar}{m\omega}\right) e^{-\frac{m\omega}{2\hbar}r^2}.} \\
P_+ &= \frac{2}{\pi}\left(\frac{2m\omega}{\hbar}\right)^2 e^{-\frac{m\omega}{2\hbar}r^2} \int_{-\infty}^{\infty} R^2 e^{-\frac{2m\omega}{\hbar}R^2}\, dR \\
&= \frac{8}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 e^{-\frac{m\omega}{2\hbar}r^2} 2\left[2\sqrt{\pi}\left(\frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\right)^3\right] = \boxed{\sqrt{\frac{2m\omega}{\pi\hbar}} e^{-\frac{m\omega}{2\hbar}r^2}.} \\
P_- &= \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 r^2 e^{-\frac{m\omega}{2\hbar}r^2} \int_{-\infty}^{\infty} e^{-\frac{2m\omega}{\hbar}R^2}\, dR \\
&= \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 r^2 e^{-\frac{m\omega}{2\hbar}r^2} 2\left[\sqrt{\pi}\left(\frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\right)\right] = \boxed{\sqrt{\frac{2}{\pi}}\left(\frac{m\omega}{\hbar}\right)^{3/2} r^2 e^{-\frac{m\omega}{2\hbar}r^2}.}
\end{aligned}$$

As we see from the graphs below, the bosons tend to be closer together, and the fermions farther apart.

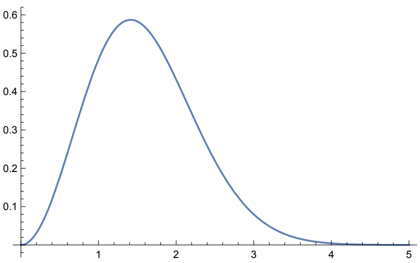
$\texttt{Plot}\left[\frac{1}{\sqrt{2\,\pi}}\,(x^2+1)\,e^{-x^2/2},\ \{x,0,5\}\right]$



$\texttt{Plot}\left[\sqrt{\frac{2}{\pi}}\,e^{-x^2/2},\ \{x,0,5\}\right]$



$\texttt{Plot}\left[\sqrt{\frac{2}{\pi}}\,x^2\,e^{-x^2/2},\ \{x,0,5\}\right]$



(d)

$$\langle n(x)\rangle = \int\int |\psi(x_1,x_2)|^2\,[\delta(x-x_1)+\delta(x-x_2)]\;dx_1\,dx_2 = \int |\psi(x,x_2)|^2\,dx_2 + \int |\psi(x_1,x)|^2\,dx_1.$$

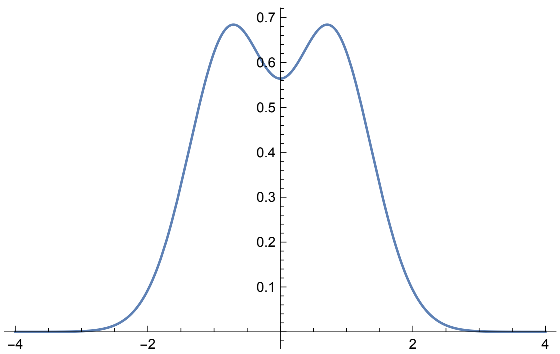
$$\begin{aligned}
\langle n(x)\rangle_d &= \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2\left[\int x^2 e^{-\frac{m\omega}{\hbar}(x^2+x_2^2)}\,dx_2 + \int x_1^2\,e^{-\frac{m\omega}{\hbar}(x_1^2+x^2)}\,dx_1\right]\\
&= \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 e^{-\frac{m\omega}{\hbar}x^2}\left[x^2\int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar}x_2^2}\,dx_2 + \int_{-\infty}^{\infty} x_1^2\,e^{-\frac{m\omega}{\hbar}x_1^2}\,dx_1\right]\\
&= \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 e^{-\frac{m\omega}{\hbar}x^2}\,2\left[x^2\sqrt{\pi}\left(\frac{1}{2}\sqrt{\frac{\hbar}{m\omega}}\right) + 2\sqrt{\pi}\left(\frac{1}{2}\sqrt{\frac{\hbar}{m\omega}}\right)^3\right]\\
&= \boxed{\frac{2}{\sqrt{\pi}}\left(\frac{m\omega}{\hbar}\right)^{3/2}\left[x^2+\frac{\hbar}{2m\omega}\right]e^{-\frac{m\omega}{\hbar}x^2}.}
\end{aligned}$$

$$\begin{aligned}
\langle n(x)\rangle_{\pm} &= \frac{1}{\pi}\left(\frac{m\omega}{\hbar}\right)^2\left[\int (x\pm x_2)^2 e^{-\frac{m\omega}{\hbar}(x^2+x_2^2)}\,dx_2 + \int (x_1\pm x)^2\, e^{-\frac{m\omega}{\hbar}(x_1^2+x^2)}\,dx_1\right]\\
&= \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 e^{-\frac{m\omega}{\hbar}x^2}\int_{-\infty}^{\infty}(x^2\pm 2x\,x_2+x_2^2)e^{-\frac{m\omega}{\hbar}x_2^2}\,dx_2\\
&= \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2 e^{-\frac{m\omega}{\hbar}x^2}\left[x^2\int_{-\infty}^{\infty}e^{-\frac{m\omega}{\hbar}x_2^2}\,dx_2 \pm 0 + \int_{-\infty}^{\infty}x_2^2\,e^{-\frac{m\omega}{\hbar}x_2^2}\,dx_2\right]\\
&= \boxed{\frac{2}{\sqrt{\pi}}\left(\frac{m\omega}{\hbar}\right)^{3/2}\left[x^2+\frac{\hbar}{2m\omega}\right]e^{-\frac{m\omega}{\hbar}x^2}.}
\end{aligned}$$

Remarkably, the density is exactly the same for all three cases! Identical bosons tend to be closer together, and fermions farther apart, but this is not reflected in the expectation value of the number density.

```
Plot[2/Sqrt[π] (x^2 + 1/2) e^(-x^2), {x, -4, 4}]
```

$$\texttt{Plot}\left[\frac{2}{\sqrt{\pi}}\left(x^2+\frac{1}{2}\right)e^{-x^2},\ \{x, -4, 4\}\right]$$



$$\int_{-\infty}^{\infty}\frac{2}{\sqrt{\pi}}\left(x^2+\frac{1}{2}\right)e^{-x^2}\,dx$$

2

(Just as a check, I integrated the density over all x: the result is 2, of course, because there are two particles here.)

Problem 5.8

(a) $\boxed{\psi(x_1,x_2,x_3)=\psi_a(x_1)\psi_b(x_2)\psi_c(x_3).}$

(b) $$\psi(x_1,x_2,x_3)=\boxed{\begin{array}{l}\frac{1}{\sqrt{6}}[\psi_a(x_1)\psi_b(x_2)\psi_c(x_3)+\psi_a(x_1)\psi_c(x_2)\psi_b(x_3)+\psi_b(x_1)\psi_a(x_2)\psi_c(x_3)\\ \quad+\psi_b(x_1)\psi_c(x_2)\psi_a(x_3)+\psi_c(x_1)\psi_b(x_2)\psi_a(x_3)+\psi_c(x_1)\psi_a(x_2)\psi_b(x_3)]\end{array}}.$$

(c) $$\psi(x_1,x_2,x_3)=\boxed{\begin{array}{l}\frac{1}{\sqrt{6}}[\psi_a(x_1)\psi_b(x_2)\psi_c(x_3)-\psi_a(x_1)\psi_c(x_2)\psi_b(x_3)-\psi_b(x_1)\psi_a(x_2)\psi_c(x_3)\\ \quad+\psi_b(x_1)\psi_c(x_2)\psi_a(x_3)-\psi_c(x_1)\psi_b(x_2)\psi_a(x_3)+\psi_c(x_1)\psi_a(x_2)\psi_b(x_3)]\end{array}}.$$

Problem 5.9

(a) **Distinguishable:**

ground state: $\psi_{11}|s\,m\rangle$, where $|s\,m\rangle$ could be $|00\rangle, |11\rangle, |10\rangle$, or $|1\,-1\rangle$. $\boxed{E = 2K,\ d = 4.}$

1st excited: $\psi_{12}|s\,m\rangle$ or $\psi_{21}|s\,m\rangle$, where $|s\,m\rangle$ could be any of the same four spin states. $\boxed{E = 5K,\ d = 8.}$

2nd excited: $\psi_{22}|s\,m\rangle$, where $|s\,m\rangle$ could be $|00\rangle, |11\rangle, |10\rangle$, or $|1\,-1\rangle$. $\boxed{E = 8K,\ d = 4.}$

3rd excited: $\psi_{13}|s\,m\rangle$ or $\psi_{31}|s\,m\rangle$, where $|s\,m\rangle$ could be any of the same four spin states. $\boxed{E = 10K,\ d = 8.}$

Identical:

ground state: $\psi_{11}|00\rangle$. $\boxed{E = 2K,\ d = 1.}$

1st excited: $\frac{1}{\sqrt{2}}(\psi_{12}+\psi_{21})|00\rangle$ or $\frac{1}{\sqrt{2}}(\psi_{12}-\psi_{21})|s\,m\rangle$, where $|s\,m\rangle$ could be $|11\rangle, |10\rangle$, or $|1\!-\!1\rangle$. $\boxed{E = 5K,\ d = 4.}$

2nd excited: $\psi_{22}|00\rangle$. $\boxed{E = 8K,\ d = 1.}$

3rd excited: $\frac{1}{\sqrt{2}}(\psi_{13}+\psi_{31})|00\rangle$ or $\frac{1}{\sqrt{2}}(\psi_{13}-\psi_{31})|s\,m\rangle$, where $|s\,m\rangle$ could be $|11\rangle, |10\rangle$, or $|1\!-\!1\rangle$. $\boxed{E = 10K,\ d = 4.}$

(b) Two particles of spin 1 can combine to make spin 0, spin 1, or spin 2. From the 1×1 C-G table:

$$\textbf{singlet: } \left\{ |00\rangle = \tfrac{1}{\sqrt{3}}|111-1\rangle - \tfrac{1}{\sqrt{3}}|1100\rangle + \tfrac{1}{\sqrt{3}}|11-11\rangle, \quad \text{(symmetric).} \right.$$

$$\textbf{triplet: } \begin{cases} |11\rangle = \frac{1}{\sqrt{2}}|1110\rangle - \frac{1}{\sqrt{2}}|1101\rangle, & \text{(antisymmetric),} \\ |10\rangle = \frac{1}{\sqrt{2}}|111-1\rangle - \frac{1}{\sqrt{2}}|11-11\rangle, & \text{(antisymmetric),} \\ |1-1\rangle = \frac{1}{\sqrt{2}}|110-1\rangle - \frac{1}{\sqrt{2}}|11-10\rangle, & \text{(antisymmetric).} \end{cases}$$

$$\textbf{quintuplet: } \begin{cases} |22\rangle = |1111\rangle, & \text{(symmetric),} \\ |21\rangle = \frac{1}{\sqrt{2}}|1110\rangle + \frac{1}{\sqrt{2}}|1101\rangle, & \text{(symmetric),} \\ |20\rangle = \frac{1}{\sqrt{6}}|111-1\rangle + \sqrt{\frac{2}{3}}|1100\rangle + \frac{1}{\sqrt{6}}|11-11\rangle, & \text{(symmetric),} \\ |2-1\rangle = \frac{1}{\sqrt{2}}|110-1\rangle + \frac{1}{\sqrt{2}}|11-10\rangle, & \text{(symmetric),} \\ |2-2\rangle = |11-1-1\rangle, & \text{(symmetric).} \end{cases}$$

Distinguishable:

ground state: $\psi_{11}|s\,m\rangle$, where $|s\,m\rangle$ could be any of the nine spin states. $\boxed{E = 2K,\ d = 9.}$

1st excited: $\psi_{12}|s\,m\rangle$ or $\psi_{21}|s\,m\rangle$, where $|s\,m\rangle$ could be any of the nine spin states. $\boxed{E = 5K,\ d = 18.}$

2nd excited: $\psi_{22}|s\,m\rangle$, where $|s\,m\rangle$ could be any of the nine spin states. $\boxed{E = 8K,\ d = 9.}$

3rd excited: $\psi_{13}|s\,m\rangle$ or $\psi_{31}|s\,m\rangle$, where $|s\,m\rangle$ could be any of the nine spin states. $\boxed{E = 10K,\ d = 18.}$

Identical:

ground state: $\psi_{11}|sm\rangle$, where $|sm\rangle$ is any of the singlet or quintuplet spin states. $\boxed{E = 2K,\ d = 6.}$

1st excited: $\frac{1}{\sqrt{2}}(\psi_{12} + \psi_{21})|sm\rangle$, where $|sm\rangle$ is any of the singlet or quintuplet spin states,
or $\frac{1}{\sqrt{2}}(\psi_{12} - \psi_{21})|s\,m\rangle$, where $|s\,m\rangle$ is any of the triplet spin states. $\boxed{E = 5K,\ d = 9.}$

2nd excited: $\psi_{22}|sm\rangle$, where $|sm\rangle$ is any of the singlet or quintuplet spin states. $\boxed{E = 8K,\ d = 6.}$

3rd excited: $\frac{1}{\sqrt{2}}(\psi_{13} + \psi_{31})|sm\rangle$, where $|sm\rangle$ is any of the singlet or quintuplet spin states,
or $\frac{1}{\sqrt{2}}(\psi_{13} - \psi_{31})|s\,m\rangle$, where $|s\,m\rangle$ is any of the triplet spin states. $\boxed{E = 10K,\ d = 9.}$

Problem 5.10

(a) $\chi(2,1,3) = a|\uparrow\uparrow\uparrow\rangle + b|\uparrow\uparrow\downarrow\rangle + c|\downarrow\uparrow\uparrow\rangle + d|\downarrow\uparrow\downarrow\rangle + e|\uparrow\downarrow\uparrow\rangle + f|\uparrow\downarrow\downarrow\rangle + g|\downarrow\downarrow\uparrow\rangle + h|\downarrow\downarrow\downarrow\rangle$.
$\chi(2,1,3) = -\chi(1,2,3) \Rightarrow a = b = g = h = 0, \quad e = -c, \quad f = -d.$
(Because the individual states are orthogonal, the associated coefficients must be equal.)
$\chi(1,3,2) = a|\uparrow\uparrow\uparrow\rangle + b|\uparrow\downarrow\uparrow\rangle + c|\uparrow\uparrow\downarrow\rangle + d|\uparrow\downarrow\downarrow\rangle + e|\downarrow\uparrow\uparrow\rangle + f|\downarrow\downarrow\uparrow\rangle + g|\downarrow\uparrow\downarrow\rangle + h|\downarrow\downarrow\downarrow\rangle$.
$\chi(1,3,2) = -\chi(1,2,3) \Rightarrow a = d = e = h = 0, \quad c = -b, \quad g = -f.$
So all 8 coefficients are zero, and $\chi(1,2,3) = 0$.
(b) You can't put all 3 in ψ_1 because this would be a symmetric combination, and we just showed that there is no antisymmetric spin state to go with it.

$$\begin{vmatrix} \psi_1(x_1)|\uparrow\rangle_1 & \psi_1(x_1)|\downarrow\rangle_1 & \psi_2(x_1)|\uparrow\rangle_1 \\ \psi_1(x_2)|\uparrow\rangle_2 & \psi_1(x_2)|\downarrow\rangle_2 & \psi_2(x_2)|\uparrow\rangle_2 \\ \psi_1(x_3)|\uparrow\rangle_3 & \psi_1(x_3)|\downarrow\rangle_3 & \psi_2(x_3)|\uparrow\rangle_3 \end{vmatrix}$$

$$\begin{aligned} = \; & \psi_1(x_1)\psi_1(x_2)\psi_2(x_3)|\uparrow\downarrow\uparrow\rangle + \psi_1(x_1)\psi_2(x_2)\psi_1(x_3)|\downarrow\uparrow\uparrow\rangle + \psi_2(x_1)\psi_1(x_2)\psi_1(x_3)|\uparrow\uparrow\downarrow\rangle \\ & - \psi_2(x_1)\psi_1(x_2)\psi_1(x_3)|\uparrow\downarrow\uparrow\rangle - \psi_1(x_1)\psi_2(x_2)\psi_1(x_3)|\uparrow\uparrow\downarrow\rangle - \psi_1(x_1)\psi_1(x_2)\psi_2(x_3)|\downarrow\uparrow\uparrow\rangle. \end{aligned}$$

The energy is $E = \dfrac{\pi^2\hbar^2}{2ma^2}(1^2+1^2+2^2) = \boxed{\dfrac{3\pi^2\hbar^2}{ma^2}}$. Degeneracy is $\boxed{d = 2,}$ (we could have started with $\psi_2(x_1)|\downarrow\rangle_1$ instead of $\psi_2(x_1)|\uparrow\rangle_1$).
(c) For normalization, divide by $\sqrt{6}$ (since the terms are orthonormal):

$$\begin{aligned} \Phi(1,2,3) = & \frac{1}{\sqrt{6}}\big[\psi_1(x_1)\psi_1(x_2)\psi_2(x_3)(|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle) + \psi_1(x_1)\psi_1(x_3)\psi_2(x_2)(|\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle) \\ & + \psi_1(x_2)\psi_1(x_3)\psi_2(x_1)(|\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\rangle)\big] \\ = & \frac{1}{\sqrt{6}}\Big[\psi_1(x_1)\psi_1(x_2)(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2)\,\psi_2(x_3)|\uparrow\rangle_3 + \psi_1(x_1)\psi_1(x_3)(|\downarrow\rangle_1|\uparrow\rangle_3 - |\uparrow\rangle_1|\downarrow\rangle_3)\,\psi_2(x_2)|\uparrow\rangle_2 \\ & + \psi_1(x_2)\psi_1(x_3)(|\uparrow\rangle_2|\downarrow\rangle_3 - |\downarrow\rangle_2|\uparrow\rangle_3)\,\psi_2(x_1)|\uparrow\rangle_1\Big] \\ = & \frac{1}{\sqrt{3}}\Big[\Phi(1,2)\,\phi(3) - \Phi(1,3)\,\phi(2) + \Phi(2,3)\,\phi(1)\Big]. \quad \checkmark \end{aligned}$$

$$\begin{aligned} \Phi(2,1,3) &= \frac{1}{\sqrt{3}}\Big[\Phi(2,1)\,\phi(3) - \Phi(2,3)\,\phi(1) + \Phi(1,3)\,\phi(2)\Big] \\ &= \frac{1}{\sqrt{3}}\Big[-\Phi(1,2)\,\phi(3) - \Phi(2,3)\,\phi(1) + \Phi(1,3)\,\phi(2)\Big] = -\Phi(1,2,3), \quad \checkmark \end{aligned}$$

and the same goes for the other two permutations.

Problem 5.11

(a) The exponential factor is obviously symmetric; the product term is

$$[(z_1 - z_2)(z_1 - z_3)\cdots(z_1 - z_N)(z_2 - z_3)\cdots(z_2 - z_N)\cdots(z_{N-1} - z_N)]^q.$$

Under $1 \leftrightarrow 2$ the first factor switches sign, while the others simply change places: $(z_1 - z_3) \leftrightarrow (z_2 - z_3)$, etc., so the term in square brackets picks up a minus sign. Since q is an *odd* positive integer, the whole thing (and hence also ψ itself) is antisymmetric. $\checkmark$

(b) $\psi(z_1,z_2,z_3)=A(z_1-z_2)(z_1-z_3)(z_2-z_3)e^{-\frac{1}{2}(|z_1|^2+|z_2|^2+|z_3|^2)}$. Now

$$(z_1-z_2)(z_1-z_3)(z_2-z_3)=z_1^2z_2+z_2^2z_3+z_3^2z_1-z_1^2z_3-z_2^2z_1-z_3^2z_2=\begin{vmatrix} z_1^2 & z_1 & 1 \\ z_2^2 & z_2 & 1 \\ z_3^2 & z_3 & 1 \end{vmatrix},$$

so

$$\psi(z_1,z_2,z_3)=A\begin{vmatrix} z_1^2e^{-\frac{1}{2}|z_1|^2} & z_1e^{-\frac{1}{2}|z_1|^2} & e^{-\frac{1}{2}|z_1|^2} \\ z_2^2e^{-\frac{1}{2}|z_2|^2} & z_2e^{-\frac{1}{2}|z_2|^2} & e^{-\frac{1}{2}|z_2|^2} \\ z_3^2e^{-\frac{1}{2}|z_3|^2} & z_3e^{-\frac{1}{2}|z_3|^2} & e^{-\frac{1}{2}|z_3|^2} \end{vmatrix}. \quad \checkmark$$

The occupied single-particle states are

$$\boxed{\psi_a(z)=A_ae^{-\frac{1}{2}|z|^2}, \quad \psi_b(z)=A_bze^{-\frac{1}{2}|z|^2}, \quad \psi_c(z)=A_cz^2e^{-\frac{1}{2}|z|^2},}$$

for appropriate normalization constants A_a, A_b, A_c.

(c) $\psi(z_1,z_2)=A(z_1-z_2)^3e^{-\frac{1}{2}(|z_1|^2+|z_2|^2)}$.

$$(z_1-z_2)^3=z_1^3-3z_1^2z_2+3z_1z_2^2-z_2^3=\begin{vmatrix} z_1^3 & 1 \\ z_2^3 & 1 \end{vmatrix}+3\begin{vmatrix} z_1 & z_1^2 \\ z_2 & z_2^2 \end{vmatrix},$$

so

$$\psi(z_1,z_2)=A\left\{\begin{vmatrix} z_1^3e^{-\frac{1}{2}|z_1|^2} & e^{-\frac{1}{2}|z_1|^2} \\ z_2^3e^{-\frac{1}{2}|z_2|^2} & e^{-\frac{1}{2}|z_2|^2} \end{vmatrix}+3\begin{vmatrix} z_1e^{-\frac{1}{2}|z_1|^2} & z_1^2e^{-\frac{1}{2}|z_1|^2} \\ z_2e^{-\frac{1}{2}(z_2|^2} & z_2^2e^{-\frac{1}{2}|z_2|^2} \end{vmatrix}\right\}. \quad \checkmark$$

Problem 5.12

(a)

$$\psi_\pm=A\big[\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\ldots,\mathbf{r}_Z)\pm\psi(\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_3,\ldots,\mathbf{r}_Z)+\psi(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_1,\ldots,\mathbf{r}_Z)+\text{etc.}\big],$$

where "etc." runs over all permutations of the arguments $\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_Z$, with a $+$ sign for all *even* permutations (even number of transpositions $\mathbf{r}_i\leftrightarrow\mathbf{r}_j$, starting from $\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_Z$), and $\pm$ for all *odd* permutations ($+$ for symmetric, $-$ for antisymmetric). At the end of the process, normalize the result to determine A. (Typically $A=1/\sqrt{Z!}$, but this may not be right if the starting function is already symmetric under some interchanges.) If ψ is symmetric in the first two arguments (or any other pair), the antisymmetric combination is zero. For example, if $Z=3$,

$$\psi_-=\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)-\psi(\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_3)+\psi(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_1)-\psi(\mathbf{r}_3,\mathbf{r}_2,\mathbf{r}_1)+\psi(\mathbf{r}_3,\mathbf{r}_1,\mathbf{r}_2)-\psi(\mathbf{r}_1,\mathbf{r}_3,\mathbf{r}_2)=0$$

(they cancel in pairs).

(b) Since there are only two possible one-particle states, $|\uparrow\rangle$ and $|\downarrow\rangle$, a configuration of three or more electrons will have to put at least two of them in the same state, which will then be symmetric under their interchange, and from that no completely antisymmetric combination can be constructed.

Problem 5.13

(a) The energy of each electron is $E=Z^2E_1/n^2=4E_1/4=E_1=-13.6\text{eV}$, so the total initial energy is $2\times(-13.6)$ eV$=-27.2$ eV. One electron drops to the ground state $Z^2E_1/1=4E_1$, so the *other* is left with $2E_1-4E_1=-2E_1=\boxed{27.2\text{ eV.}}$

(b) He^+ has *one* electron; it's a hydrogenic ion (Problem 4.19) with $Z = 2$, so the spectrum is $\boxed{1/\lambda = 4R\left(1/n_f^2 - 1/n_i^2\right),}$ where R is the hydrogen Rydberg constant, and n_i, n_f are the initial and final quantum numbers (1, 2, 3, ...).

Problem 5.14

(a) The ground state (Eq. 5.41) is spatially *symmetric*, so it goes with the symmetric (triplet) spin configuration. Thus the ground state is *ortho*helium, and it is triply degerate. The excited states (Eq. 5.43) come in ortho (triplet) and para (singlet) form; since the former go with the symmetric spatial wave function, the orthohelium states are *higher* in energy than the corresponding (nondegenerate) para states.

(b) The ground state (Eq. 5.41) and all excited states (Eq. 5.43) come in both ortho and para form. All are quadruply degenerate (or at any rate we have no way *a priori* of knowing whether ortho or para are higher in energy, since we don't know which goes with the symmetric spatial configuration).

Problem 5.15

(a)

$$\left\langle \frac{1}{|r_1 - r_2|} \right\rangle = \left(\frac{8}{\pi a^3}\right)^2 \int \underbrace{\left[\int \frac{e^{-4(r_1+r_2)/a}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}}\, d^3\mathbf{r}_2\right]}_{\blacklozenge} d^3\mathbf{r}_1$$

$$\blacklozenge = 2\pi \int_0^\infty e^{-4(r_1+r_2)/a} \underbrace{\left[\int_0^\pi \frac{\sin\theta_2}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}} d\theta_2\right]}_{\star} r_2^2\, dr_2$$

$$\star = \frac{1}{r_1 r_2}\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}\,\Big|_0^\pi = \frac{1}{r_1 r_2}\left[\sqrt{r_1^2 + r_2^2 + 2r_1 r_2} - \sqrt{r_1^2 + r_2^2 - 2r_1 r_2}\right]$$

$$= \frac{1}{r_1 r_2}\left[(r_1 + r_2) - |r_1 - r_2|\right] = \begin{cases} 2/r_1 & (r_2 < r_1) \\ 2/r_2 & (r_2 > r_1) \end{cases}$$

$$\blacklozenge = 4\pi e^{-4r_1/a}\left[\frac{1}{r_1}\int_0^{r_1} r_2^2 e^{-4r_2/a} dr_2 + \int_{r_1}^\infty r_2 e^{-4r_2/a} dr_2\right].$$

$$\frac{1}{r_1}\int_0^{r_1} r_2^2 e^{-4r_2/a} dr_2 = \frac{1}{r_1}\left[-\frac{a}{4} r_2^2 e^{-4r_2/a} + \frac{a}{2}\left(\frac{a}{4}\right)^2 e^{-4r_2/a}\left(-\frac{4r_2}{a} - 1\right)\right]\Bigg|_0^{r_1}$$

$$= -\frac{a}{4r_1}\left[r_1^2 e^{-4r_1/a} + \frac{ar_1}{2}e^{-4r_1/a} + \frac{a^2}{8}e^{-4r_1/a} - \frac{a^2}{8}\right].$$

$$\int_{r_1}^{\infty} r_2 e^{-4r_2/a} dr_2 = \left(\frac{a}{4}\right)^2 e^{-4r_2/a}\left(-\frac{4r_2}{a} - 1\right)\Big|_{r_1}^{\infty} = \frac{ar_1}{4}e^{-4r_1/a} + \frac{a^2}{16}e^{-4r_1/a}.$$

$$\blacklozenge = 4\pi\left\{\frac{a^3}{32r_1}e^{-4r_1/a} + \left[-\frac{ar_1}{4} - \frac{a^2}{8} - \frac{a^3}{32r_1} + \frac{ar_1}{4} + \frac{a^2}{16}\right]e^{-8r_1/a}\right\}$$

$$= \frac{\pi a^2}{8}\left\{\frac{a}{r_1}e^{-4r_1/a} - \left(2 + \frac{a}{r_1}\right)e^{-8r_1/a}\right\}.$$

$$\left\langle\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\right\rangle = \frac{8}{\pi a^4}\cdot 4\pi\int_0^{\infty}\left[\frac{a}{r_1}e^{-4r_1/a} - \left(2 + \frac{a}{r_1}\right)e^{-8r_1/a}\right]r_1^2\, dr_1$$

$$= \frac{32}{a^4}\left\{a\int_0^{\infty} r_1 e^{-4r_1/a}dr_1 - 2\int_0^{\infty} r_1^2 e^{-8r_1/a}dr_1 - a\int_0^{\infty} r_1 e^{-8r_1/a}dr_1\right\}$$

$$= \frac{32}{a^4}\left\{a\cdot\left(\frac{a}{4}\right)^2 - 2\cdot 2\left(\frac{a}{8}\right)^3 - a\cdot\left(\frac{a}{8}\right)^2\right\} = \frac{32}{a}\left(\frac{1}{16} - \frac{1}{128} - \frac{1}{64}\right) = \boxed{\frac{5}{4a}.}$$

(b)

$$V_{ee} \approx \frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\right\rangle = \boxed{\frac{5}{4}\frac{e^2}{4\pi\epsilon_0}\frac{1}{a}} = \frac{5}{4}\frac{m}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = \frac{5}{2}(-E_1) = \frac{5}{2}(13.6\,\text{eV}) = \boxed{34 \text{ eV.}}$$

$E_0 + V_{ee} = (-109 + 34)\text{eV} = \boxed{-75 \text{ eV},}$ which is pretty close to the experimental value (-79 eV).

Problem 5.16

$\psi_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \psi_{100}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2)\psi_{200}(\mathbf{r}_3)$, where $\psi_{n\ell m}$ is the hydrogenic wave function with "Bohr radius" $\bar{a} = a/Z = a/3$. The energy (expressed in terms of Bohr levels) is $E = Z^2(E_1 + E_1 + E_2) = 9(2E_1 + \frac{E_1}{4}) = \boxed{\frac{81}{4}E_1 = -275\,\text{eV}.}$ In the notation of Problem 5.10:

$$\psi_1(r) = \psi_{100}(\mathbf{r}) = \frac{1}{\sqrt{\pi\bar{a}^3}}e^{-r/\bar{a}}; \quad \psi_2(r) = \psi_{200}(\mathbf{r}) = R_{20}Y_0^0 = \frac{1}{\sqrt{2}}\,\bar{a}^{-3/2}\left(1 - \frac{r}{2\bar{a}}\right)e^{-r/2\bar{a}}\frac{1}{\sqrt{4\pi}},$$

$$\Phi(i,j) \equiv \psi_1(r_i)\psi_1(r_j)|00\rangle_{ij} = \frac{27}{\pi a^3} e^{-3(r_i+r_j)/a}|00\rangle_{ij}$$

(where $|00\rangle_{ij}$ denotes the singlet configuration of spins i and j), and

$$\phi(j) \equiv \psi_2(r_j)|\tfrac{1}{2}\,\tfrac{1}{2}\rangle_j = \frac{1}{2\sqrt{2\pi}}\left(\frac{3}{a}\right)^{3/2}\left(1-\frac{3r_j}{2a}\right)e^{-3r_j/2a}|\tfrac{1}{2}\,\tfrac{1}{2}\rangle_j.$$

The complete ground state, then, is (quoting the result of Problem 5.10(c)):

$$\Phi(1,2,3) = \frac{1}{\sqrt{3}}\Big[\Phi(1,2)\,\phi(3) - \Phi(1,3)\,\phi(2) + \Phi(2,3)\,\phi(1)\Big].$$

It is $\boxed{\text{doubly degenerate,}}$ since for $\phi(j)$ we could have used $|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle$.

Problem 5.17

(a) Hydrogen: $(1s)$; helium: $(1s)^2$; lithium: $(1s)^2(2s)$; beryllium: $(1s)^2(2s)^2$; boron: $(1s)^2(2s)^2(2p)$; carbon: $(1s)^2(2s)^2(2p)^2$; nitrogen: $(1s)^2(2s)^2(2p)^3$; oxygen: $(1s)^2(2s)^2(2p)^4$; fluorine: $(1s)^2(2s)^2(2p)^5$; neon: $(1s)^2(2s)^2(2p)^6$. These values agree with those in Table 5.1—no surprises so far.

(b) Hydrogen: ${}^2S_{1/2}$; helium: ${}^1S_0$; lithium: ${}^2S_{1/2}$; beryllium ${}^1S_0$. (These four are unambiguous, because the *orbital* angular momentum is zero in all cases.) For boron, the spin (1/2) and orbital (1) angular momenta could add to give 3/2 or 1/2, so the possibilities are $\boxed{{}^2P_{3/2} \text{ or } {}^2P_{1/2}.}$ For carbon, the two p electrons could combine for orbital angular momentum 2, 1, or 0, and the spins could add to 1 or 0: $\boxed{{}^1S_0, {}^3S_1, {}^1P_1, {}^3P_2, {}^3P_1, {}^3P_0, {}^1D_2, {}^3D_3, {}^3D_2, {}^3D_1.}$ For nitrogen, the 3 p electrons can add to orbital angular momentum 3, 2, 1, or 0, and the spins to 3/2 or 1/2:

$$\boxed{\begin{array}{l} {}^2S_{1/2}, {}^4S_{3/2}, {}^2P_{1/2}, {}^2P_{3/2}, {}^4P_{1/2}, {}^4P_{3/2}, {}^4P_{5/2}, {}^2D_{3/2}, {}^2D_{5/2}, \\ {}^4D_{1/2}, {}^4D_{3/2}, {}^4D_{5/2}, {}^4D_{7/2}, {}^2F_{5/2}, {}^2F_{7/2}, {}^4F_{3/2}, {}^4F_{5/2}, {}^4F_{7/2}, {}^4F_{9/2}. \end{array}}$$

Problem 5.18

(a) Orthohelium should have lower energy than parahelium, for corresponding states (which is true).

(b) Hund's first rule says $S = 1$ for the ground state of carbon. But this (the triplet) is symmetric, so the orbital state will have to be antisymmetric. Hund's second rule favors $L = 2$, but this is symmetric, as you can see most easily by going to the "top of the ladder": $|2\,2\rangle = |1\,1\rangle_1|1\,1\rangle_2$. So the ground state of carbon will be $S = 1, L = 1$. This leaves three possibilities: ${}^3P_2, {}^3P_1$, and ${}^3P_0$.

(c) For boron there is only one electron in the $2p$ subshell (which can accommodate a total of 6), so Hund's third rule says the ground state will have $J = |L - S|$. We found in Problem 5.17(b) that $L = 1$ and $S = 1/2$, so $J = 1/2$, and the configuration is $\boxed{{}^2P_{1/2}.}$

(d) For carbon we know that $S = 1$ and $L = 1$, and there are only two electrons in the outer subshell, so Hund's third rule says $J = 0$, and the ground state configuration must be $\boxed{{}^3P_0.}$

For nitrogen Hund's first rule says $S = 3/2$, which is symmetric (the top of the ladder is $|\tfrac{3}{2}\,\tfrac{3}{2}\rangle = |\tfrac{1}{2}\,\tfrac{1}{2}\rangle_1|\tfrac{1}{2}\,\tfrac{1}{2}\rangle_2|\tfrac{1}{2}\,\tfrac{1}{2}\rangle_3$). Hund's second rule favors $L = 3$, but this is also symmetric. In fact, the only *anti*symmetric orbital configuration here is $L = 0$. [You can check this directly by working out the Clebsch-Gordan coefficients, but it's easier to reason as follows: Suppose the three outer electrons are in the "top of the ladder" spin state, so each one has spin up ($|\frac{1}{2}\,\frac{1}{2}\rangle$); then (since the spin states are all the same) the orbital states *have* to be different: $|1\,1\rangle$, $|1\,0\rangle$, and $|1\,{-1}\rangle$. In particular, the total z-component of orbital angular momentum has to be zero. But the only configuration that restricts L_z to zero is $L = 0$.] The outer subshell is exactly half filled (three electrons with $n = 2$, $l = 1$), so Hund's third rule says $J = |L - S| = |0 - \frac{3}{2}| = 3/2$. *Conclusion:* The ground state of nitrogen is $\boxed{{}^4S_{3/2}.}$ (Table 5.1 confirms this.)

Problem 5.19

$\boxed{S = 2;\ L = 6;\ J = 8.}\ \underbrace{(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(3d)^{10}(4s)^2(4p)^6}_{\text{definite (36 electrons)}}\ \underbrace{(4d)^{10}(5s)^2(5p)^6(4f)^{10}(6s)^2}_{\text{likely (30 electrons)}}.$

Problem 5.20

Divide Eq. 5.56 by Eq. 5.54, using Eq. 5.53:

$$\frac{E_{\text{tot}}/Nq}{E_F} = \frac{\hbar^2(3\pi^2 Nq)^{5/3}}{10\pi^2 m V^{2/3}}\frac{1}{Nq}\frac{2m}{\hbar^2(3\pi^2 Nq/V)^{2/3}} = \boxed{\frac{3}{5}.}$$

Problem 5.21

(a) $E_F = \dfrac{\hbar^2}{2m}(3\rho\pi^2)^{2/3}$. $\rho = \dfrac{Nq}{V} = \dfrac{N}{V} = \dfrac{\text{atoms}}{\text{mole}} \times \dfrac{\text{moles}}{\text{gm}} \times \dfrac{\text{gm}}{\text{volume}} = \dfrac{N_A}{M} \cdot d$, where N_A is Avogadro's number (6.02×10^{23}), M = atomic mass = 63.5 gm/mol, d = density = 8.96 gm/cm^3.

$$\rho = \frac{(6.02 \times 10^{23})(8.96\ \text{gm/cm}^3)}{(63.5\ \text{gm})} = 8.49 \times 10^{22}/\text{cm}^3 = 8.49 \times 10^{28}/\text{m}^3.$$

$$E_F = \frac{(1.055 \times 10^{-34}\text{J}\cdot\text{s})(6.58 \times 10^{-16}\text{eV}\cdot\text{s})}{(2)(9.109 \times 10^{-31}\text{kg})}(3\pi^2\, 8.49 \times 10^{28}/\text{m}^3)^{2/3} = \boxed{7.04\ \text{eV}.}$$

(b)

$$7.04\ \text{eV} = \frac{1}{2}(0.511 \times 10^6\text{eV}/c^2)v^2 \Rightarrow \frac{v^2}{c^2} = \frac{14.08}{.511 \times 10^6} = 2.76 \times 10^{-5} \Rightarrow \frac{v}{c} = 5.25 \times 10^{-3},$$

so it's $\boxed{\text{nonrelativistic.}}$ $v = (5.25 \times 10^{-3}) \times (3 \times 10^8) = \boxed{1.57\ \times 10^6\ \text{m/s.}}$

(c)

$$T = \frac{7.04\,\text{eV}}{8.62 \times 10^{-5}\,\text{eV/K}} = \boxed{8.17 \times 10^4\,\text{K.}}$$

(d)

$$P = \frac{(3\pi^2)^{2/3}\hbar^2}{5m}\rho^{5/3} = \frac{(3\pi^2)^{2/3}(1.055 \times 10^{-34})^2}{5(9.109 \times 10^{-31})}(8.49 \times 10^{28})^{5/3}\text{N/m}^2 = \boxed{3.84 \times 10^{10}\ \text{N/m}^2.}$$

Problem 5.22

$T_F = \dfrac{E_F}{k_B} = \dfrac{\hbar^2}{2mk_B}(3\rho\pi^2)^{2/3}$ (Equation 5.54). The number density $\rho = \frac{\text{atoms}}{\text{mass}} \times \frac{\text{mass}}{\text{volume}} = \frac{\rho_m}{m}$, where ρ_m is the mass density and m is the atomic mass—3 times the mass of the proton: $m = 3m_p$ (well, OK, two protons and a neutron, and two electrons, and some binding energy ... but 3 protons is close enough). So

$$T_F = \frac{\hbar^2}{6m_pk_B}\left(\frac{\pi^2\rho_m}{m_p}\right)^{2/3} = \frac{(1.055\times10^{-34})^2}{6(1.673\times10^{-27})(1.381\times10^{-23})}\left(\frac{\pi^2(82)}{1.673\times10^{-27}}\right)^{2/3} = \boxed{4.95\,\mathrm{K}.}$$

Problem 5.23

$$P = \frac{(3\pi^2)^{2/3}\hbar^2}{5m}\left(\frac{Nq}{V}\right)^{5/3} = AV^{-5/3} \Rightarrow B = -V\frac{dP}{dV} = -VA\left(\frac{-5}{3}\right)V^{-5/3-1} = \frac{5}{3}AV^{-5/3} = \frac{5}{3}P.$$

For copper, $B = \frac{5}{3}(3.84\times10^{10}\,\mathrm{N/m^2}) = \boxed{6.4\times10^{10}\ \mathrm{N/m^2}.}$

Problem 5.24

(a) Equations 5.66 and 5.70 $\Rightarrow \psi = A\sin kx + B\cos kx;\quad A\sin ka = \left[e^{iqa} - \cos ka\right]B.$ So

$$\psi = A\sin kx + \frac{A\sin ka}{(e^{iqa}-\cos ka)}\cos kx = \frac{A}{(e^{iqa}-\cos ka)}\left[e^{iqa}\sin kx - \sin kx\cos ka + \cos kx\sin ka\right]$$

$$= C\left\{\sin kx + e^{-iqa}\sin[k(a-x)]\right\},\ \text{where } C \equiv \frac{Ae^{iqa}}{e^{iqa}-\cos ka}.$$

(b) If $z = ka = j\pi$, then $\sin ka = 0$, Eq. 5.71 $\Rightarrow \cos qa = \cos ka = (-1)^j \Rightarrow \sin qa = 0$, so $e^{iqa} = \cos qa + i\sin qa = (-1)^j$, and the constant C involves division by zero. In this case we must go back to Eq. 5.70, which is a tautology (0=0) yielding no constraint on A or B, Eq. 5.68 holds automatically, and Eq. 5.69 gives

$$kA - (-1)^jk\left[A(-1)^j - 0\right] = \frac{2m\alpha}{\hbar^2}B \Rightarrow B = 0.\quad \text{So}\quad \boxed{\psi = A\sin kx.}$$

Here ψ is *zero* at each delta spike, so the wave function never "feels" the potential at all.

Problem 5.25

We're looking for a solution to Eq. 5.73 with $\beta = 10$ and $z \lesssim \pi$: $f(z) = \cos z + 10\dfrac{\sin z}{z} = 1.$

Mathematica gives $z = 2.62768$. So $\quad E = \dfrac{\hbar^2k^2}{2m} = \dfrac{\hbar^2z^2}{2ma^2} = \dfrac{z^2}{2\beta}\dfrac{\alpha}{a} = \dfrac{(2.62768)^2}{20}\,\mathrm{eV} = \boxed{0.345\ \mathrm{eV}.}$

Problem 5.26

Positive-energy solutions. These are the same as before, except that α (and hence also β) is now a negative number.

Negative-energy solutions. On $0 < x < a$ we have

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi, \quad \text{where} \quad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \quad \Rightarrow \quad \psi(x) = A\sinh\kappa x + B\cosh\kappa x.$$

According to Bloch's theorem the solution on $-a < x < 0$ is

$$\psi(x) = e^{-iqa}\left[A\sinh\kappa(x+a) + B\cosh\kappa(x+a)\right].$$

Continuity at $x = 0 \Rightarrow$

$$B = e^{-iqa}\left[A\sinh\kappa a + B\cosh\kappa a\right], \quad \text{or} \quad A\sinh\kappa a = B\left[e^{iqa} - \cosh\kappa a\right]. \qquad [\bigstar]$$

The discontinuity in ψ' (Eq. 2.128) $\Rightarrow$

$$\kappa A - e^{-iqa}\kappa\left[A\cosh\kappa a + B\sinh\kappa a\right] = \frac{2m\alpha}{\hbar^2}B, \text{ or } A\left[1 - e^{-iqa}\cosh\kappa a\right] = B\left[\frac{2m\alpha}{\hbar^2\kappa} + e^{-iqa}\sinh\kappa a\right]. \qquad [\blacklozenge]$$

Plugging $\bigstar$ into $\blacklozenge$ and cancelling B:

$$\left(e^{iqa} - \cosh\kappa a\right)\left(1 - e^{-iqa}\cosh\kappa a\right) = \frac{2m\alpha}{\hbar^2\kappa}\sinh\kappa a + e^{-iqa}\sinh^2\kappa a.$$

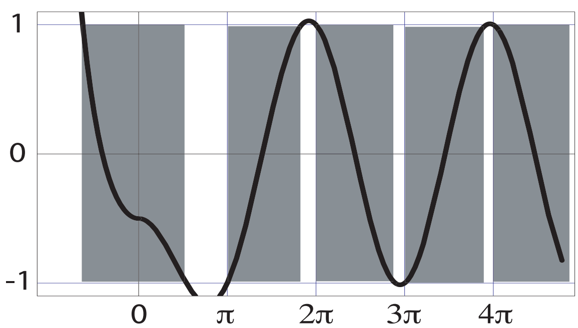
$$e^{iqa} - 2\cosh\kappa a + e^{-iqa}\cosh^2\kappa a - e^{-iqa}\sinh^2\kappa a = \frac{2m\alpha}{\hbar^2\kappa}\sinh\kappa a.$$

$$e^{iqa} + e^{-iqa} = 2\cosh\kappa a + \frac{2ma}{\hbar^2\kappa}\sinh\kappa a, \qquad \boxed{\cos qa = \cosh\kappa a + \frac{m\alpha}{\hbar^2\kappa}\sinh\kappa a.}$$

This is the analog to Eq. 5.71. As before, we let $\beta \equiv m\alpha a/\hbar^2$ (but remember it's now a *negative* number), and this time we define $z \equiv -\kappa a$, extending Eq. 5.72 to negative z, where it represents negative-energy solutions. In this region we define

$$f(z) = \cosh z + \beta\,\frac{\sinh z}{z}. \qquad [\bigstar\bigstar]$$

In the figure below I have plotted $f(z)$ for $\beta = -1.5$, using Eq. 5.73 for positive z and $\bigstar\bigstar$ for negative z. As before, allowed energies are restricted to the range $-1 \le f(z) \le 1$, and occur at intersections of $f(z)$ with the N horizontal lines $\cos qa = \cos(2\pi n/Na)$, with $n = 0, 1, 2 \ldots N-1$. Evidently the first band (partly negative, and partly positive) contains N states, as do all the higher bands.



Problem 5.27

Equation 5.63 says $q = \dfrac{2\pi n}{Na} \Rightarrow qa = 2\pi\dfrac{n}{N}$; on page 223 we found that $n = 0, 1, 2, \ldots, N-1$. Each value of n corresponds to a distinct state. To find the allowed energies we draw N horizontal lines on Figure 5.5, at heights $\cos qa = \cos(2\pi n/N)$, and look for intersections with $f(z)$. The point is that *almost* all of these lines come in pairs—two different n's yielding the same value of $\cos qa$:

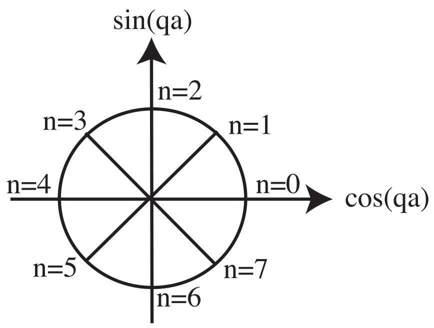
$\underline{N=1}$ $\Rightarrow n = 0 \Rightarrow \cos qa = 1.$ Nondegenerate.

$\underline{N=2}$ $\Rightarrow n = 0, 1 \Rightarrow \cos qa = 1, -1.$ Nondegenerate.

$\underline{N=3}$ $\Rightarrow n = 0, 1, 2 \Rightarrow \cos qa = 1, -\frac{1}{2}, -\frac{1}{2}.$ The first is nondegenerate, the other two are degenerate.

$\underline{N=4}$ $\Rightarrow n = 0, 1, 2, 3 \Rightarrow \cos qa = 1, 0, -1, 0.$ Two are nondegenerate, the others are degenerate.

Evidently they are doubly degenerate (two different n's give same $\cos qa$) *except* when $\cos qa = \pm 1$, i.e., at the $\boxed{\text{top or bottom of a band.}}$ The Bloch factors e^{iqa} lie at equal angles in the complex plane, starting with 1 (see figure below, drawn for the case $N = 8$); by symmetry, there is always one with negative imaginary part symmetrically opposite each one with positive imaginary part; these two have the same *real* part ($\cos qa$). Only points which fall *on* the real axis have no twins.



Problem 5.28

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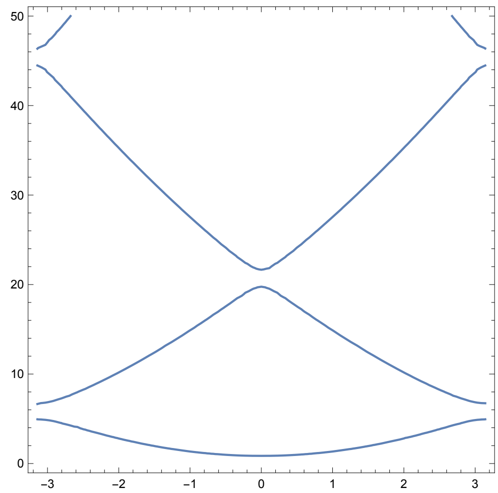
ContourPlot[Cos[x] == Cos[√(2 y)] + (Sin[√(2 y)]) / √(2 y), {x, -π, π}, {y, 0, 50}]
```



Problem 5.29

(a) Each particle has 3 possible states: $3 \times 3 \times 3 = \boxed{27.}$

(b) All in same state: $aaa,\ bbb,\ ccc \Rightarrow 3.$

2 in one state: $aab,\ aac,\ bba,\ bbc,\ cca,\ ccb \Rightarrow 6$ (each symmetrized).

3 different states: abc (symmetrized) $\Rightarrow 1.$

Total: $\boxed{10.}$

(c) Only abc (antisymmetrized) $\Longrightarrow \boxed{1.}$

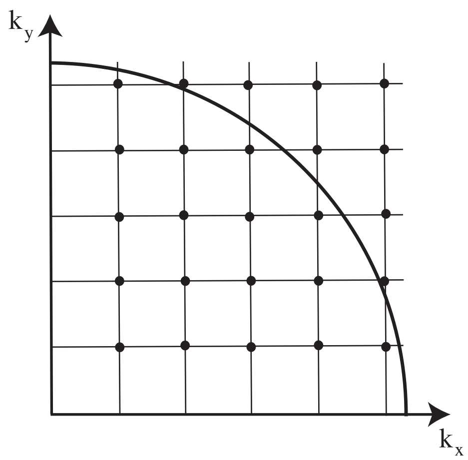
Problem 5.30

Equation 5.50 $\Rightarrow E_{n_x n_y} = \dfrac{\pi^2\hbar^2}{2m}\left(\dfrac{n_x^2}{l_x^2}+\dfrac{n_y^2}{l_y^2}\right) = \dfrac{\hbar^2 k^2}{2m}$, with $\mathbf{k} = \left(\dfrac{\pi n_x}{l_x}, \dfrac{\pi n_y}{l_y}\right)$. Each state is represented by an intersection on a grid in "**k**-space"—this time a *plane*—and each state occupies an area $\pi^2/l_x l_y = \pi^2/A$ (where $A \equiv l_x l_y$ is the area of the well). Two electrons per state means

$$\frac{1}{4}\pi k_F^2 = \frac{Nq}{2}\left(\frac{\pi^2}{A}\right), \text{ or } k_F = \left(2\pi\frac{Nq}{A}\right)^{1/2} = (2\pi\sigma)^{1/2},$$

where $\sigma \equiv Nq/A$ is the number of free electrons per unit area.

$$\therefore E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}2\pi\sigma = \boxed{\frac{\pi\hbar^2\sigma}{m}.}$$



Problem 5.31

(a) The energy of a particle in the ground state of an infinite cubical well of side a is (Equation5.50)
$E_{111} = \frac{\pi^2\hbar^2}{2m}\left(\frac{1}{a^2}+\frac{1}{a^2}+\frac{1}{a^2}\right) = \frac{3\pi^2\hbar^2}{2ma^2}$. So the energy of N such particles is $\boxed{E_a = N\frac{3\pi^2\hbar^2}{2ma^2}.}$

(b) Now we put the N electrons in a single cubical box of volume V; according to Equation 5.56 the total energy is
$E_b = \frac{\hbar^2(3\pi^2N)^{5/3}}{10\,\pi^2 m}V^{-2/3}$. Here V is the total volume of N cubes, each of volume a^3, so $V = Na^3$, and hence
$E_b = \frac{\hbar^2(3\pi^2N)^{5/3}}{10\pi^2 m(Na^3)^{2/3}} = \boxed{N\frac{\pi^2\hbar^2}{2ma^2}\frac{3}{5}\left(\frac{3}{\pi}\right)^{2/3}.}$

(c) $\frac{\Delta E}{N} = \frac{E_a - E_b}{N} = \boxed{\frac{3\pi^2\hbar^2}{2ma^2}\left[1-\frac{1}{5}\left(\frac{3}{\pi}\right)^{2/3}\right].}$

(d) In Problem 2.58(d) we found that $\frac{\pi^2\hbar^2}{3ma^2} = 1.6\,\text{eV}$, so $\frac{\Delta E}{N} = \frac{9}{2}\left[1-\frac{1}{5}\left(\frac{3}{\pi}\right)^{2/3}\right]\times 1.6\,\text{eV} = \boxed{5.8\,\text{eV}.}$

Problem 5.32

(a) Repeat the calculation of Section 5.3.1 separately for N_+ and N_- (setting $Nd \to N_\pm$), and then add the energies. Start with the equation before 5.52, with no 1/2 on the right side:
$\frac{1}{8}\left(\frac{4}{3}\pi k_{F_\pm}^3\right) = N_\pm\left(\frac{\pi^3}{V}\right) \Rightarrow k_{F_\pm} = (6\rho_\pm\pi^2)^{1/3}$, where $\rho_\pm = \frac{N_\pm}{V}$. So Equation 5.54 becomes
$E_{F_\pm} = \frac{\hbar^2}{2m}(6\rho_\pm\pi^2)^{2/3}$. The number of states in the shell is $\frac{[\frac{1}{2}\pi k^2\,dk]}{(\pi^3/V)} = \frac{V}{2\pi^2}k^2\,dk$, Equation 5.55 becomes
$dE = \frac{\hbar^2k^2}{2m}\frac{V}{2\pi^2}k^2\,dk$, and

$$E_{\text{tot}_\pm} = \frac{\hbar^2 V}{4m\pi^2}\int_0^{k_{F_\pm}} k^4\,dk = \frac{\hbar^2 V}{20\pi^2 m}k_{F_\pm}^5 = \frac{\hbar^2(6\pi^2N_\pm)^{5/3}}{20\pi^2 m}V^{-2/3}; \boxed{E_{\text{tot}} = \frac{\hbar^2(6\pi^2)^{5/3}}{20\pi^2 m}V^{-2/3}\left[N_+^{5/3}+N_-^{5/3}\right].}$$

If $N_+ = N_- = (Nd)/2$, this reduces to $E_{\text{tot}} = \frac{\hbar^2(6\pi^2)^{5/3}}{20\pi^2 m}V^{-2/3}2\left(\frac{Nd}{2}\right)^{5/3} = \frac{\hbar^2}{10\pi^2 m}(3\pi^2 Nd)^{5/3}V^{-2/3}$, in agreement with Equation 5.56.

(b) Let $N \equiv (N_+ + N_-)$, $\Delta N \equiv (N_+ - N_-)$, so $N_\pm = \frac{1}{2}(N\pm\Delta N) = \frac{N}{2}(1\pm\epsilon)$, where $\epsilon \equiv \frac{\Delta N}{N} \ll 1$. Expanding in powers of ϵ:

$$N_+^{5/3}+N_-^{5/3} = \left(\frac{N}{2}\right)^{5/3}\left[(1+\epsilon)^{5/3}+(1-\epsilon)^{5/3}\right] \approx \left(\frac{N}{2}\right)^{5/3}\Big[\left(1+\tfrac{5}{3}\epsilon+\tfrac{1}{2}\left(\tfrac{5}{3}\right)\left(\tfrac{2}{3}\right)\epsilon^2\right)$$
$$+\left(1-\tfrac{5}{3}\epsilon+\tfrac{1}{2}\left(\tfrac{5}{3}\right)\left(\tfrac{2}{3}\right)\epsilon^2\right)\Big] = 2\left(\frac{N}{2}\right)^{5/3}\left(1+\frac{5}{9}\epsilon^2\right).$$

Therefore

$$\frac{E_{\text{tot}}}{V} = \frac{\hbar^2(6\pi^2)^{5/3}}{20\pi^2 m}V^{-5/3}\,2\left(\frac{N}{2}\right)^{5/3}\left[1+\frac{5}{9}\left(\frac{\Delta N}{N}\right)^2\right] = \frac{\hbar^2}{10\pi^2 m}\left(\frac{3\pi^2 N}{V}\right)^{5/3}\left[1+\frac{5}{9}\left(\frac{\Delta N}{N}\right)^2\right],$$

or, using $\rho = \dfrac{N}{V}$ and $\Delta N = -\dfrac{MV}{\mu_B} \Rightarrow \dfrac{\Delta N}{N} = -\dfrac{MV}{\mu_B \rho V} = -\dfrac{M}{\mu_B \rho}$, $\dfrac{E_{\text{tot}}}{V} = \dfrac{\hbar^2(3\pi^2\rho)^{5/3}}{10\pi^2 m}\left[1 + \dfrac{5}{9}\left(\dfrac{M}{\rho\mu_B}\right)^2\right]$. ✓
(Note that M is the *z-component* of $\mathbf{M}$, not its magnitude.)

Problem 5.33

(a) The extra energy is $\mu_B B(N_+ - N_-) = -BMV$, so $\dfrac{E_{\text{tot}}}{V} = \dfrac{\hbar^2(3\pi^2\rho)^{5/3}}{10\pi^2 m}\left[1 + \dfrac{5}{9}\left(\dfrac{M}{\rho\mu_B}\right)^2\right] - BM$. The minimum energy is given by

$$\frac{1}{V}\frac{\partial E_{\text{tot}}}{\partial M} = \frac{\hbar^2(3\pi^2\rho)^{5/3}}{10\pi^2 m}\left(\frac{5}{9}\right)\frac{2M}{(\rho\mu_B)^2} - B = 0 \Rightarrow M = B\frac{10\pi^2 m}{\hbar^2(3\pi^2\rho)^{5/3}}\left(\frac{9}{10}\right)(\rho\mu_B)^2 = \boxed{B\left(\frac{3\rho}{\pi}\right)^{1/3}\left(\frac{m\mu_B^2}{\pi\hbar^2}\right).}$$

(b) $\chi = \mu_0\left(\dfrac{3\rho}{\pi}\right)^{1/3}\left(\dfrac{m\mu_B^2}{\pi\hbar^2}\right)$. The numbers are

$$\begin{aligned}
\mu_0 &= 4\pi \times 10^{-7}\,\text{N/A}^2,\\
\rho &= 18.1 \times 10^{28}\,\text{m}^{-3},\\
m &= 9.11 \times 10^{-31}\,\text{kg},\\
\hbar &= 1.055 \times 10^{-34}\,\text{J s},\\
\mu_B &= 5.788 \times 10^{-5}\,\text{eV/T} = 9.272 \times 10^{-24}\,\text{J/T}.
\end{aligned}$$

Putting them into the formula, $\boxed{\chi = 15.7 \times 10^{-6}.}$ This is not wildly far from the experimental value (16, as compared to 22).

Problem 5.34

(a) In the notation of Problem 5.32: $N^2 = (N_+ + N_-)^2 = N_+^2 + 2N_+N_- + N_-^2$,

$(\Delta N)^2 = (N_+ - N_-)^2 = N_+^2 - 2N_+N_- + N_-^2$, so $4N_+N_- = N^2 - (\Delta N)^2 = \rho^2 V^2 - \left(\dfrac{MV}{\mu_B}\right)^2$,

and hence $\boxed{\Delta E = \dfrac{U}{4}\left[\rho^2 - \left(\dfrac{M}{\mu_B}\right)^2\right] V^2.}$

(b) Quoting the result of Problem 5.32(b):

$$\frac{E_{\text{tot}}}{V} = \frac{\hbar^2(3\pi^2\rho)^{5/3}}{10\pi^2 m}\left[1 + \frac{5}{9}\left(\frac{M}{\rho\mu_B}\right)^2\right] + \frac{UV}{4}\left[\rho^2 - \left(\frac{M}{\mu_B}\right)^2\right] = A(1 + \tfrac{5}{9}x^2) + B(1 - x^2),$$

where

$$A \equiv \frac{\hbar^2(3\pi^2\rho)^{5/3}}{10\pi^2 m}, \quad x \equiv \frac{M}{\rho\,\mu_B}, \quad B \equiv \tfrac{1}{4}UV\rho^2.$$

Thus

$$\frac{E_{\text{tot}}}{V} = (A + B) + (\tfrac{5}{9}A - B)x^2).$$

If the coefficient of x^2 is positive, then the minimum occurs $x = 0$, and $M = 0$. To get spontaneous magnetization we need $B > \frac{5}{9}A$, which is to say,

$$U > \frac{4}{V\rho^2}\frac{5}{9}\frac{\hbar^2(3\pi^2\rho)^{5/3}}{10\pi^2 m} = \boxed{\frac{2\pi\hbar^2}{mV}\left(\frac{\pi}{3\rho}\right)^{1/3}.}$$

Problem 5.35

(a)

$$V = \frac{4}{3}\pi R^3, \quad \text{so } E = \frac{\hbar^2(3\pi^2 Nq)^{5/3}}{10\pi^2 m}\left(\frac{4}{3}\pi R^3\right)^{-2/3} = \boxed{\frac{2\hbar^2}{15\pi m R^2}\left(\frac{9}{4}\pi N q\right)^{5/3}.}$$

(b) Imagine building up a sphere by layers. When it has reached mass m, and radius r, the work necessary to bring in the next increment dm is: $dW = -(Gm/r)\,dm$. In terms of the mass density ρ, $m = \frac{4}{3}\pi r^3\rho$, and $dm = 4\pi r^2 dr\rho$, where dr is the resulting increase in radius. Thus:

$$dW = -G\frac{4}{3}\pi r^3\rho\, 4\pi r^2\rho\,\frac{dr}{r} = -\frac{16\pi^2}{3}\rho^2 G r^4 dr,$$

and the *total* energy of a sphere of radius R is therefore

$$E_{\text{grav}} = -\frac{16\pi^2}{3}\rho^2 G\int_0^R r^4\,dr = -\frac{16\pi^2\rho^2 R^5}{15}G. \quad \text{But } \rho = \frac{NM}{4/3\pi R^3}, \text{ so}$$

$$E_{\text{grav}} = -\frac{16\pi^2 R^5}{15}G\frac{9N^2M^2}{16\pi^2 R^6} = \boxed{-\frac{3}{5}G\frac{N^2M^2}{R}.}$$

(c)

$$E_{\text{tot}} = \frac{A}{R^2} - \frac{B}{R}, \quad \text{where } A \equiv \frac{2\hbar^2}{15\pi m}\left(\frac{9}{4}\pi Nq\right)^{5/3} \quad \text{and} \quad B \equiv \frac{3}{5}GN^2M^2.$$

$$\frac{dE_{\text{tot}}}{dR} = -\frac{2A}{R^3} + \frac{B}{R^2} = 0 \Rightarrow 2A = BR, \quad \text{so} \quad R = \frac{2A}{B} = \frac{4\hbar^2}{15\pi m}\left(\frac{9}{4}\pi Nq\right)^{5/3}\frac{5}{3GN^2M^2}.$$

$$R = \left[\left(\frac{4}{9\pi}\right)\left(\frac{9\pi}{4}\right)^{5/3}\right]\left(\frac{N^{5/3}}{N^2}\right)\frac{\hbar^2}{GmM^2}q^{5/3} = \boxed{\left(\frac{9\pi}{4}\right)^{2/3}\frac{\hbar^2}{GmM^2}\frac{q^{5/3}}{N^{1/3}}.}$$

$$R = \left(\frac{9\pi}{4}\right)^{2/3}\frac{(1.055\times10^{-34}\,\text{J}\cdot\text{s})^2(1/2)^{5/3}}{(6.673\times10^{-11}\,\text{Nm}^2/\text{kg}^2)(9.109\times10^{-31}\,\text{kg})(1.674\times10^{-27}\,\text{kg})^2}N^{-1/3}$$
$$= \boxed{(7.58\times10^{25}\,\text{m})N^{-1/3}.}$$

(d) Mass of sun: 1.989×10^{30} kg, so $N = \dfrac{1.989\times10^{30}}{1.674\times10^{-27}} = 1.188\times10^{57}$; $N^{-1/3} = 9.44\times10^{-20}$.

$R = (7.58\times10^{25})(9.44\times10^{-20})\,\text{m} = \boxed{7.16\times10^6\,\text{m}}$ (slightly larger than the earth).

(e)

$$\text{From Eq. 5.54:}\quad E_F = \frac{\hbar^2}{2m}\left(3\pi^2\frac{Nq}{4/3\pi R^3}\right)^{2/3} = \frac{\hbar^2}{2mR^2}\left(\frac{9\pi}{4}Nq\right)^{2/3}.\quad \text{Numerically:}$$

$$E_F = \frac{(1.055\times10^{-34}\,\mathrm{J\cdot s})^2}{2(9.109\times10^{-31}\,\mathrm{kg})(7.16\times10^6\,\mathrm{m})^2}\left[\frac{9\pi}{4}(1.188\times10^{57})\frac{1}{2}\right]^{2/3} = 3.102\times10^{-14}\,\mathrm{J},$$

$$\text{or, in electron volts:}\quad E_F = \frac{3.102\times10^{-14}}{1.602\times10^{-19}}\,\mathrm{eV} = \boxed{1.94\times10^5\ \mathrm{eV}.}$$

$E_{\text{rest}} = mc^2 = 5.11\times10^5$ eV, so the Fermi energy (which is the energy of the most energetic electrons) is comparable to the rest energy, so they are getting fairly relativistic.

Problem 5.36

(a)

$$dE = (\hbar ck)\frac{V}{\pi^2}k^2\,dk \Rightarrow E_{\text{tot}} = \frac{\hbar cV}{\pi^2}\int_0^{k_F}k^3\,dk = \frac{\hbar cV}{4\pi^2}k_F^4;\quad k_F = \left(\frac{3\pi^2Nq}{V}\right)^{1/3}.$$

$$\text{So } E_{\text{tot}} = \boxed{\frac{\hbar c}{4\pi^2}(3\pi^2Nq)^{4/3}V^{-1/3}.}$$

(b)

$$V = \frac{4}{3}\pi R^3 \Rightarrow E_{\text{deg}} = \frac{\hbar c}{4\pi^2 R}(3\pi^2Nq)^{4/3}\left(\frac{4\pi}{3}\right)^{-1/3} = \frac{\hbar c}{3\pi R}\left(\frac{9}{4}\pi Nq\right)^{4/3}.$$

Adding in the gravitational energy, from Problem 5.35(b),

$$E_{\text{tot}} = \frac{A}{R} - \frac{B}{R},\quad \text{where } A \equiv \frac{\hbar c}{3\pi}\left(\frac{9}{4}\pi Nq\right)^{4/3} \text{ and } B \equiv \frac{3}{5}GN^2M^2.\quad \frac{dE_{\text{tot}}}{dR} = -\frac{(A-B)}{R^2} = 0 \Rightarrow A = B,$$

but there is no special value of R for which E_{tot} is minimal. Critical value: $A = B(E_{\text{tot}} = 0) \Rightarrow$ $\frac{\hbar c}{3\pi}\left(\frac{9}{4}\pi Nq\right)^{4/3} = \frac{3}{5}GN^2M^2$, or

$$\boxed{N_c = \frac{15}{16}\sqrt{5\pi}\left(\frac{\hbar c}{G}\right)^{3/2}\frac{q^2}{M^3}} = \frac{15}{16}\sqrt{5\pi}\left(\frac{1.055\times10^{-34}\,\mathrm{J\cdot s}\times2.998\times10^8\,\mathrm{m/s}}{6.673\times10^{-11}\,\mathrm{N\cdot m^2/kg^2}}\right)^{3/2}\frac{(1/2)^2}{(1.674\times10^{-27}\,\mathrm{kg})^3}$$

$= \boxed{2.04\times10^{57}.}$ (About *twice* the value for the sun—Problem 5.35(d).)

(c) Same as Problem 5.35(c), with $m \to M$ and $q \to 1$, so multiply old answer by $(2)^{5/3}m/M$:

$$R = 2^{5/3}\frac{(9.109\times10^{-31})}{(1.674\times10^{-27})}(7.58\times10^{25}\,\mathrm{m})N^{-1/3} = (1.31\times10^{23}\,\mathrm{m})N^{-1/3}.\quad \text{Using } N = 1.188\times10^{57},$$

$R = (1.31 \times 10^{23}\,\text{m})(9.44 \times 10^{-20}) = \boxed{12.4\text{ km.}}$ To get E_F, use Problem 5.35(e) with $q = 1$, the new R, and the neutron mass in place of m:

$$E_F = 2^{2/3}\left(\frac{7.16 \times 10^6}{1.24 \times 10^4}\right)^2 \left(\frac{9.11 \times 10^{-31}}{1.67 \times 10^{-27}}\right)(1.94 \times 10^5\,\text{eV}) = 5.60 \times 10^7\,\text{eV} = \boxed{56.0\text{ MeV.}}$$

The rest energy of a neutron is 940 MeV, so a neutron star is reasonably nonrelativistic.

Problem 5.37

(a) From Equation 5.71, $\cos(qa) = \cos(ka) \Rightarrow q = \pm k = \pm\frac{\sqrt{2mE}}{\hbar}$; $\quad E = \frac{\hbar^2 q^2}{2m} \Rightarrow \frac{dE}{dq} = \frac{\hbar^2 q}{m}$.

$$\frac{1}{Na}G_{\text{free}}(E) = \frac{1}{\pi}\frac{m}{\hbar^2|q|} = \frac{m\hbar}{\pi\hbar^2\sqrt{2mE}} = \frac{1}{\pi\hbar}\sqrt{\frac{m}{2E}}. \quad \checkmark$$

(b) $-a\sin(qa) = \left\{-a\sin(ka) + \frac{m\alpha}{\hbar^2}\left[-\frac{1}{k^2}\sin(ka) + \frac{a}{k}\cos(ka)\right]\right\}\frac{dk}{dq}$. Equation (5.65): $\frac{dk}{dq} = \frac{\sqrt{2m}}{2\hbar\sqrt{E}}\frac{dE}{dq}$.

$$\sin(qa) = \left\{\sin(ka) + \frac{m\alpha}{\hbar^2 k}\left[\frac{1}{ka}\sin(ka) - \cos(ka)\right]\right\}\frac{m}{\hbar^2 k}\frac{dE}{dq}.$$

$$\frac{dE}{dq} = \frac{\sin(qa)}{\sin(ka) + \frac{m\alpha}{\hbar^2 k}\left(\frac{1}{ka}\sin(ka) - \cos(ka)\right)}\frac{\hbar^2 k}{m}.$$

$$\begin{aligned}
\sin(qa) &= \sqrt{1-\cos^2(qa)} = \sqrt{1-\left[\cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka)\right]^2} \\
&= \sqrt{1-\cos^2(ka) - \frac{2m\alpha}{\hbar^2 k}\cos(ka)\sin(ka) - \left(\frac{m\alpha}{\hbar^2 k}\right)^2\sin^2(ka)} \\
&= \sin(ka)\sqrt{1-\frac{2m\alpha}{\hbar^2 k}\cot(ka) - \left(\frac{m\alpha}{\hbar^2 k}\right)^2}.
\end{aligned}$$

$$\begin{aligned}
\frac{1}{Na}G(E) &= \frac{1}{\pi}\left(\frac{m}{\hbar^2 k}\right)\frac{\left|\sin(ka) + \frac{m\alpha}{\hbar^2 k}\left(\frac{1}{ka}\sin(ka) - \cos(ka)\right)\right|}{\sin(ka)\sqrt{1-\frac{2m\alpha}{\hbar^2 k}\cot(ka) - \left(\frac{m\alpha}{\hbar^2 k}\right)^2}} \\
&= \boxed{\frac{m}{\pi\hbar^2 k}\frac{\left|1 + \frac{m\alpha}{\hbar^2 k}\left[\frac{1}{ka} - \cot(ka)\right]\right|}{\sqrt{1-\frac{2m\alpha}{\hbar^2 k}\cot(ka) - \left(\frac{m\alpha}{\hbar^2 k}\right)^2}}.}
\end{aligned}$$

(c) With $m = \hbar = a = 1$, the expressions in (a) and (b) reduce to

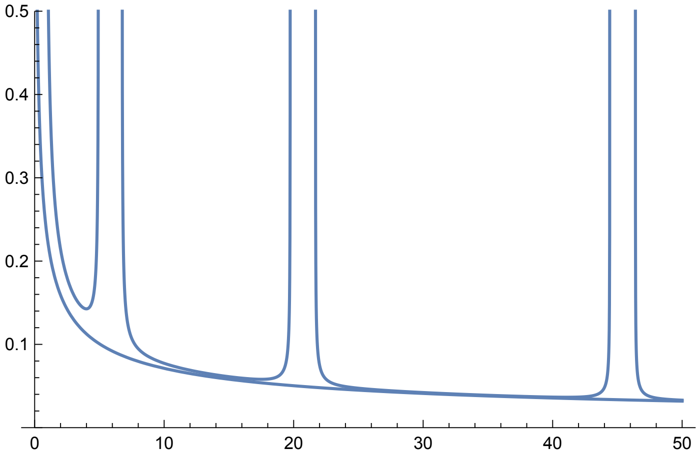
$$\alpha = 0: \quad \frac{1}{\pi\sqrt{2E}}; \qquad \alpha = 1: \quad \frac{1}{\pi\sqrt{2E}}\left[\frac{1 + \frac{1}{2E} - \frac{1}{\sqrt{2E}}\cot(\sqrt{2E})}{\sqrt{1 - \frac{1}{2E} - \frac{2}{\sqrt{2E}}\cot(\sqrt{2E})}}\right].$$

In the graph, the lower curve is for $\alpha = 0$, the upper one (with the breaks) is for $\alpha = 1$.

```
Plot[1/(π √(2 x)), {x, 0, 50}, PlotRange → {0, .5}]

Plot[1/(π √(2 x)) (1 + 1/(2 x) - 1/√(2 x) Cot[√(2 x)]) / √(1 - 1/(2 x) - 2/√(2 x) Cot[√(2 x)]),
 {x, 0, 50}, PlotRange → {0, .5}]

Show[%3, %4]
```



Problem 5.38

(a) Consider

$$\frac{1}{N}\sum_{j=1}^{N} e^{i\,2\,\pi\,j\,r/N} = \frac{1}{N}\sum_{j=1}^{N}\left(e^{i\,2\,\pi\,r/N}\right)^j = \frac{1}{N}\frac{e^{2\,i\,\pi\,r}-1}{1-e^{-2\,i\,\pi\,r/N}}$$

For any integer r the numerator vanishes and the sum must be zero *unless* the denominator also vanishes. The denominator vanishes for $r = m\,N$ where m is any integer; when $r = m\,N$ it is easy to see that the expression evaluates to 1. Now, to prove the first identity, $k - k' = m\,N$ only when $m = 0$ and hence $k = k'$. In the second case, $k + k' = m\,N$ only when $m = 1$ and $k' = N - k$.

(b) We first consider

$$[a_{k-}, a_{k'+}] = \frac{1}{N}\sum_{j,\,j'} e^{i\,2\,\pi\left(j'\,k' - j\,k\right)/N}\,\frac{1}{2}\left\{-\sqrt{\frac{\omega_k}{\omega_{k'}}}\left[x_j, \frac{\partial}{\partial x_{j'}}\right] + \sqrt{\frac{\omega_k'}{\omega_k}}\left[\frac{\partial}{\partial x_j}, x_{j'}\right]\right\}$$

where I've dropped the two terms involving commutators of two coordinates or two derivatives. The remaining commutators are $-\delta_{jj'}$ and $\delta_{jj'}$ respectively and we have

$$[a_{k-}, a_{k'+}] = \left(\frac{1}{N}\sum_j e^{i\,2\,\pi\,j\left(k'-k\right)/N}\right)\,\frac{1}{2}\left[\sqrt{\frac{\omega_k}{\omega_{k'}}} + \sqrt{\frac{\omega_{k'}}{\omega_k}}\right].$$

We can now do the sum on j using the result from part (a), and that gives the first commutator. Next we take

$$[a_{k-}, a_{k'-}] = \frac{1}{N}\sum_{j,\,j'} e^{-i\,2\,\pi\left(j'\,k'+j\,k\right)/N}\,\frac{1}{2}\left\{\sqrt{\frac{\omega_k}{\omega_{k'}}}\left[x_j, \frac{\partial}{\partial x_{j'}}\right] + \sqrt{\frac{\omega_k'}{\omega_k}}\left[\frac{\partial}{\partial x_j}, x_{j'}\right]\right\}$$

Evaluating the two commutators we have

$$[a_{k-}, a_{k'-}] = \left(\frac{1}{N}\sum_j e^{-i\,2\,\pi\,j\left(k'+k\right)/N}\right)\frac{1}{2}\left[-\sqrt{\frac{\omega_k}{\omega_{k'}}} + \sqrt{\frac{\omega_k'}{\omega_k}}\right]$$

Doing the sum on j now gives the result that $k' = N - k$ (or $k' = k$ if $k = N$) but since $\omega_{N-k} = \omega_k$ this vanishes, proving the second result. The final commutator works out the same way.

(c)

$$\begin{aligned}(a_{k_-} + a_{N-k_+}) = \frac{1}{\sqrt{N}}\sum_{j=1}^{N}\Bigg\{ & e^{-i2\pi jk/N}\left[\sqrt{\frac{m\omega_k}{2\hbar}}\,x_j + \sqrt{\frac{\hbar}{2m\omega_k}}\,\frac{\partial}{\partial x_j}\right] \\ & + e^{i2\pi j(N-k)/N}\left[\sqrt{\frac{m\omega_{N-k}}{2\hbar}}x_j - \sqrt{\frac{\hbar}{2m\omega_{N-k}}}\,\frac{\partial}{\partial x_j}\right]\Bigg\}.\end{aligned}$$

But $\omega_{N-k} = \omega_k$, and $e^{i2\pi j(N-k)/N} = e^{i2\pi j}e^{-i2\pi jk/N} = e^{-i2\pi jk/N}$, so

$$(a_{k_-} + a_{N-k_+}) = \frac{2}{\sqrt{N}}\sum_{j=1}^{N}\sqrt{\frac{m\omega_k}{2\hbar}}\,e^{-i2\pi jk/N}\,x_j.$$

$$\begin{aligned}\frac{1}{\sqrt{N}}\sum_{k=1}^{N-1}\sqrt{\frac{\hbar}{2m\omega_k}}(a_{k_-} + a_{N-k_+})e^{i2\pi jk/N} &= \frac{1}{\sqrt{N}}\sum_{k=1}^{N-1}\sqrt{\frac{\hbar}{2m\omega_k}}\,\frac{2}{\sqrt{N}}\sum_{j'=1}^{N}\sqrt{\frac{m\omega_k}{2\hbar}}e^{-i2\pi j'k/N}\,x_{j'}\,e^{i2\pi jk/N} \\ = \frac{1}{N}\sum_{j'=1}^{N}\sum_{k=1}^{N-1}e^{i2\pi(j-j')k/N}\,x_{j'} &= \frac{1}{N}\sum_{j'=1}^{N}\left(\sum_{k=1}^{N}e^{i2\pi(j-j')k/N} - e^{i2\pi(j-j')}\right)x_{j'} \\ = \sum_{j'=1}^{N}\left(\frac{1}{N}\sum_{k=1}^{N}e^{i2\pi(j-j')k/N}\right)x_{j'} - \frac{1}{N}\sum_{j'=1}^{N}x_{j'} &= \sum_{j'=1}^{N}\delta_{jj'}\,x_{j'} - R = x_j - R.\end{aligned}$$

That proves the first relation; to prove the second, we repeat these steps, starting with

$$\begin{aligned}(a_{k_-} - a_{N-k_+}) = \frac{1}{\sqrt{N}}\sum_{j=1}^{N}\Bigg\{ & e^{-i2\pi jk/N}\left[\sqrt{\frac{m\omega_k}{2\hbar}}\,x_j + \sqrt{\frac{\hbar}{2m\omega_k}}\,\frac{\partial}{\partial x_j}\right] \\ & - e^{i2\pi j(N-k)/N}\left[\sqrt{\frac{m\omega_{N-k}}{2\hbar}}x_j - \sqrt{\frac{\hbar}{2m\omega_{N-k}}}\,\frac{\partial}{\partial x_j}\right]\Bigg\} \\ = \frac{2}{\sqrt{N}}\sum_{j=1}^{N}\sqrt{\frac{\hbar}{2m\omega_k}}\,e^{-i2\pi jk/N}\,\frac{\partial}{\partial x_j}.\end{aligned}$$

$$\frac{1}{\sqrt{N}}\sum_{k=1}^{N-1}\sqrt{\frac{m\omega_k}{2\hbar}}(a_{k_-}-a_{N-k_+})e^{i2\pi jk/N}=\frac{1}{\sqrt{N}}\sum_{k=1}^{N-1}\sqrt{\frac{m\omega_k}{2\hbar}}\frac{2}{\sqrt{N}}\sum_{j'=1}^{N}\sqrt{\frac{\hbar}{2m\omega_k}}e^{-i2\pi j'k/N}\frac{\partial}{\partial x_{j'}}\,e^{i2\pi jk/N}$$
$$=\frac{1}{N}\sum_{j'=1}^{N}\sum_{k=1}^{N-1}e^{i2\pi(j-j')k/N}\frac{\partial}{\partial x_{j'}}=\frac{1}{N}\sum_{j'=1}^{N}\left(\sum_{k=1}^{N}e^{i2\pi(j-j')k/N}-e^{i2\pi(j-j')}\right)\frac{\partial}{\partial x_{j'}}$$
$$=\sum_{j'=1}^{N}\left(\frac{1}{N}\sum_{k=1}^{N}e^{i2\pi(j-j')k/N}\right)\frac{\partial}{\partial x_{j'}}-\frac{1}{N}\sum_{j'=1}^{N}\frac{\partial}{\partial x_{j'}}=\sum_{j'=1}^{N}\delta_{jj'}\frac{\partial}{\partial x_{j'}}-\frac{1}{N}\sum_{j'=1}^{N}\frac{\partial}{\partial x_{j'}}=\frac{\partial}{\partial x_j}-\frac{1}{N}\frac{\partial}{\partial R}.$$

In the last step I used $\dfrac{\partial}{\partial R}=\displaystyle\sum_{j=1}^{N}\frac{\partial x_j}{\partial R}\frac{\partial}{\partial x_j}$, and $\dfrac{\partial x_j}{\partial R}=1$ (for instance, if $N=2, R=\frac{1}{2}(x_1+x_2)$, and $r=\frac{1}{2}(x_1-x_2)$, so $x_1=R+r$ and $x_2=R-r\Rightarrow \partial x_i/\partial R=1$).

(d)

$$(x_{j+1}-x_j)=\frac{1}{\sqrt{N}}\sum_{k=1}^{N-1}\sqrt{\frac{\hbar}{2m\omega_k}}(a_{k_-}+a_{N-k_+})e^{i2\pi jk/N}\left(e^{i2\pi k/N}-1\right),$$
$$(x_{j+1}-x_j)^2=\frac{1}{N}\sum_{k,k'}^{N-1}\frac{\hbar}{2m\sqrt{\omega_k\omega_{k'}}}(a_{k_-}+a_{N-k_+})(a_{k'_-}+a_{N-k'_+})e^{i2\pi j(k+k')/N}$$
$$\times\left(e^{i2\pi k/N}-1\right)\left(e^{i2\pi k'/N}-1\right),$$
$$\sum_{j=1}^{N}\frac{1}{2}m\omega^2(_{j+1}-x_j)^2=\sum_{k,k'}^{N-1}\frac{\hbar\omega^2}{4\sqrt{\omega_k\omega_{k'}}}(a_{k_-}+a_{N-k_+})(a_{k'_-}+a_{N-k'_+})\delta_{k',N-k}$$
$$\times\left(e^{i2\pi k/N}-1\right)\left(e^{i2\pi k'/N}-1\right)$$
$$=\sum_{k=1}^{N-1}\frac{\hbar\omega^2}{4\omega_k}(a_{k_-}+a_{N-k_+})(a_{N-k_-}+a_{k_+})\frac{\omega_k^2}{\omega^2}$$
$$=\sum_{k=1}^{N-1}\frac{\hbar\omega_k}{4}\left(a_{k_-}a_{k_+}+a_{N-k_+}a_{k_+}+a_{k_-}a_{N-k_-}+a_{N-k_+}a_{N-k_-}\right).$$

In the penultimate line I used

$$\left(e^{i2\pi k/N}-1\right)\left(e^{i2\pi(N-k)/N}-1\right)=e^{i\pi k/N}\left(e^{i\pi k/N}-e^{-i\pi k/N}\right)e^{-i\pi k/N}\left(e^{-i\pi k/N}-e^{i\pi k/N}\right)$$
$$=\left(2i\sin(\pi k/N)\right)\left(-2i\sin(\pi k/N)\right)=\left[2\sin(\pi k/N)\right]^2=\left(\frac{\omega_k}{\omega}\right)^2.$$

Meanwhile,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_j^2}=\frac{1}{N}\sum_{k,k'}^{N-1}\left(-\frac{\hbar^2}{2m}\right)\frac{m}{2\hbar}\sqrt{\omega_k\omega_{k'}}(a_{k_-}-a_{N-k_+})(a_{k'_-}-a_{N-k'_+})e^{i2\pi j(k+k')/N}$$
$$-\frac{\hbar^2}{2m}\frac{1}{N^{3/2}}\left[\frac{\partial}{\partial R}\sum_{k=1}^{N-1}\sqrt{\frac{m\omega_k}{2\hbar}}\left(a_{k_-}-a_{N-k_+}\right)e^{i2\pi jk/N}\right.$$
$$\left.+\sum_{k=1}^{N-1}\sqrt{\frac{m\omega_k}{2\hbar}}\left(a_{k_-}-a_{N-k_+}\right)e^{i2\pi jk/N}\frac{\partial}{\partial R}\right]-\frac{\hbar^2}{2m}\frac{1}{N^2}\frac{\partial^2}{\partial R^2}.$$

The middle terms vanish when summed over j $\left(\sum_{j=1}^{N} e^{i2\pi jk/N} = N\delta_{k,0} = 0\right)$, leaving

$$-\frac{\hbar^2}{2m}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2} = \sum_{k=1}^{N-1}\left(-\frac{\hbar\omega_k}{4}\right)\left(a_{k_-} - a_{N-k_+}\right)\left(a_{N-k_-} - a_{k_+}\right) - \frac{\hbar^2}{2Nm}\frac{\partial^2}{\partial R^2}$$
$$= \sum_{k=1}^{N-1}\frac{\hbar\omega_k}{4}\left(a_{k_-}a_{k_+} - a_{N-k_+}a_{k_+} - a_{k_-}a_{N-k_-} + a_{N-k_+}a_{N-k_-}\right) - \frac{\hbar^2}{2Nm}\frac{\partial^2}{\partial R^2}.$$

Adding the two results:

$$\hat{H} = -\frac{\hbar^2}{2Nm}\frac{\partial^2}{\partial R^2} + \sum_{k=1}^{N-1}\frac{\hbar\omega_k}{2}\left(a_{k_-}a_{k_+} + a_{N-k_+}a_{N-k_-}\right) = -\frac{\hbar^2}{2Nm}\frac{\partial^2}{\partial R^2} + \sum_{k=1}^{N-1}\frac{\hbar\omega_k}{2}\left(a_{k_-}a_{k_+} + a_{k_+}a_{k_-}\right)$$

(the change in the final two subscripts just means adding these terms in reverse order, given that $\omega_{N-k} = \omega_k$). Thus

$$\hat{H} = -\frac{\hbar^2}{2(Nm)}\frac{\partial^2}{\partial R^2} + \sum_{k=1}^{N-1}\hbar\omega_k\left(a_{k_+}a_{k_-} + \frac{1}{2}\right). \quad \checkmark$$

Problem 5.39

(a)

$$\psi(x + l_x, y, z) = \frac{1}{\sqrt{l_x l_y l_z}}e^{i[k_x(x+l_x)+k_y y+k_z z]} = \psi(x, y, z) = \frac{1}{\sqrt{l_x l_y l_z}}e^{i(k_x x+k_y y+k_z z)} \Rightarrow e^{ik_x l_x} = 1,$$

so $k_x l_x = 0, \pm 2\pi, \pm 4\pi, \ldots = 2n_x\pi$; likewise $k_y l_y = 2n_y\pi$, $k_z l_z = 2n_z\pi$.

$$\Delta k_x \Delta k_y \Delta k_z = \frac{2\pi}{l_x}\frac{2\pi}{l_y}\frac{2\pi}{l_z} = \boxed{\frac{8\pi^3}{V}.}$$

(b) Because n_x, n_y, and n_z run negative as well as positive, we want the *whole* sphere, not just one octant:

$$\frac{4}{3}\pi k_F^3 = \frac{8\pi^3}{V}\frac{Nd}{2} \Rightarrow k_F = \left(\frac{3\pi^2 Nd}{V}\right)^{1/3} = \boxed{(3\rho\pi^2)^{1/3},}$$

where $\rho \equiv Nd/V$ (same as Equation 5.52). $E_F = \frac{\hbar^2}{2m}k_F^2 = \boxed{\frac{\hbar^2}{2m}(3\rho\pi^2)^{2/3}}$ (same as Equation 5.54). A shell of thickness dk contains a volume $4\pi k^2\, dk$ of k-space, so the number of electron states in the shell is $2\frac{4\pi k^2\, dk}{8\pi^3/V} = \frac{V}{\pi^2}k^2\, dk$ (same as in the text), so $\boxed{E_{\text{tot}} = \frac{\hbar^2(3\pi^2 Nd)^{5/3}}{10\pi^2 m}V^{-2/3}}$ (same as Equation 5.56). Each state occupies an 8-times larger volume of k-space (because of the 2's in part (a)), but the k-space itself is 8 times larger (because negative n's are allowed, so with periodic boundary conditions all 8 octants are accessible).

Chapter 6

Symmetries and Conservation Laws

Problem 6.1

(a) A mirror reflection across the x-y plane produces

$$\hat{M}\,\psi(x,y,z) = \psi'(x,y,z) = \psi(x,y,-z)\ .$$

A 180° rotation in the x-y plane has the effect

$$\hat{R}\,\psi(x,y,z) = \psi'(x,y,z) = \psi(-x,-y,z)\ .$$

Composing these two operations gives

$$\hat{M}\,\hat{R}\,\psi(x,y,z) = \psi(-x,-y,-z) = \hat{\Pi}\,\psi(x,y,z)\ .$$

(b) In polar coordinates

$$\begin{aligned} x &= r\,\sin\theta\,\cos\phi \\ y &= r\,\sin\theta\,\sin\phi \\ z &= r\,\cos\theta\,. \end{aligned}$$

Replacing θ with $\pi-\theta$ and ϕ with $\phi+\pi$ gives

$$\begin{aligned} x &\to r\,\underbrace{\sin(\pi-\theta)}_{\sin\theta}\,\underbrace{\cos(\phi+\pi)}_{-\cos\phi} = -x \\ y &\to r\,\underbrace{\sin(\pi-\theta)}_{\sin\theta}\,\underbrace{\sin(\phi+\pi)}_{-\sin\phi} = -y \\ z &\to r\,\underbrace{\cos(\pi-\theta)}_{-\cos\theta} = -z \end{aligned}$$

so this transformation is equivalent to changing the sign of each Cartesian coordinate. One could also solve this problem by drawing a careful picture in spherical coordinates and showing that the transformed angles identify the point $-\mathbf{r}$.

(c) The Hydrogenic orbitals may be written as

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\ Y_\ell^m(\theta,\phi)$$

so that

$$\hat{\Pi}\,\psi_{n\ell m}(r,\theta,\phi) = R_{n\,\ell}(r)\;Y_\ell^m(\pi-\theta,\phi+\pi)\ .$$

The spherical harmonics are defined in Equation 4.32,

$$Y_\ell^m(\theta,\phi) = K_\ell^m\,e^{i\,m\,\phi}P_\ell^m(\cos\theta)$$

where K_ℓ^m is the normalization constant, and therefore

$$Y_\ell^m(\pi-\theta,\phi+\pi) = K_\ell^m\,(-1)^m\;e^{i\,m\,\phi}\;P_\ell^m(-\cos\theta)\ .$$

Furthermore, from Equation 4.27 we see that

$$P_\ell^m(-x) = (-1)^m\left(1-x^2\right)^{m/2}\left(-\frac{d}{dx}\right)^m P_\ell(-x)\ ,$$

and from Equation 4.28 that $P_\ell(-x) = (-1)^\ell\;P_\ell(x)$, so that

$$P_\ell^m(-x) = (-1)^{\ell+m}\;P_\ell^m(x)$$

(which you could also infer from Table 4.2). Combining these results,

$$\boxed{\hat{\Pi}\,\psi_{n\ell m}(r,\theta,\phi) = (-1)^\ell\;\psi_{n\ell m}(r,\theta,\phi)\ .}$$

Problem 6.2

We define the exponential of an operator by its power series so that

$$\hat{U} = 1 + i\,\hat{\Omega} - \frac{1}{2}\,\hat{\Omega}\,\hat{\Omega} - \frac{i}{3!}\,\hat{\Omega}\,\hat{\Omega}\,\hat{\Omega} + \dots$$

Taking the adjoint, we complex conjugate all numbers, reverse the order of all operators and replace each one with its adjoint. Therefore

$$\begin{aligned}\hat{U}^\dagger &= 1 - i\,\hat{\Omega}^\dagger - \frac{1}{2}\,\hat{\Omega}^\dagger\,\hat{\Omega}^\dagger + \frac{i}{3!}\,\hat{\Omega}^\dagger\,\hat{\Omega}^\dagger\,\hat{\Omega}^\dagger + \dots\\ &= 1 - i\,\hat{\Omega} - \frac{1}{2}\,\hat{\Omega}\,\hat{\Omega} + \frac{i}{3!}\,\hat{\Omega}\,\hat{\Omega}\,\hat{\Omega} + \dots\\ &= e^{-i\,\hat{\Omega}}\end{aligned}$$

where we've used the fact that $\hat{\Omega}$ is hermitian in the second line. Now, we know (from Problem 3.29) that $e^{\hat{A}}\,e^{\hat{B}} = e^{\hat{A}+\hat{B}}$ if $\hat{A}$ and $\hat{B}$ commute. Since $i\,\hat{\Omega}$ clearly commutes with $-i\,\hat{\Omega}$ we may then write

$$\hat{U}\,\hat{U}^\dagger = e^{i\,\hat{\Omega}}\,e^{-i\,\hat{\Omega}} = e^{i\,\hat{\Omega}-i\,\hat{\Omega}} = e^0 = 1\,.$$

(One could also multiply the two series directly if you haven't seen Problem 3.29).

Problem 6.3

We consider how the operator $\hat{p}'$ acts on an arbitrary function $f(x)$.

$$\begin{aligned}\hat{p}' &= \hat{T}^\dagger(a)\,\frac{\hbar}{i}\,\frac{d}{dx}\,\hat{T}(a)\;f(x)\\ &= \hat{T}^\dagger(a)\,\frac{\hbar}{i}\,\frac{d}{dx}\,f(x-a)\\ &= \hat{T}(-a)\,\frac{\hbar}{i}\,f'(x-a)\\ &= \frac{\hbar}{i}\,f'(x)\\ &= \frac{\hbar}{i}\,\frac{d}{dx}\,f(x)\end{aligned}$$

(An alternative proof would quote Equation 6.3 and prove that $\hat{p}$ must commute with $\hat{T}$ from there.)

Problem 6.4

We start by writing

$$\hat{T}^\dagger\,\hat{\Omega}\,\hat{T} = \sum_{mn} a_{mn}\,\hat{T}^\dagger\,\hat{x}^m\,\hat{p}^n\,\hat{T}\,.$$

The idea is that we're then free to insert copies of $\hat{T}\,\hat{T}^\dagger = 1$ wherever necessary. For example, consider the term

$$\hat{T}^\dagger\,\hat{x}^3\,\hat{p}^2\,\hat{T} = \underbrace{\hat{T}^\dagger\,\hat{x}\,\hat{T}}_{\hat{x}'}\,\hat{T}^\dagger\,\hat{x}\,\hat{T}\,\hat{T}^\dagger\,\hat{x}\,\hat{T}\,\hat{T}^\dagger\,\hat{p}\,\hat{T}\,\hat{T}^\dagger\,\hat{p}\,\hat{T} = \hat{x}'^3\,\hat{p}'^3\,.$$

It is then clear that

$$\hat{T}^\dagger\,\hat{\Omega}\,\hat{T} = \sum_{mn} a_{mn}\left(\hat{T}^\dagger\,\hat{x}\,\hat{T}\right)^m\left(\hat{T}^\dagger\,\hat{p}\,\hat{T}\right)^n = \sum_{mn} a_{mn}\,(\hat{x}')^m\,(\hat{p}')^n\;.$$

so that

$$\boxed{\hat{\Omega}'(\hat{x},\hat{p}) = \hat{T}^\dagger\,\hat{\Omega}(\hat{x},\hat{p})\;\hat{T} = \hat{\Omega}(\hat{x}',\hat{p}')\;.}$$

Problem 6.5

We insert $\psi(x) = e^{i\,q\,x}\,u(x)$ into Equation 6.11 to get

$$\begin{aligned}e^{i\,q(x-a)}\,u(x-a) &= e^{-i\,q\,a}\,e^{i\,q\,x}\,u(x)\\ u(x-a) &= u(x)\;.\end{aligned}$$

This shows that $u(x)$ is in fact a periodic function.

Problem 6.6

(a) First note that

$$
\begin{aligned}
\frac{d^2}{dx^2}\psi &= \frac{d^2}{dx^2} e^{i\,q\,x}\, u(x) \\
&= \frac{d}{dx}\left[i\,q\,e^{i\,q\,x}\,u(x) + e^{i\,q\,x}\,u'(x)\right] \\
&= -q^2\,e^{i\,q\,x}\,u(x) + 2\,i\,q\,e^{i\,q\,x}\,u'(x) + e^{i\,q\,x}\,u''(x)\ .
\end{aligned}
$$

Plugging this into the time-independent Schrödinger equation we get

$$
\begin{aligned}
-\frac{\hbar^2}{2\,m}\frac{d^2\psi}{dx^2} + V(x)\ \psi &= E\,\psi \\
-\frac{\hbar^2}{2\,m}\frac{d^2 u}{dx^2} + \frac{\hbar\,q}{m}\,\frac{\hbar}{i}\,\frac{du}{dx} + V(x)\ u &= \left(E - \frac{\hbar^2 q^2}{2\,m}\right)\ u
\end{aligned}
$$

after cancelling the common factor of $e^{i\,q\,x}$. This is the desired result.

(b) First we will non-dimensionalize our equation. Let $x = a\,s$ where s will range from 0 to 1. Then we get a proper dimensionless Equation

$$
-\frac{d^2 u}{ds^2} + 2\,(q\,a)\ \frac{1}{i}\,\frac{du}{ds} + \frac{2\,m\,a}{\hbar^2}\ V(x) = \left[E\,\frac{2\,m\,a}{\hbar^2}\ -(q\,a)^2\right]\ u\,.
$$

The numerical solution to this equation for the requested values of n and q follows.

Set the number of samples:

```
In[·]:= Num = 100; dx = 1./(Num + 1);
```

Define the potential function:

```
In[·]:= Potential[x_] := If[x > .25 && x < .75, -20 , 0];
```

The first derivative operator (with appropriate periodic boundary conditions)

```
In[·]:= D1 = 1/(2 dx) Table[If[i == j + 1, 1, If[i == j - 1, -1, 0]], {i, 1, Num}, {j, 1, Num}];
D1[[1, Num]] = 1/(2 dx);
D1[[Num, 1]] = -1/(2 dx);
```

The second derivative operator

```
In[·]:= D2 = 1/dx^2 Table[
    If[i == j, -2, If[i == j + 1, 1, If[i == j - 1, 1, 0]]], {i, 1, Num}, {j, 1, Num}];
D2[[1, Num]] = D2[[Num, 1]] = 1/dx^2;
```

The potential operator

```
In[·]:= V = Table[If[i == j, Potential[i dx], 0], {i, 1, Num}, {j, 1, Num}];
```

Solve the effective Schrodinger equation to get the nth solution for a given choice of q

```
In[·]:= Energy[q_, n_] := q^2 - Sort[Eigenvalues[D2 + 2. I q D1 - V] // Chop][[Num + 1 - n]]

In[·]:= TableForm[Table[Energy[q, n], {n, 1, 2}, {q, {-Pi, -Pi / 2, 0, Pi / 2, Pi}}],
  TableHeadings → {{1, 2}, {-Pi, -Pi / 2, 0, Pi / 2, Pi}}]
```

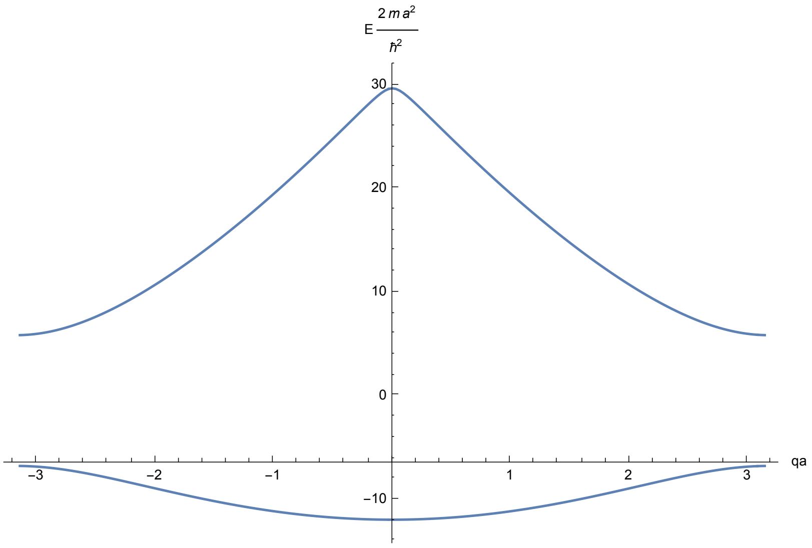
Out[·]//TableForm=

	$-\pi$	$-\frac{\pi}{2}$	0	$\frac{\pi}{2}$	π
1	-6.77261	-10.0067	-11.9549	-10.0067	-6.77261
2	5.84137	14.1147	29.6386	14.1147	5.84137

(c) Running this program for 100 different values of q generates this plot.

```
In[∘]:= Show[
  ListPlot[Table[{q, Energy[q, 1]}, {q, -Pi, Pi, Pi / 100}], Joined → True],
  ListPlot[Table[{q, Energy[q, 2]}, {q, -Pi, Pi, Pi / 100}], Joined → True],
  PlotRange → All, AxesLabel → {"qa", "E 2 m a^2/ħ^2"}
 ]
```

Out[∘]=



Problem 6.7

(a) We can expand $\hat{T}$ in a Taylor series just as we did in the single-particle case:

$$\begin{aligned}\hat{T}(a)\ \psi(x_1,x_2) &= \psi(x_1-a,x_2-a)\\ &= \sum_{m,n}\frac{1}{m!\,n!}\,\frac{\partial^{m+n}}{\partial x_1^m\,\partial x_2^n}\psi(x_1,x_2)\,(-a)^{m+n}\ .\end{aligned}$$

We can write this in terms of the two momenta as

$$\hat{T}(a)\ \psi(x_1,x_2) = \sum_{mn}\frac{1}{m!\,n!}\left(-\frac{i\,a}{\hbar}\right)^{m+n}\ \hat{p}_1^m\,\hat{p}_2^n\,\psi(x_1,x_2)$$

and then split up the sums as

$$\begin{aligned}\hat{T}(a)\ \psi(x_1,x_2) &= \sum_m\frac{1}{m!}\left(-\frac{i\,a}{\hbar}\right)^m\ \hat{p}_1^m\ \sum_n\frac{1}{n!}\left(-\frac{i\,a}{\hbar}\right)^n\ \hat{p}_2^n\,\psi(x_1,x_2)\\ &= e^{-i\,a\,\hat{p}_1/\hbar}\,e^{-i\,a\,\hat{p}_2/\hbar}\,\psi(x_1,x_2)\ .\end{aligned}$$

Finally, since $\hat{p}_1$ and $\hat{p}_2$ commute we can write

$$\boxed{\hat{T}(a) = e^{-i\,a\,\hat{p}_1/\hbar}\,e^{-i\,a\,\hat{p}_2/\hbar} = e^{-i\,a(\hat{p}_1+\hat{p}_2)/\hbar} = e^{-i\,a\,\hat{P}/\hbar}\,.}$$

(b) We first need to show that the Hamiltonian is translationally invariant. Acting on a test function $f(x_1, x_2)$,

$$\begin{aligned}
\hat{H}'\, f(x_1, x_2) =& \hat{T}^\dagger(a)\ \hat{H}\, \hat{T}(a)\ f(x_1, x_2) \\
=& \hat{T}(-a)\ \left[-\frac{\hbar^2}{2\,m} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2\,m} \frac{\partial^2}{\partial x_2^2} \right. \\
& \left. + V(|x_1 - x_2|) \right]\ f(x_1 - a, x_2 - a) \\
=& \left[-\frac{\hbar^2}{2\,m} \frac{\partial^2}{\partial x_1'^2} - \frac{\hbar^2}{2\,m} \frac{\partial^2}{\partial x_2'^2} \right. \\
& \left. + V(|x_1 + a - (x_2 + a)|) \right]\ f(x_1 + a - a, x_2 + a - a)
\end{aligned}$$

where $x_1' = x_1 + a$ and $x_2' = x_2 + a$. Since

$$\frac{\partial}{\partial x_1'} = \frac{\partial x_1}{\partial x_1'} \frac{\partial}{\partial x_1} = \frac{\partial}{\partial x_1}$$

(and similarly for x_2') we have

$$\hat{H}'\, f(x) = \left[-\frac{\hbar^2}{2\,m} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2\,m} \frac{\partial^2}{\partial x_2^2} + V(|x_1 - x_2|) \right]\ f(x_1, x_2)$$

so that $\hat{H}' = \hat{H}$. Of course, this is all rather pedantic. Just as in the single-particle case the momentum (and therefore kinetic energy) is invariant under a translation and since the potential in this case depends only on the *distance between particles*, it is invariant as well.

Since the Hamiltonian has a continuous translational symmetry, it is invariant under an infinitessimal transformation

$$\begin{aligned}
\hat{T}^\dagger(\delta)\ \hat{H}\, \hat{T}(\delta) &= \hat{H} \\
\hat{H} + i\,\frac{\delta}{\hbar}\,\hat{P}\,\hat{H} - i\,\frac{\delta}{\hbar}\,\hat{H}\,\hat{P} &= \hat{H} \\
\left[\hat{H}, \hat{P}\right] &= 0
\end{aligned}$$

and therefore, according to the generalized Ehrenfest theorem, the total momentum is conserved.

Problem 6.8

(a) We consider

$$\begin{aligned}
\left\langle f \,\middle|\, \hat{\Pi} g \right\rangle &= \int f^*(x)\ \left[\hat{\Pi}\, g(x)\right]\ dx \\
&= \int_{-\infty}^{\infty} f^*(x)\ g(-x)\ dx \\
&= \int_{\infty}^{-\infty} f^*(-x)\ g(x)\,(-\,dx)
\end{aligned}$$

where we have changed the integration variable from x to $-x$ in then last line. Then using the minus sign to reverse the limits of integration we have

$$\begin{aligned}\left\langle f \,\middle|\, \hat{\Pi} g\right\rangle &= \int_{-\infty}^{\infty} \left[f(-x)\right]^* \, g(x) \; dx \\ &= \int_{-\infty}^{\infty} \left[\hat{\Pi} f(x)\right]^* \, g(x) \; dx \\ &= \left\langle \hat{\Pi} f \,\middle|\, g\right\rangle \,,\end{aligned}$$

showing that the parity operator is hermitian.

(b) Because the operator is hermitian and its own inverse, it must also be unitary. A hermitian operator has eigenvalues λ that are *real* and a unitary operator has eigenvalues λ such that $|\lambda| = 1$. The only way to satisfy both these conditions is if the eigenvalues are ± 1. Clearly both cases occur: all even functions are eigenfunctions of the parity operator with eigenvalue 1 and all odd functions are eigenfunctions of the parity operator with eigenvalue -1.

Problem 6.9

(a) For a "true" scalar operator,

$$\begin{aligned}\hat{\Pi}^\dagger \, \hat{f} \, \hat{\Pi} &= \hat{f} \\ \underbrace{\hat{\Pi} \, \hat{\Pi}^\dagger}_{1} \, \hat{f} \, \hat{\Pi} &= \hat{\Pi} \, \hat{f} \\ \hat{f} \, \hat{\Pi} &= \hat{\Pi} \, \hat{f} \\ \left[\hat{\Pi}, \hat{f}\right] &= 0 \,,\end{aligned}$$

and for a pseudoscalar operator:

$$\begin{aligned}\hat{\Pi}^\dagger \, \hat{f} \, \hat{\Pi} &= -\hat{f} \\ \underbrace{\hat{\Pi} \, \hat{\Pi}^\dagger}_{1} \, \hat{f} \, \hat{\Pi} &= -\hat{\Pi} \, \hat{f} \\ \hat{f} \, \hat{\Pi} &= -\hat{\Pi} \, \hat{f} \\ \left\{\hat{\Pi}, \hat{f}\right\} &= 0 \,.\end{aligned}$$

(b) For a "true" vector operator

$$\begin{aligned}\hat{\Pi}^\dagger \, \hat{\mathbf{V}} \, \hat{\Pi} &= -\hat{\mathbf{V}} \\ \underbrace{\hat{\Pi} \, \hat{\Pi}^\dagger}_{1} \, \hat{\mathbf{V}} \, \hat{\Pi} &= -\hat{\Pi} \, \hat{\mathbf{V}} \\ \hat{\mathbf{V}} \, \hat{\Pi} &= -\hat{\Pi} \, \hat{\mathbf{V}} \\ \left\{\hat{\Pi}, \hat{\mathbf{V}}\right\} &= 0 \,,\end{aligned}$$

and for a pseudvector operator:

$$
\begin{aligned}
\hat{\Pi}^\dagger\, \hat{\mathbf{V}}\, \hat{\Pi} &= \hat{\mathbf{V}} \\
\underbrace{\hat{\Pi}\, \hat{\Pi}^\dagger}_{1}\, \hat{\mathbf{V}}\, \hat{\Pi} &= \hat{\Pi}\, \hat{\mathbf{V}} \\
\hat{\mathbf{V}}\, \hat{\Pi} &= \hat{\Pi}\, \hat{\mathbf{V}} \\
\left[\hat{\Pi}, \hat{\mathbf{V}}\right] &= 0\,.
\end{aligned}
$$

Problem 6.10

Applying $\hat{x}'$ to a test function we have

$$\hat{x}'\, f(x) = \hat{\Pi}^\dagger\, \hat{x}\, \hat{\Pi}\, f(x) = \hat{\Pi}\, x\, f(-x) = (-x)\ f(x) = -\hat{x}\, f(x)$$

so that $\hat{x}' = \hat{x}$. Applying $\hat{p}'$ to a test function we have

$$
\begin{aligned}
\hat{p}'\, f(x) &= \hat{\Pi}^\dagger\, \hat{p}\, \hat{\Pi}\, f(x) = \hat{\Pi}\left(-i\,\hbar\, \frac{d}{dx}\right)\ f(-x) \\
&= i\,\hbar\, \frac{d}{d(-x)}\ f(x) = -i\,\hbar\, \frac{d}{dx} f(x) = -\hat{p}\, f(x)
\end{aligned}
$$

so that $\hat{p}' = -\hat{p}$.

The same calculation works in three dimensions.

$$
\begin{aligned}
\hat{x}'\, f(x,y,z) &= \hat{\Pi}^\dagger\, \hat{x}\, \hat{\Pi}\, f(x,y,z) = \hat{\Pi}\, x\, f(-x,-y,-z) \\
&= (-x)\ f(x,y,z) = -\hat{x}\, f(x,y,z) \\
\hat{y}'\, f(x,y,z) &= \hat{\Pi}^\dagger\, \hat{y}\, \hat{\Pi}\, f(x,y,z) = \hat{\Pi}\, y\, f(-x,-y,-z) \\
&= (-y)\ f(x,y,z) = -\hat{y}\, f(x,y,z) \\
\hat{z}'\, f(x,y,z) &= \hat{\Pi}^\dagger\, \hat{z}\, \hat{\Pi}\, f(x,y,z) = \hat{\Pi}\, y\, f(-x,-y,-z) \\
&= (-z)\ f(x,y,z) = -\hat{z}\, f(x,y,z)
\end{aligned}
$$

so that $\hat{\mathbf{r}}' = -\hat{\mathbf{r}}$. And

$$
\begin{aligned}
\hat{p}_x'\, f(x,y,z) &= \hat{\Pi}^\dagger\, \hat{p}_x\, \hat{\Pi}\, f(x,y,z) = \hat{\Pi}\left(-i\,\hbar\, \frac{\partial}{\partial x}\right)\ f(-x,-y,-z) \\
&= i\,\hbar\, \frac{\partial}{\partial(-x)}\ f(x,y,z) = -i\,\hbar\, \frac{\partial}{\partial x} f(x,y,z) = -\hat{p}_x\, f(x,y,z) \\
\hat{p}_y'\, f(x,y,z) &= \hat{\Pi}^\dagger\, \hat{p}_y\, \hat{\Pi}\, f(x,y,z) = \hat{\Pi}\left(-i\,\hbar\, \frac{\partial}{\partial y}\right)\ f(-x,-y,-z) \\
&= i\,\hbar\, \frac{\partial}{\partial(-y)}\ f(x,y,z) = -i\,\hbar\, \frac{\partial}{\partial y} f(x,y,z) = -\hat{p}_y\, f(x,y,z) \\
\hat{p}_z'\, f(x,y,z) &= \hat{\Pi}^\dagger\, \hat{p}_z\, \hat{\Pi}\, f(x,y,z) = \hat{\Pi}\left(-i\,\hbar\, \frac{\partial}{\partial z}\right)\ f(-x,-y,-z) \\
&= i\,\hbar\, \frac{\partial}{\partial(-z)}\ f(x,y,z) = -i\,\hbar\, \frac{\partial}{\partial z} f(x,y,z) = -\hat{p}_z\, f(x,y,z)
\end{aligned}
$$

so that $\hat{\mathbf{p}}' = -\hat{\mathbf{p}}$.

Problem 6.11

From Equation 6.24 we have

$$\hat{\Pi}^\dagger\,\hat{\mathbf{L}}\,\hat{\Pi} = \hat{\mathbf{L}}\,.$$

Sandwiching this statement in between two parity eigenstates we have

$$\begin{aligned}\left\langle n'\ell'm'\,\middle|\,\hat{\Pi}^\dagger\,\hat{\mathbf{L}}\,\hat{\Pi}\,\middle|\,n\ell m\right\rangle &= \left\langle n'\ell'm'\,\middle|\,\hat{\mathbf{L}}\,\middle|\,n\ell m\right\rangle \\ \left\langle n'\ell'm'\,\middle|(-1)^{\ell'}\,\hat{\mathbf{L}}\,(-1)^{\ell}\middle|\,n\ell m\right\rangle &= \left\langle n'\ell'm'\,\middle|\,\hat{\mathbf{L}}\,\middle|\,n\ell m\right\rangle\end{aligned}$$

so that

$$\left[1-(-1)^{\ell+\ell'}\right]\left\langle n'\ell'm'\,\middle|\,\hat{\mathbf{L}}\,\middle|\,n\ell m\right\rangle = 0\,.$$

Therefore, the matrix element vanishes unless $\ell+\ell'$ is even (equivalently, it vanishes unless the two states have the *same* parity).

Problem 6.12

We need to find a Hermitian 2×2 matrix $\mathsf{\Pi}$ that commutes with each component of $\mathbf{S}$. So let

$$\mathsf{\Pi} = \begin{pmatrix} a & b \\ b^* & c\end{pmatrix}$$

with a and b real. Then

$$\begin{aligned}[\mathsf{\Pi},\mathsf{S}_x] &= \begin{pmatrix} a & b \\ b^* & c\end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}\begin{pmatrix} a & b \\ b^* & c\end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} b-b^* & a-c \\ -a+c & -b+b^*\end{pmatrix}.\end{aligned}$$

Since this must be zero we see that $a=c$ and $b=b^*$ (so that b is real) if we are to have $\mathsf{\Pi}$ and S_x commute. Next

$$\begin{aligned}[\mathsf{\Pi},\mathsf{S}_y] &= \begin{pmatrix} a & b \\ b & a\end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0\end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0\end{pmatrix}\begin{pmatrix} a & b \\ b & a\end{pmatrix} \\ &= i\,\frac{\hbar}{2}\begin{pmatrix} 2\,b & 0 \\ 0 & -2\,b\end{pmatrix}.\end{aligned}$$

so that, in addition, b must be zero if $\mathsf{\Pi}$ is to commute with S_x. That means that $\mathsf{\Pi} = a\,\mathsf{1}$, which clearly commutes with the remaining spin matrix S_z.

Problem 6.13

(a) The ground state is non-degenerate and, by Equation 6.26,

$$\langle \mathbf{p}_e\rangle = \langle 100\,|\,\mathbf{p}_e\,|\,100\rangle = \mathbf{0}\,.$$

(b) The $n = 2$ state is degenerate. Consider a state with a mixture of ℓ values: $(|200\rangle + |210\rangle)/\sqrt{2}$. For this state,

$$\begin{aligned}\langle \mathbf{p}_e \rangle &= \left(\frac{\langle 200| + \langle 210|}{\sqrt{2}}\right) \mathbf{p}_e \left(\frac{|200\rangle + |210\rangle}{\sqrt{2}}\right)\\ &= \frac{1}{2}\left(\langle 200\,|\,\mathbf{p}_e\,|\,200\rangle + 2\,\mathrm{Re}\left[\langle 210\,|\,\mathbf{p}_e\,|\,200\rangle\right] + \langle 210\,|\,\mathbf{p}_e\,|\,210\rangle\right),\end{aligned}$$

and by Equation 6.26:

$$\langle \mathbf{p}_e \rangle = \mathrm{Re}\left[\langle 210\,|\,\mathbf{p}_e\,|\,200\rangle\right].$$

The parity selection rule tells us nothing about the remaining matrix element. We can go ahead and actually compute it:

$$\begin{aligned}\langle \mathbf{p}_e \rangle =& \mathrm{Re}\left[\langle 210\,|\,\mathbf{p}_e\,|\,200\rangle\right]\\ =&\mathrm{Re}\left[-e \int \psi^*_{210}(\mathbf{r})\; r\,\sin\theta\,\cos\phi\,\psi_{200}(\mathbf{r})\; d^3\mathbf{r}\,\hat{\imath}\right.\\ &- e \int \psi^*_{210}(\mathbf{r})\; r\,\sin\theta\,\sin\phi\,\psi_{200}(\mathbf{r})\; d^3\mathbf{r}\,\hat{\jmath}\\ &\left.-e \int \psi^*_{210}(\mathbf{r})\; r\,\cos\theta\,\psi_{200}(\mathbf{r})\; d^3\mathbf{r}\,\hat{k}\right]\\ =& 3\,e\,a\,\hat{k}\,.\end{aligned}$$

Problem 6.14

(a) We first compute the eigenvalues of M.

$$0 = |\mathsf{M} - \lambda\,\mathsf{1}| = \begin{vmatrix} 1-\lambda & -\varphi/N \\ \varphi/N & 1-\lambda \end{vmatrix} = \left(1 - \lambda^2\right) + \left(\frac{\varphi}{N}\right)^2$$

so that $\lambda = 1 \pm i\,\varphi/N$. The corresponding eigenvectors are

$$\begin{aligned}\mathsf{M}\,\mathbf{v}_\pm =& (1 \pm i\,\varphi/N)\;\mathbf{v}_\pm\\ \begin{pmatrix} 1 & -\varphi/N \\ \varphi/N & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} =& (1 \pm i\,\varphi/N)\begin{pmatrix} a \\ b \end{pmatrix}\\ \begin{pmatrix} a - \varphi/N b \end{pmatrix} =& \begin{pmatrix} a \pm i\,\varphi/N\,a \end{pmatrix}\end{aligned}$$

so that $b = \mp i\,a$. The matrix S^{-1} is then

$$\mathsf{S} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}$$

and the matrix M' is

$$\begin{aligned}\mathsf{M}' &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}\begin{pmatrix} 1 & -\varphi/N \\ \varphi/N & 1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}\\ &= \begin{pmatrix} 1 + i\,\varphi/N & 0 \\ 0 & 1 - i\,\varphi/N \end{pmatrix}.\end{aligned}$$

(b) Now

$$\left(1 \pm i\,\frac{\varphi}{N}\right)^N = \sum_{k=0}^{N} \binom{N}{k} \left(\pm i\,\frac{\varphi}{N}\right)^k = \sum_{k=0}^{N} \frac{N!}{(N-k)!N^k}\,\frac{(\pm i\,\varphi)^k}{k!}$$

The coefficient

$$\frac{N!}{(N-k)!N^k} = \prod_{i=0}^{k-1}\left(1 - \frac{i}{N}\right)$$

becomes 1 in the limit that $N \to \infty$ and

$$\lim_{N\to\infty}\left(1 \pm i\,\frac{\varphi}{N}\right)^N = \sum_{k=0}^{\infty} \frac{(\pm i\,\varphi)^k}{k!} = e^{\pm i\,\varphi}\,.$$

Therefore

$$\lim_{N\to\infty} (\mathsf{M}')^N = \begin{pmatrix} e^{i\,\varphi} & 0 \\ 0 & e^{-i\,\varphi} \end{pmatrix}\,.$$

(c) Finally we transform back to the original basis to get

$$\begin{aligned}
\lim_{N\to\infty} \mathsf{M}^N &= \mathsf{S}^{-1} \lim_{N\to\infty} (\mathsf{M}')^N\,\mathsf{S} \\
&= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}\begin{pmatrix} e^{i\,\varphi} & 0 \\ 0 & e^{-i\,\varphi} \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \\
&= \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}\,.
\end{aligned}$$

Problem 6.15

Consider an infinitesimal rotation applied to the scalar operator $\hat{f}$. To first order in δ we have

$$\begin{aligned}
\hat{R}_{\mathbf{n}}(\delta)^\dagger\;\hat{f}\,\hat{R}_{\mathbf{n}}(\delta) &= \left(1 + \frac{i\,\delta}{\hbar}\,\mathbf{n}\cdot\hat{\mathbf{L}}\right)\,\hat{f}\,\left(1 - \frac{i\,\delta}{\hbar}\,\mathbf{n}\cdot\hat{\mathbf{L}}\right) \\
&= \hat{f} + \frac{i\,\delta}{\hbar}\,\mathbf{n}\cdot\hat{\mathbf{L}}\,\hat{f} - \frac{i\,\delta}{\hbar}\,\hat{f}\,\mathbf{n}\cdot\hat{\mathbf{L}} \\
&= \hat{f} + \frac{i\,\delta}{\hbar}\,\mathbf{n}\cdot\left[\hat{\mathbf{L}}, f\right]
\end{aligned}$$

so that if $\hat{f}$ commutes with $\mathbf{L}$ then it is invariant under a rotation by an infinitesimal angle δ and by extension, for any finite angle φ as well.

Problem 6.16

For an infinitesimal rotation about the y axis

$$\begin{aligned}
\hat{\mathbf{V}}' &= \left(1 + \frac{i\,\delta}{\hbar}\,L_y\right)\,\mathbf{V}\,\left(1 - \frac{i\,\delta}{\hbar}\,L_y\right) \\
&= \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} + \frac{i\,\delta}{\hbar}\begin{pmatrix} [L_y, V_x] \\ [L_y, V_y] \\ [L_y, V_z] \end{pmatrix} \\
&= \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} + \frac{i\,\delta}{\hbar}\begin{pmatrix} -i\,\hbar\,V_z \\ 0 \\ i\,\hbar\,V_x \end{pmatrix} \\
&= \begin{pmatrix} V_x + \delta\,V_z \\ V_y \\ V_z - \delta V_x \end{pmatrix}
\end{aligned}$$

so that the matrix for an infinitesimal rotation about the y axis is

$$D(\delta) = \begin{pmatrix} 1 & 0 & \delta \\ 0 & 1 & 0 \\ -\delta & 0 & 1 \end{pmatrix} .$$

Compare to Equations 6.30 and 6.31. This is clearly the infinitesimal version of

$$D(\varphi) = \begin{pmatrix} \cos\varphi & 0 & \sin\varphi \\ 0 & 1 & 0 \\ -\sin\varphi & 0 & \cos\varphi \end{pmatrix} .$$

Problem 6.17

Consider the infinitesimal rotation of the state $\psi_{n\ell m}$

$$\begin{aligned}
R_{\mathbf{n}}(\delta)\;\psi_{n\ell m} &= \left(1 - \frac{i\,\delta}{\hbar}\,\mathbf{n}\cdot\mathbf{L}\right)\;\psi_{n\,\ell m} \\
&= \psi_{n\ell m} - \frac{i\,\delta}{\hbar}\,(n_x\,L_x + n_y\,L_y + n_z\,L_z)\;\psi_{n\ell m} \\
&= \psi_{n\ell m} - \frac{i\,\delta}{\hbar}\left(\frac{n_x - i\,n_y}{2}\,L_+ + \frac{n_x + i\,n_y}{2}\,L_- + n_z\,L_z\right)\;\psi_{n\ell m}\,.
\end{aligned}$$

Then from Equations 4.121 we have

$$\begin{aligned}
R_{\mathbf{n}}(\delta)\;\psi_{n\ell m} =& (1 - i\,\delta\,m)\;\psi_{n\,\ell m} \\
& - i\,\delta\,\frac{n_x - i\,n_y}{2}\,\sqrt{\ell\,(\ell+1) - m\,(m+1)}\,\psi_{n\ell m+1} \\
& - i\,\delta\,\frac{n_x + i\,n_y}{2}\,\sqrt{\ell\,(\ell+1) - m\,(m-1)}\,\psi_{n\ell m-1} \\
\equiv& \sum_{m'} D_{m'm}\,\psi_{n\ell m'}
\end{aligned}$$

so that

$$\begin{aligned} D_{m'm} &= (1 - i\,\delta\, m)\ \delta_{m',m} \\ &\quad - i\,\delta\,\frac{n_x - i\,n_y}{2}\,\sqrt{\ell\,(\ell+1) - m\,(m+1)}\,\delta_{m',m+1} \\ &\quad - i\,\delta\,\frac{n_x + i\,n_y}{2}\,\sqrt{\ell\,(\ell+1) - m\,(m-1)}\,\delta_{m',m-1}\,. \end{aligned}$$

Problem 6.18

(a) Consider operating with the commutator on a test function $f(x)$:

$$\begin{aligned} \left[\hat{\Pi}, \hat{T}\right]\ f(x) &= \hat{\Pi}\,\hat{T}\,f(x) - \hat{T}\,\hat{\Pi}\,f(x) \\ &= \hat{\Pi}\,f(x-a) - \hat{T}\,f(-x) \\ &= f(-x-a) - f(-(x-a)) \\ &= f(-x-a) - f(-x+a)\ . \end{aligned}$$

So these two operators don't commute.

(b) Acting on one of the states $f_p(x)$ we have

$$\hat{\Pi}\,f_p(x) = \hat{\Pi}\,\frac{1}{\sqrt{2\,\pi\,\hbar}}\,e^{i\,p\,x/\hbar} = \frac{1}{\sqrt{2\,\pi\,\hbar}}\,e^{-i\,p\,x/\hbar} = f_{-p}(x)\ .$$

(c) The translation operator applied to the first state gives

$$\begin{aligned} \hat{T}\,\frac{1}{\sqrt{\pi\,\hbar}}\,\cos\!\left(\frac{p\,x}{\hbar}\right) &= \frac{1}{\sqrt{\pi\,\hbar}}\,\cos\!\left(\frac{p\,(x-a)}{\hbar}\right) \\ &= \cos\!\left(\frac{p\,a}{\hbar}\right)\,\frac{1}{\sqrt{\pi\,\hbar}}\,\cos\!\left(\frac{p\,x}{\hbar}\right) \\ &\quad + \sin\!\left(\frac{p\,a}{\hbar}\right)\,\frac{1}{\sqrt{\pi\,\hbar}}\,\sin\!\left(\frac{p\,x}{\hbar}\right) \end{aligned}$$

and

$$\begin{aligned} \hat{T}\,\frac{1}{\sqrt{\pi\,\hbar}}\,\sin\!\left(\frac{p\,x}{\hbar}\right) &= \frac{1}{\sqrt{\pi\,\hbar}}\,\sin\!\left(\frac{p\,(x-a)}{\hbar}\right) \\ &= \cos\!\left(\frac{p\,a}{\hbar}\right)\,\frac{1}{\sqrt{\pi\,\hbar}}\,\sin\!\left(\frac{p\,x}{\hbar}\right) \\ &\quad - \sin\!\left(\frac{p\,a}{\hbar}\right)\,\frac{1}{\sqrt{\pi\,\hbar}}\,\cos\!\left(\frac{p\,x}{\hbar}\right)\ . \end{aligned}$$

Therefore, the translation operator mixes these two states together.

Probelm 6.19

(a) First,

$$
\begin{aligned}
[L_z, V_\pm] &= [L_z, V_x] \pm i\,[L_z, V_y] = i\,\hbar\,V_y \pm i\,(-i\,\hbar\,V_x) \\
&= \hbar\,(\pm V_x + i\,V_y) = \pm\hbar\,(V_x \pm i\,V_y) = \pm\hbar\,V_\pm\,.
\end{aligned}
$$

If you're comfortable working with index notation, the next part could be quicker, but I'll do it the long way. Here we go:

$$
\begin{aligned}
\left[L^2, V_\pm\right] &= \left[L_x^2 + L_y^2 + L_z^2, V_x \pm iV_y\right] \\
&= \left[L_x^2, V_x\right] \pm i\,\left[L_x^2, V_y\right] + \left[L_y^2, V_x\right] \pm i\,\left[L_y^2, V_y\right] + \left[L_z^2, V_\pm\right] \\
&= 0 \pm i\,L_x\,[L_x, V_y] \pm i\,[L_x, V_y]\,L_x + L_y\,[L_y, V_x] + [L_y, V_x]\,L_y \\
&\quad + 0 + L_z\,[L_z, V_\pm] + [L_z, V_\pm]\,L_z \\
&= \pm\,i\,L_x\,i\,\hbar\,V_z \pm i\,(i\,\hbar\,V_z)\,L_x + L_y\,(-i\,\hbar\,V_z) + (-i\,\hbar\,V_z)\,L_y \\
&\quad + L_z\,(\pm\hbar\,V_\pm) \pm \hbar\,V_\pm\,L_z
\end{aligned}
$$

where we've used the result proved above. Finally we need to get all L's to the right of all V's:

$$
\begin{aligned}
\left[L^2, V_\pm\right] &= \mp\,\hbar\,V_z\,L_x \mp \hbar\,[L_x, V_z] \mp \hbar\,V_z\,L_x - i\,\hbar\,V_z\,L_y - i\,\hbar\,[L_y, V_z] \\
&\quad - i\,\hbar\,V_z\,L_y \pm \hbar\,V_\pm\,L_z \pm\,\hbar\,[L_z, V_\pm] \pm \hbar\,V_\pm\,L_z \\
&= \hbar\,V_z(\mp 2\,L_x - 2\,i\,L_y) \mp \hbar(-i\,\hbar\,V_y) - i\,\hbar\,i\,\hbar\,V_x \\
&\quad \pm 2\,\hbar\,V_\pm\,L_z \pm\,\hbar\,(\pm\hbar\,V_\pm) \\
&= \mp\,2\,\hbar\,V_z\,(L_x \pm i\,L_y) + \hbar^2\,(V_x \pm i\,V_y) \pm 2\,\hbar\,V_\pm\,L_z + \hbar^2\,V_\pm \\
&= 2\,\hbar^2\,V_\pm \pm 2\,\hbar\,V_\pm\,L_z \mp 2\,\hbar\,V_z\,L_\pm\,.
\end{aligned}
$$

This is the desired result.

(b) Acting on a state $\psi_{n\ell\ell}$ with each of the commutator relations form part a we get

$$
\begin{aligned}
[L_z, V_+]\;\psi_{n\ell\ell} &= \hbar\,V_+\,\psi_{n\ell\ell} \\
L_z\,V_+\,\psi_{n\ell\ell} - V_+\,\underbrace{L_z\,\psi_{n\ell\ell}}_{\ell\,\hbar\,\psi_{n\ell\ell}} &= \hbar\,V_+\,\psi_{n\ell\ell} \\
L_z\,(V_+\,\psi_{n\ell\ell}) &= (\ell+1)\;\hbar\,(V_+\,\psi_{n\ell\ell})
\end{aligned}
$$

and

$$
\begin{aligned}
\left[L^2, V_+\right]\;\psi_{n\ell\ell} &= \left(2\,\hbar^2\,V_+ + 2\,\hbar\,V_+\,L_z - 2\,\hbar\,V_z\,L_+\right)\;\psi_{n\ell\ell} \\
L^2\,V_+\,\psi_{n\ell\ell} - V_+\;\underbrace{L^2\,\psi_{n\ell\ell}}_{\ell(\ell+1)\,\hbar^2\,\psi_{n\ell\ell}} &= 2\,\hbar^2\,V_+\,\psi_{n\ell\ell} + 2\,\hbar\,V_+\;\underbrace{L_z\,\psi_{n\ell\ell}}_{\ell\,\hbar\,\psi_{n\ell\ell}} - 2\,\hbar\,V_z\;\underbrace{L_+\,\psi_{n\ell\ell}}_{0} \\
L^2\,(V_+\,\psi_{n\ell\ell}) &= [\ell\,(\ell+1) + 2 + 2\,\ell]\;\hbar^2\,(V_+\,\psi_{n\ell\ell}) \\
&= (\ell+1)\,(\ell+2)\;\hbar^2\,(V_+\,\psi_{n\ell\ell})\;.
\end{aligned}
$$

From these results, the state $V_+\,\psi_{n\ell\ell}$ has an m value of $\ell+1$ and an ℓ value of $\ell+1$.

Problem 6.20

Sandwiching the commutator between two angular momentum eigenstates gives

$$\begin{aligned}\langle n'\ell'm' \,|\, [L_-, f] \,|\, n\ell m\rangle &= 0 \\ \langle n'\ell'm' \,|\, L_- \, f \,|\, n\ell m\rangle - \langle n'\ell'm' \,|\, f \, L_- \,|\, n\ell m\rangle &= 0 \\ A_{\ell'}^{m'} \;\langle n'\ell'm'+1 \,|\, f \,|\, n\ell m\rangle - B_\ell^m \;\langle n'\ell'm' \,|\, f \,|\, n\ell m-1\rangle &= 0\end{aligned}$$

Now we know that these matrix elements vanish unless $m'{+}1 = m$ and $\ell' = \ell$. When those are equal $A_\ell^{m-1} = B_\ell^m$ and

$$\langle n'\ell m \,|\, f \,|\, n\ell m\rangle = \langle n'\ell m-1 \,|\, f \,|\, n\ell m-1\rangle \ .$$

Since m is arbitrary, this is equivalent to Equation 6.46.

Problem 6.21

The expectation value of r is

$$\begin{aligned}\langle \psi \,|\, r \,|\, \psi\rangle &= \frac{1}{2}\left(\langle 211| + \langle 21-1|\right) r \left(|211\rangle + |21-1\rangle\right) \\ &= \frac{1}{2}\;\langle 211 \,|\, r \,|\, 211\rangle + \mathrm{Re}\left[\langle 211 \,|\, r \,|\, 21-1\rangle\right] + \langle 21-1 \,|\, r \,|\, 21-1\rangle\end{aligned}$$

and applying Equation 6.47 we get

$$\langle \psi \,|\, r \,|\, \psi\rangle = \langle 21 \,\|\, r \,\|\, 21\rangle \ .$$

Now we need to actually evaluate the reduced matrix element. We can choose any value of m to do so:

$$\langle 21 \,\|\, r \,\|\, 21\rangle = \langle 210 \,|\, r \,|\, 210\rangle = \int \psi_{210}^*(\mathbf{r}) \; r \, \psi_{210}^*(\mathbf{r}) \; d^3\mathbf{r} = 5\,a \, .$$

Therefore

$$\boxed{\langle \psi \,|\, r \,|\, \psi\rangle = \langle 21 \,\|\, r \,\|\, 21\rangle = 5\,a \, .}$$

Problem 6.22

(a)

$$\begin{aligned}[L_z, V_z] &= 0 \\ [L_z, V_\pm] &= [L_z, V_x] \pm i\;[L_z, V_y] = i\,\hbar\,V_y \pm i\,(-i\,\hbar\,V_x) \\ &= \pm\hbar\,(V_x \pm i\,V_y) = \pm\,\hbar\,V_\pm \\ [L_\pm, V_\pm] &= [L_x, V_x] \pm i\;[L_x, V_y] \pm i\;[L_y, V_x] - [L_y, V_y] \\ &= 0 \pm i\,(i\,\hbar\,V_z) \pm i\,(-i\,\hbar\,V_z) - 0 = 0 \\ [L_\pm, V_z] &= [L_x, V_z] \pm i\;[L_y, V_z] = -i\,\hbar\,V_y \pm i\,(i\,\hbar\,V_x) \\ &= \mp\hbar\,(V_x \pm i\,V_y) = \mp\,\hbar\,V_\pm \\ [L_\pm, V_\mp] &= [L_x, V_x] \mp i\;[L_x, V_y] \pm i\;[L_y, V_x] + [L_y, V_y] \\ &= 0 \mp i\,(i\,\hbar\,V_z) \pm i\,(-i\,\hbar\,V_z) = \pm 2\,\hbar\,V_z \, .\end{aligned}$$

(b) Sandwiching 6.50 in between two angular-momentum eigenstates we get

$$\begin{aligned}\langle n'\ell' m' \,|\, [L_z, V_z] \,|\, n\ell m\rangle &= 0\\ \langle n'\ell' m' \,|\, L_z\, V_z \,|\, n\ell m\rangle - \langle n'\ell' m' \,|\, V_z\, L_z \,|\, n\ell m\rangle &= 0\\ m'\; \langle n'\ell' m' \,|\, V_z \,|\, n\ell m\rangle - m\; \langle n'\ell' m' \,|\, V_z \,|\, n\ell m\rangle &= 0\end{aligned}$$

so that $\langle n'\ell' m'|V_z|n\ell m\rangle = 0$ unless $m = m'$.

Problem 6.23

(a) This is nothing more than Fourier's trick. Taking an inner product with an arbitrary state from the sum and using the orthonormality,

$$\begin{aligned}\langle j_1\, j_2\, m_1'\, m_2' \,|\, J\, M\rangle &= \sum_{m_1, m_2} C^{j_1\, j_2\, J}_{m_1\, m_2\, M}\; \underbrace{\langle j_1\, j_2\, m_1'\, m_2' \,|\, j_1\, j_2\, m_1\, m_2\rangle}_{\delta_{m_1, m_1'}\, \delta_{m_2, m_2'}}\\ &= C^{j_1\, j_2, J}_{m_1'\, m_2'\, M}\,.\end{aligned}$$

(b) Applying $J_\pm$ to Equation 6.64 we get

$$J_\pm\; |J\, M\rangle = \sum_{m_1, m_2} C^{j_1 j_2 J}_{m_1 m_2 M} \left[J_\pm^{(1)}\; |j_1\, j_2\, m_1\, m_2\rangle + J_\pm^{(2)}\; |j_1\, j_2\, m_1\, m_2\rangle\right]\,.$$

(a) For the plus case, Equation 4.121 gives

$$A_J^M\; |J\, M+1\rangle = \sum_{m_1\, m_2} C^{j_1 j_2 J}_{m_1\, m_2\, M}\; \left[A_{j_1}^{m_1}\; |j_1\, j_2\, m_1+1\, m_2\rangle + A_{j_2}^{m_2}\; |j_1\, j_2\, m_1\, m_2+1\rangle\right]\,.$$

Next we take the inner product with $\langle j_1 j_2 m_1' m_2'|$ to get

$$\begin{aligned}A_J^M\, C^{j_1\, j_2\, J}_{m_1'\, m_2'\, M+1} &= \sum_{m_1\, m_2} C^{j_1 j_2 J}_{m_1\, m_2\, M}\; \left[A_{j_1}^{m_1}\, \delta_{m_1+1, m_1'}\, \delta_{m_2, m_2'} + A_{j_2}^{m_2}\, \delta_{m_1, m_1'}\, \delta_{m_2+1, m_2'}\right]\\ &= A_{j_1}^{m_1'-1}\, C^{j_1\, j_2\, J}_{m_1'-1\, m_2\, M} + A_{j_2}^{m_2'-1}\, C^{j_1\, j_2\, J}_{m_1'\, m_2'-1\, M}\,.\end{aligned}$$

Now $A_j^{m-1} = B_j^m$ and dropping the primes we have

$$\boxed{A_J^M\, C^{j_1\, j_2\, J}_{m_1\, m_2\, M+1} = B_{j_1}^{m_1}\, C^{j_1\, j_2\, J}_{m_1-1\, m_2\, M} + B_{j_2}^{m_2}\, C^{j_1\, j_2\, J}_{m_1\, m_2-1\, M}}$$

which is the first desired equality.

(b) For the minus case, Equation 4.121 gives

$$B_J^M\; |J\, M-1\rangle = \sum_{m_1\, m_2} C^{j_1 j_2 J}_{m_1\, m_2\, M}\; \left[B_{j_1}^{m_1}\; |j_1\, j_2\, m_1-1\, m_2\rangle + B_{j_2}^{m_2}\; |j_1\, j_2\, m_1\, m_2-1\rangle\right]\,.$$

Next we take the inner product with $\langle j_1 j_2 m_1' m_2'|$ to get

$$\begin{aligned}B_J^M\, C^{j_1\, j_2\, J}_{m_1'\, m_2'\, M-1} &= \sum_{m_1\, m_2} C^{j_1 j_2 J}_{m_1\, m_2\, M}\; \left[B_{j_1}^{m_1}\, \delta_{m_1-1, m_1'}\, \delta_{m_2, m_2'} + B_{j_2}^{m_2}\, \delta_{m_1, m_1'}\, \delta_{m_2-1, m_2'}\right]\\ &= B_{j_1}^{m_1'+1}\, C^{j_1\, j_2\, J}_{m_1'+1\, m_2\, M} + B_{j_2}^{m_2'+1}\, C^{j_1\, j_2\, J}_{m_1'\, m_2'+1\, M}\,.\end{aligned}$$

Now $B_j^{m+1} = A_j^m$ and dropping the primes we have

$$\boxed{B_J^M\, C^{j_1\, j_2\, J}_{m_1\, m_2\, M-1} = A_{j_1}^{m_1}\, C^{j_1\, j_2\, J}_{m_1+1\, m_2\, M} + A_{j_2}^{m_2}\, C^{j_1\, j_2\, J}_{m_1\, m_2+1\, M}}$$

which is the second desired equality.

Problem 6.24

(a) i. From Equation 6.52 (upper signs),

$$\begin{aligned}\langle n'\ell' m' \,|\, L_+\, V_+ - V_+\, L_+ \,|\, n\ell m\rangle &= 0 \\ B_{\ell'}^{m'}\ \langle n'\ell' m' - 1 \,|\, V_+ \,|\, n\ell m\rangle &= A_\ell^m\ \langle n'\ell' m' \,|\, V_+ \,|\, n\ell m + 1\rangle\ .\end{aligned}$$

ii. From Equation 6.52 (lower signs),

$$\begin{aligned}\langle n'\ell' m' \,|\, L_-\, V_- - V_-\, L_- \,|\, n\ell m\rangle &= 0 \\ A_{\ell'}^{m'}\ \langle n'\ell' m' + 1 \,|\, V_- \,|\, n\ell m\rangle &= B_\ell^m\ \langle n'\ell' m' \,|\, V_+ \,|\, n\ell m - 1\rangle\ .\end{aligned}$$

iii. From Equation 6.53 (upper signs),

$$\begin{aligned}\langle n'\ell' m' \,|\, L_+\, V_z - V_z\, L_+ \,|\, n\ell m\rangle &= -\hbar\ \langle n'\ell' m' \,|\, V_+ \,|\, n\ell m\rangle \\ B_{\ell'}^{m'}\ \langle n'\ell' m' - 1 \,|\, V_z \,|\, n\ell m\rangle &= A_\ell^m\ \langle n'\ell' m' \,|\, V_z \,|\, n\ell m + 1\rangle - \hbar\ \langle n'\ell' m' \,|\, V_+ \,|\, n\ell m\rangle\ .\end{aligned}$$

iv. From Equation 6.53 (lower signs),

$$\begin{aligned}\langle n'\ell' m' \,|\, L_-\, V_z - V_z\, L_- \,|\, n\ell m\rangle &= \hbar\ \langle n'\ell' m' \,|\, V_- \,|\, n\ell m\rangle \\ A_{\ell'}^{m'}\ \langle n'\ell' m' + 1 \,|\, V_z \,|\, n\ell m\rangle &= B_\ell^m\ \langle n'\ell' m' \,|\, V_z \,|\, n\ell m - 1\rangle + \hbar\ \langle n'\ell' m' \,|\, V_- \,|\, n\ell m\rangle\ .\end{aligned}$$

v. From Equation 6.54 (upper signs),

$$\begin{aligned}\langle n'\ell' m' \,|\, L_+\, V_- - V_-\, L_+ \,|\, n\ell m\rangle &= 2\,\hbar\ \langle n'\ell' m' \,|\, V_z \,|\, n\ell m\rangle \\ B_{\ell'}^{m'}\ \langle n'\ell' m' - 1 \,|\, V_- \,|\, n\ell m\rangle &= A_\ell^m\ \langle n'\ell' m' \,|\, V_- \,|\, n\ell m + 1\rangle + 2\,\hbar\ \langle n'\ell' m' \,|\, V_z \,|\, n\ell m\rangle\ .\end{aligned}$$

vi. From Equation 6.54 (lower signs),

$$\begin{aligned}\langle n'\ell' m' \,|\, L_-\, V_+ - V_+\, L_- \,|\, n\ell m\rangle &= -2\,\hbar\ \langle n'\ell' m' \,|\, V_z \,|\, n\ell m\rangle \\ A_{\ell'}^{m'}\ \langle n'\ell' m' + 1 \,|\, V_+ \,|\, n\ell m\rangle &= B_\ell^m\ \langle n'\ell' m' \,|\, V_+ \,|\, n\ell m - 1\rangle - 2\,\hbar\ \langle n'\ell' m' \,|\, V_z \,|\, n\ell m\rangle\ .\end{aligned}$$

(b) i. Plugging in Equation 6.59 to the result from a.i,

$$B_{\ell'}^{m'}\, C^{\ell\ 1\ell'}_{m1m'-1} \stackrel{?}{=} A_\ell^m\, C^{\ell\ \ \ 1\ell'}_{m+11m'}$$

and applying Equation 6.66,

$$A_\ell^m\, C^{\ell\ \ \ 1\ell'}_{m+11m'} + A_1^1\, C^{\ell\ 1\ell'}_{m2m'} \stackrel{?}{=} A_\ell^m\, C^{\ell\ \ \ 1\ell'}_{m+11m'}\ .$$

Since $A_1^1 = 0$, the equation is satisfied.

ii. Plugging in Equation 6.60 to the result from a.ii,

$$A^{m'}_{\ell'}\, C^{\ell\ 1\ \ell'}_{m\,-1\,m'+1} \stackrel{?}{=} B^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ \ell'}_{m-1\,-1\,m'}$$

and applying Equation 6.66,

$$B^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ \ell'}_{m-1\,-1\,m'} + B^{-}_{1}1\, C^{\ell\ 1\ \ell'}_{m\,-2\,m'} \stackrel{?}{=} B^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ \ell'}_{m-1\,-1\,m'}\ .$$

Since $B^{-1}_{1} = 0$, the equation is satisfied.

iii. Plugging in Equation 6.59 and 6.61 to the result from a.iii,

$$B^{m'}_{\ell'}\, C^{\ell\ 1\ \ell'}_{m\,0\,m'-1} \stackrel{?}{=} A^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ell'}_{m+1\,0\,m'} + \sqrt{2}\,\hbar\, C^{\ell\ 1\ \ell'}_{m\,1\,m'}$$

and applying Equation 6.66,

$$A^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ell'}_{m+1\,0\,m'} + A^{0}_{1}\, C^{\ell\ 1\ \ell'}_{m\,1\,m'} \stackrel{?}{=} A^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ell'}_{m+1\,0\,m'} + \sqrt{2}\,\hbar\, C^{\ell\ 1\ \ell'}_{m\,1\,m'}\ .$$

Since $A^{0}_{1} = \sqrt{2}\,\hbar$, the equation is satisfied.

iv. Plugging in Equation 6.60 and 6.61 to the result from a.iv,

$$A^{m'}_{\ell'}\, C^{\ell\ 1\ \ell'}_{m\,0\,m'+1} \stackrel{?}{=} B^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ell'}_{m-1\,0\,m'} + \sqrt{2}\,\hbar\, C^{\ell\ 1\ \ell'}_{m\,-1\,m'}$$

and applying Equation 6.66,

$$B^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ell'}_{m-1\,0\,m'} + B^{0}_{1}\, C^{\ell\ 1\ \ell'}_{m\,-1\,m'} \stackrel{?}{=} B^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ell'}_{m-1\,0\,m'} + \sqrt{2}\,\hbar\, C^{\ell\ 1\ \ell'}_{m\,-1\,m'}\ .$$

Since $B^{0}_{1} = \sqrt{2}\,\hbar$, the equation is satisfied.

v. Plugging in Equation 6.60 and 6.61 to the result from a.v,

$$B^{m'}_{\ell'}\, C^{\ell\ 1\ \ell'}_{m\,-1\,m'-1} \stackrel{?}{=} A^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ \ell'}_{m+1\,-1\,m'} + \sqrt{2}\,\hbar\, C^{\ell\ 1\ \ell'}_{m\,0\,m'}\ ,$$

and applying Equation 6.66,

$$A^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ \ell'}_{m+1\,-1\,m'} + A^{-1}_{1}\, C^{\ell\ 1\ \ell'}_{m\,0\,m'} \stackrel{?}{=} A^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ \ell'}_{m+1\,-1\,m'} + \sqrt{2}\,\hbar\, C^{\ell\ 1\ \ell'}_{m\,0\,m'}\ .$$

Since $A^{-1}_{1} = \sqrt{2}\,\hbar$, the equation is satisfied.

vi. Finally, plugging in Equations 6.59 and 6.61 to the result from a.vi,

$$A^{m'}_{\ell'}\, C^{\ell\ 1\ \ell'}_{m\,1\,m'+1} \stackrel{?}{=} B^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ell'}_{m-1\,1\,m'} + \sqrt{2}\,\hbar\, C^{\ell\ 1\ \ell'}_{m\,0\,m'}\ ,$$

and applying Equation 6.66,

$$B^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ell'}_{m-1\,1\,m'} + B^{1}_{1}\, C^{\ell\ 1\ \ell'}_{m\,0\,m'} \stackrel{?}{=} B^{m}_{\ell}\, C^{\ell\ \ \ 1\ \ell'}_{m-1\,1\,m'} + \sqrt{2}\,\hbar\, C^{\ell\ 1\ \ell'}_{m\,0\,m'}\ .$$

Since $B^{1}_{1} = \sqrt{2}\,\hbar$, the equation is satisfied.

Problem 6.25

The expectation value of the dipole moment $\mathbf{p}_e$ is

$$\begin{aligned}\langle\psi\,|\,\mathbf{p}_e\,|\,\psi\rangle &= \frac{1}{2}\left(\langle 211| + \langle 200|\right)\,\mathbf{p}_e\left(|211\rangle + |200\rangle\right)\\ &= \frac{1}{2}\left(\langle 211\,|\,\mathbf{p}_e\,|\,211\rangle + 2\,\mathrm{Re}\left[\langle 211\,|\,\mathbf{p}_e\,|\,200\rangle\right] + \langle 210\,|\,\mathbf{p}_e\,|\,200\rangle\right)\,.\end{aligned}$$

Now because of Laporte's rule, the first and last matrix elements vanish and

$$\langle\psi\,|\,\mathbf{p}_e\,|\,\psi\rangle = \mathrm{Re}\left[\langle 211\,|\,\mathbf{p}_e\,|\,200\rangle\right]\,.$$

We can now write out the operator

$$\langle\psi\,|\,\mathbf{p}_e\,|\,\psi\rangle = -e\left(\mathrm{Re}\left[\langle 211\,|\,x\,|\,200\rangle\;\hat{\imath} + \langle 211\,|\,y\,|\,200\rangle\;\hat{\jmath} + \langle 211\,|\,z\,|\,200\rangle\;\hat{k}\right]\right)\,.$$

Now, according to Equation 6.57 the last term vanishes and we may write $r_\pm = x \pm i\,y$ so that

$$\langle\psi\,|\,\mathbf{p}_e\,|\,\psi\rangle = -e\left(\mathrm{Re}\left[\left\langle 211\,\middle|\,\frac{r_+ + r_-}{2}\,\middle|\,200\right\rangle\;\hat{\imath} + \left\langle 211\,\middle|\,\frac{r_+ - r_-}{2\,i}\,\middle|\,200\right\rangle\;\hat{\jmath}\right]\right)\,.$$

Now according to Equation 6.58, the matrix elements of r_- vanish and

$$\langle\psi\,|\,\mathbf{p}_e\,|\,\psi\rangle = -e\,\mathrm{Re}\left[\langle 211\,|\,r_+\,|\,200\rangle\;\frac{\hat{\imath} - i\,\hat{\jmath}}{2}\right]$$

We can then use Equation 6.59 to write

$$\begin{aligned}\langle\psi\,|\,\mathbf{p}_e\,|\,\psi\rangle &= -e\,\mathrm{Re}\left[-\sqrt{2}\,C^{011}_{011}\;\langle 21\,\|\,r\,\|\,21\rangle\;\frac{\hat{\imath} - i\,\hat{\jmath}}{2}\right]\\ &= e\,\mathrm{Re}\left[\langle 21\,\|\,r\,\|\,20\rangle\;\frac{\hat{\imath} - i\,\hat{\jmath}}{\sqrt{2}}\right] = \frac{e}{\sqrt{2}}\;\langle 21\,\|\,r\,\|\,21\rangle\;\hat{\imath}\end{aligned}$$

since, as we'll prove in just a second, the reduced matrix element is real in this case. To evaluate the reduced matrix element, we choose the simplest instance:

$$\langle 210\,|\,z\,|\,100\rangle = C^{011}_{000}\;\langle 21\,\|\,r\,\|\,21\rangle = \langle 21\,\|\,r\,\|\,21\rangle$$

or

$$\begin{aligned}\langle 21\,\|\,r\,\|\,20\rangle &= \sqrt{2}\;\langle 210\,|\,z\,|\,200\rangle\\ &= \sqrt{2}\int \psi^*_{210}(\mathbf{r})\;r\;\cos\theta\,\psi_{200}(\mathbf{r})\;d^3\mathbf{r} = -3\,a\end{aligned}$$

and

$$\boxed{\langle\psi\,|\,\mathbf{p}_e\,|\,\psi\rangle = -\frac{3\,e\,a}{\sqrt{2}}\,.}$$

Problem 6.26

We can follow the same steps as in Example 6.7. We have

$$\begin{aligned}
p_H(t)\ \psi_n(x) &= U^\dagger\, p\, U\, \psi_n(x) \\
&= U^\dagger\, i\,\sqrt{\frac{\hbar\, m\,\omega}{2}}\ (a_+ - a_-)\ e^{-i\,E_n\,t/\hbar}\,\psi_n(x) \\
&= U^\dagger\, i\,\sqrt{\frac{\hbar\, m\,\omega}{2}}\ e^{-i\,E_n\,t/\hbar}\left(\sqrt{n+1}\,\psi_{n+1}(x) - \sqrt{n}\,\psi_n(x)\right) \\
&= i\,\sqrt{\frac{\hbar\, m\,\omega}{2}}\ e^{-i\,E_n\,t/\hbar}\left(\sqrt{n+1}\,e^{i\,E_{n+1}\,t/\hbar}\,\psi_{n+1}(x) - \sqrt{n}\,e^{i\,E_{n-1}\,t/\hbar}\,\psi_n(x)\right) \\
&= i\,\sqrt{\frac{\hbar\, m\,\omega}{2}}\left(e^{i\,\omega\,t}\,\sqrt{n+1}\,\psi_{n+1}(x) - e^{-i\,\omega\,t}\,\sqrt{n}\,\psi_{n-1}(x)\right) \\
&= i\,\sqrt{\frac{\hbar\, m\,\omega}{2}}\left(e^{i\,\omega\,t}\,a_+ - e^{-i\,\omega\,t}\,a_-\right)\ \psi_n(x)
\end{aligned}$$

so that

$$\begin{aligned}
p_H(t) &= i\,\sqrt{\frac{\hbar\, m\,\omega}{2}}\left(e^{i\,\omega\,t}\,a_+ - e^{-i\,\omega\,t}\,a_-\right) \\
&= i\,\sqrt{\frac{\hbar\, m\,\omega}{2}}\left(e^{i\,\omega\,t}\,\frac{1}{\sqrt{2\,\hbar\,m\,\omega}}(-i\,p + m\,\omega\,x) - e^{-i\,\omega\,t}\,\frac{1}{\sqrt{2\,\hbar\,m\,\omega}}(i\,p + m\,\omega\,x)\right) \\
&= p\,\cos(\omega\,t) - m\,\omega\,x\,\sin(\omega\,t)
\end{aligned}$$

and

$$\boxed{p_H(t) = p_H(0)\,\cos(\omega\,t) - m\,\omega\,x_H(0)\,\sin(\omega\,t)\ .}$$

This is identical to the solution of the classical equations of motion with the classical variables x and p replaced by the quantum operators x_H and p_H.

Problem 6.27

For the free particle

$$\begin{aligned}
[p, H] &= \left[p, \frac{p^2}{2\,m}\right] = 0 \\
[x, H] &= \left[x, \frac{p^2}{2\,m}\right] = \frac{1}{2\,m}\,([x,p]\ p + p\ [x,p]) = \frac{i\,\hbar}{m}\,p
\end{aligned}$$

and

$$\begin{aligned}
\left[x, H^2\right] &= [x,H]\ H + H\ [x,H] = \frac{i\,\hbar}{m}p\,H + H\,\frac{i\,\hbar}{m}\,p = 2\,\frac{i\,\hbar}{m}\,p\,H \\
\left[x, H^3\right] &= [x,H]\ H^2 + H\ \left[x,H^2\right] = \frac{i\,\hbar}{m}\,p\,H^2 + H\,2\,\frac{i\,\hbar}{m}\,p\,H = 3\,\frac{i\,\hbar}{m}\,p\,H^2\,.
\end{aligned}$$

Now that we see the pattern we can do a proof by induction. Assume that $[x, H^n] = n\, i\, \hbar\, p\, H^{n-1}/m$ (which we've already verified for $n = 1, 2, 3$) and show that if it holds for n, then it holds for $n+1$. Well

$$\begin{aligned}
\left[x, H^{n+1}\right] &= H\ [x, H^n] + [x, H]\ H^n \\
&= H\, n\, \frac{i\,\hbar}{m}\, p\, H^{n-1} + \frac{i\,\hbar}{m}\, p\, H^n \\
&= (n+1)\ \frac{i\,\hbar}{m}\, p\, H^n
\end{aligned}$$

so that the proof by induction holds. Now from this

$$\begin{aligned}
[x, U] &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\, t\right)^n\ [x, H^n] \\
&= 1 + \frac{i\,\hbar}{m}\, p \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left(-\frac{i}{\hbar}\, t\right)^n\ H^{n-1} \\
&= 1 + \frac{p\, t}{m}\ \underbrace{\sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left(-\frac{i}{\hbar}\, t\right)^{n-1}\ H^{n-1}}_{U}
\end{aligned}$$

and since p commutes with H we also have $[p, U] = 0$. We are then finally in a position to compute

$$\begin{aligned}
x_H(t) &= U^\dagger\, x\, U = U^\dagger\, (U\, x + [x, U]) = x + U^\dagger\, \frac{p\, t}{m}\, U = x + \frac{p\, t}{m} \\
p_H(t) &= U^\dagger\, p\, U = U^\dagger\, (U\, p + [p, U]) = p\,.
\end{aligned}$$

Writing everything in terms of Heisenberg picture operators we have

$$\boxed{x_H(t) = x_H(0) + \frac{1}{m}\, p_H(0)\ t \qquad p_H(t) = p_H(0)\ .}$$

Problem 6.28

Taylor expanding $\Psi(x, t)$ we have

$$\begin{aligned}
\Psi(x, t_0 + \delta) &= \Psi(x, t_0) + \delta\ \left.\frac{\partial \Psi}{\partial t}\right|_{t_0} + \ldots \\
&= \Psi(x, t_0) + \delta\, \frac{1}{i\,\hbar}\, \hat{H}(t_0)\ \Psi(x, t_0) + \ldots \\
&= \left[1 - \frac{i\,\delta}{\hbar}\, \hat{H}(t_0) + \ldots\right]\ \Psi(x, t_0)
\end{aligned}$$

and comparing to Equation 6.75 we may read off

$$\boxed{\hat{U}(t_0 + \delta, t_0) \approx 1 - \frac{i\,\delta}{\hbar}\, \hat{H}(t_0)\ .}$$

Problem 6.29

We start with

$$\begin{aligned} i\hbar \frac{d}{dt}\hat{Q}_H(t) &= i\hbar \frac{d}{dt}\left[\hat{U}^\dagger(t)\ \hat{Q}\,\hat{U}(t)\right] \\ &= i\hbar \frac{dU^\dagger}{dt}\,\hat{Q}\,\hat{U}(t) + \hat{U}^\dagger(t)\ \hat{Q}\, i\hbar \frac{d\hat{U}}{dt} \end{aligned}$$

Since $\hat{H}$ is time independent,

$$\frac{dU}{dt} = \frac{d}{dt} e^{-i\hat{H}t/\hbar} = -\frac{i}{\hbar}\,\hat{H}\, e^{-i\hat{H}t/\hbar} = -\frac{i}{\hbar}\,\hat{H}\,\hat{U}(t)\ ,$$

and taking the adjoint of this expression

$$\frac{dU^\dagger}{dt} = \frac{i}{\hbar}\,\hat{U}^\dagger(t)\ \hat{H}\,.$$

$\hat{H}$ clearly commutes with $\hat{U}$ or $\hat{U}^\dagger$ and therefore

$$\begin{aligned} i\hbar \frac{d}{dt}\,\hat{Q}_H(t) &= -\hat{U}^\dagger(t)\ \hat{H}\,\hat{Q}\,\hat{U}(t) + \hat{U}^\dagger(t)\ \hat{Q}\,\hat{H}\,\hat{U}(t) \\ &= \hat{U}^\dagger(t)\ \hat{Q}\,\hat{U}(t)\ \hat{H} - \hat{H}\,\hat{U}^\dagger(t)\ \hat{Q}\,\hat{U}(t) \\ &= \hat{Q}_H(t)\ \hat{H} - \hat{H}\,\hat{Q}_H(t) \end{aligned}$$

which is the desired result.

For the operator $\hat{x}$,

$$\begin{aligned} \frac{d}{dt}\hat{x}_H &= \frac{1}{i\hbar}\left[\hat{x}_H, \hat{H}\right] = \frac{1}{i\hbar}\left[\hat{U}^\dagger\,\hat{x}\,\hat{U}, \hat{H}\right] \\ &= \frac{1}{i\hbar}\left(\hat{U}^\dagger\,\hat{x}\,\underbrace{\left[\hat{U}, \hat{H}\right]}_{0} + \hat{U}^\dagger\left[\hat{x}, \hat{H}\right]\hat{U} + \underbrace{\left[U^\dagger, \hat{H}\right]}_{0}\,\hat{x}\,\hat{U}\right) \\ &= \frac{1}{i\hbar}\,\hat{U}^\dagger\left[\hat{x}, \frac{\hat{p}^2}{2m} + V\right]\hat{U} \\ &= \frac{1}{i\hbar}\,\hat{U}^\dagger\left(\frac{1}{2m}\left[\hat{x}, \hat{p}^2\right] + \underbrace{\left[\hat{x}, V\right]}_{0}\right)\hat{U} \\ &= \frac{1}{i\hbar}\,\hat{U}^\dagger\,\frac{1}{2m}\left(\hat{p}\,\underbrace{\left[\hat{x}, \hat{p}\right]}_{i\hbar} + \left[\hat{x}, \hat{p}\right]\,\hat{p}\right)\hat{U} \\ &= \frac{1}{m}\,\hat{U}^\dagger\,\hat{p}\,\hat{U} = \frac{1}{m}\,\hat{p}_H(t)\ . \end{aligned}$$

And for the operator $\hat{p}$ we reproduce the first two lines of the above calculation to arrive at

$$\begin{aligned}
\frac{d}{dt}\hat{p}_H &= \frac{1}{i\,\hbar}\,\hat{U}^\dagger \left[\hat{p}, \frac{\hat{p}^2}{2\,m} + V\right] \hat{U} \\
&= \frac{1}{i\,\hbar}\,\hat{U}^\dagger \left(\underbrace{\left[\hat{p}, \frac{\hat{p}^2}{2\,m}\right]}_{0} + [\hat{p}, V]\right) \hat{U} \\
&= \frac{1}{i\,\hbar}\,\hat{U}^\dagger \left(-i\,\hbar\,\frac{dV}{dx}\right) \hat{U} = \left(-\frac{dV}{dx}\right)_H (t)\ .
\end{aligned}$$

These have an identical structure to the classical equations of motion for the dynamic variables x and p:

$$\boxed{m\,\frac{d\hat{x}_H}{dt} = \hat{p}_H(t) \qquad \frac{d\hat{p}_H}{dt} = \left(-\frac{dV}{dx}\right)_H\ .}$$

Problem 6.30

(a) We can express $\Psi(x,0)$ as a linear combination of stationary states

$$\Psi(x,0) = \sum_n c_n\,\psi_n(x)$$

where

$$c_n = \int \psi_n^*(x)\ \Psi(x,0)\ dx\,.$$

Then we have

$$\begin{aligned}
\Psi(x,t) &= \sum_n c_n\,\psi_n(x)\ e^{-i\,E_n\,t/\hbar} \\
&= \sum_n \left[\int \psi_n^*(x')\ \Psi(x',0)\ dx'\right]\ \psi_n(x)\ e^{-i\,E_n\,t/\hbar} \\
&= \int \sum_n\ \psi_n^*(x')\ e^{-i\,E_n\,t/\hbar}\,\psi_n(x)\ \Psi(x',0)\ dx' \\
&= \int K(x,x',t)\ \Psi(x',0)\ dx'
\end{aligned}$$

which is the desired result.

(b) For the simpler harmonic oscillator, the stationary states are

$$\psi_n = A_n\,H_n(\xi)\ e^{-\xi^2/2}$$

where $\xi = \sqrt{m\,\omega/\hbar}\,x$. Then

$$K(x,x',t) = \sum_{n=0}^{\infty} A_n\,H_n(\eta)\ e^{-\eta^2/2}\ e^{-i(n+1/2)\,\omega\,t}\ A_n\,H_n(\xi)\ e^{-\xi^2/2} \qquad [\bigstar]$$

where $\eta = \sqrt{m\,\omega/\hbar}\,x$. We define $z = e^{-i\,\omega\,t}$ and recalling that $A_n = (m\,\omega/\pi\,\hbar)^{1/4}\;1/\sqrt{2^n\,n!}$ (Equation 2.86) we have

$$\begin{aligned}
K(x,x',t) &= e^{\left(\eta^2+\xi^2\right)/2}\sqrt{\frac{m\,\omega}{\pi\,\hbar}}\,\sqrt{z}\,e^{-\left(\eta^2+\xi^2\right)}\sum_{n=0}^{\infty}\frac{z^n}{2^n\,n!}H_n(\xi)\;H_n(\eta)\\
&= \sqrt{\frac{m\,\omega}{\pi\,\hbar}}\sqrt{\frac{z}{1-z^2}}\,\exp\left[\frac{\eta^2+\xi^2}{2}-\frac{\eta^2+\xi^2-2\,\eta\,\xi\,z}{1-z^2}\right]\\
&= \sqrt{\frac{m\,\omega}{\pi\,\hbar}}\sqrt{\frac{z}{1-z^2}}\,\exp\left[-\frac{1}{2}\,\frac{\left(1+z^2\right)\left(\eta^2+\xi^2\right)-4\,\eta\,\xi\,z}{1-z^2}\right].
\end{aligned}$$

Lets clean this up a little bit. We note that $z\,z^* = 1$ so

$$K(x,x',t) = \sqrt{\frac{m\,\omega}{\pi\,\hbar}}\sqrt{\frac{1}{z^*-z}}\,\exp\left[-\frac{1}{2}\,\frac{\left(z^*+z\right)\left(\eta^2+\xi^2\right)-4\,\eta\,\xi}{z^*-z}\right].$$

We then further note that $z^*-z = 2\,i\,\sin(\omega\,t)$ and $z+z^* = 2\,\cos(\omega\,t)$ and we have

$$\boxed{K(x,x',t) = \sqrt{\frac{1}{\pi}\,\frac{m\,\omega}{2\,\hbar}}\sqrt{\frac{1}{i\,\sin(\omega\,t)}}\;\exp\left[-\frac{m\,\omega}{2\,\hbar}\,\frac{\cos(\omega\,t)\left(x^2+x'^2\right)-2\,x x'}{i\,\sin(\omega\,t)}\right].}$$

(c) For the given initial state we have

$$\begin{aligned}
\Psi(x,t) &= \int_{-\infty}^{\infty}K(x,x',t)\;\Psi(x',0)\;dx'\\
&= \sqrt{\frac{1}{\pi}\,\frac{m\,\omega}{2\,\hbar}}\sqrt{\frac{1}{i\,\sin(\omega\,t)}}\int_{-\infty}^{\infty}\exp\left[-\frac{m\,\omega}{2\,\hbar}\,\frac{\cos(\omega\,t)\left(x^2+x'^2\right)-2\,x x'}{i\,\sin(\omega\,t)}\right]\left(\frac{2\,a}{\pi}\right)^{1/4}\;e^{-a\left(x'-x_0\right)^2}\;dx'\\
&= \sqrt{\frac{1}{\pi}\,\frac{m\,\omega}{2\,\hbar}}\sqrt{\frac{1}{i\,\sin(\omega\,t)}}\left(\frac{2\,a}{\pi}\right)^{1/4}\;\exp\left[-\frac{m\,\omega}{2\,\hbar}\,\frac{x^2}{i\,\tan(\omega\,t)}-a\,x_0^2\right]\\
&\quad\times\int_{-\infty}^{\infty}\exp\left[-\left(\frac{m\,\omega}{2\,\hbar}\,\frac{1}{i\,\tan(\omega\,t)}+a\right)x'^2+\left(\frac{m\,\omega}{\hbar}\,\frac{x}{i\,\sin(\omega\,t)}+2a\,x_0\right)x'\right]dx'
\end{aligned}$$

Even though the constants are complicated, this is nothing more than the Gaussian integral given in the problem statement and we have

$$\begin{aligned}
\Psi(x,t) &= \sqrt{\frac{1}{\pi}\,\frac{m\,\omega}{2\,\hbar}}\sqrt{\frac{1}{i\,\sin(\omega\,t)}}\left(\frac{2\,a}{\pi}\right)^{1/4}\;\exp\left[-\frac{m\,\omega}{2\,\hbar}\,\frac{x^2}{i\,\tan(\omega\,t)}-a\,x_0^2\right]\\
&\quad\times\sqrt{\frac{\pi}{\frac{m\,\omega}{2\,\hbar}\,\frac{1}{i\,\tan(\omega\,t)}+a}}\;\exp\left[\frac{\left(\frac{m\,\omega}{\hbar}\,\frac{x}{i\,\sin(\omega\,t)}+2a\,x_0\right)^2}{4\left(\frac{m\,\omega}{2\,\hbar}\,\frac{1}{i\,\tan(\omega\,t)}+a\right)}\right].
\end{aligned}$$

This simplifies to

$$\boxed{\Psi(x,t) = \left(\frac{2\,a}{\pi}\right)^{1/4}\;\frac{\exp\left[-a\,\frac{\left(x^2+x_0^2\right)\,\cos(\omega\,t)-2\,x\,x_0+\frac{i\,m\,\omega}{2\,\hbar\,a}\,\sin(\omega\,t)\,x^2}{\cos(\omega\,t)+\frac{2\,i\,a\,\hbar}{m\,\omega}\,\sin(\omega\,t)}\right]}{\sqrt{\cos(\omega\,t)+\frac{2\,i\,a\,\hbar}{m\,\omega}\,\sin(\omega\,t)}}.}$$

Now, Problem 2.49 is a special case of this equation. Plugging in $t = 0$ we see

$$\Psi(x,0) = \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{1/4} \exp\left[-\frac{m\,\omega}{2\,\hbar}\,(x-x_0)^2\right]$$

so that this corresponds to choosing $a = m\,\omega/2\,\hbar$. If we plug $a = m\,\omega/2\,\hbar$ into our general solution we get

$$\begin{aligned}
\Psi(x,t) &= \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{1/4} \frac{\exp\left[-\frac{m\,\omega}{2\,\hbar}\,\frac{\left(x^2+x_0^2\right)\,\cos(\omega\,t)-2\,x\,x_0+i\,\sin(\omega\,t)\,x^2}{e^{i\,\omega\,t}}\right]}{\sqrt{e^{i\,\omega\,t}}} \\
&= \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{1/4} \exp\left[-\frac{m\,\omega}{2\,\hbar}\,\left[\left(x^2+x_0^2\right)\left(1+e^{-2\,i\,\omega\,t}\right)/2 - 2\,x\,x_0\,e^{-i\,\omega\,t}\right.\right. \\
&\quad \left.\left. +\left(1-e^{-2\,i\,\omega\,t}\right)\,x^2/2\right] + \frac{i\,\omega\,t}{2}\right] \\
&= \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{1/4} \exp\left[-\frac{m\,\omega}{2\,\hbar}\left(x^2 + \frac{x_0^2}{2}\left(1+e^{-2\,i\,\omega\,t}\right) + \frac{i\,\hbar\,t}{m} - 2\,e^{-i\,\omega\,t}\,x\,x_0\right)\right]\,,
\end{aligned}$$

exactly as in Problem 2.49.

(d) For the free particle

$$\begin{aligned}
K(x,x',t) &= \int_{-\infty}^{\infty} f_p(x')^*\; e^{-i\,E_p\,t/\hbar}\, f_p(x)\; dp \\
&= \int_{-\infty}^{\infty} \frac{e^{-i\,p\,x'/\hbar}}{\sqrt{2\,\pi\,\hbar}}\; e^{-i\,p^2\,t/(2\,m\,\hbar)}\; \frac{e^{i\,p\,x/\hbar}}{\sqrt{2\,\pi\,\hbar}}\, dp \\
&= \frac{1}{2\,\pi\,\hbar}\int_{-\infty}^{\infty} \exp\left[-i\,\frac{p^2\,t}{2\,m\,\hbar} + i\,\frac{p}{\hbar}\,(x-x')\right]\, dp \\
&= \frac{1}{2\,\pi\,\hbar}\sqrt{\frac{\pi}{i\,t/2\,m\,\hbar}}\,\exp\left[-\frac{(x-x')^2\,/\hbar^2}{2\,i\,t/(m\,\hbar)}\right]
\end{aligned}$$

where we have used the general expression given for the Gaussian integral. So, for the free particle

$$\boxed{K(x,x',t) = \sqrt{\frac{m}{2\,\pi\,i\,\hbar\,t}}\,\exp\left[\frac{i\,m}{2\,\hbar\,t}\,(x-x')^2\right]\,.}$$

(e) For this initial state,

$$\begin{aligned}
\Psi(x,t) &= \int_{-\infty}^{\infty} K(x,x',t)\;\Psi(x',0)\; dx' \\
&= \int_{-\infty}^{\infty} \sqrt{\frac{m}{2\,\pi\,i\,\hbar\,t}}\,\exp\left[\frac{i\,m}{2\,\hbar\,t}\,(x-x')^2\right]\left(\frac{2\,a}{\pi}\right)^{1/4} e^{-a\,x'^2}\; dx' \\
&= \sqrt{\frac{m}{2\,\pi\,i\,\hbar\,t}}\left(\frac{2\,a}{\pi}\right)^{1/4}\exp\left[\frac{i\,m}{2\,\hbar\,t}\,x^2\right]\int_{-\infty}^{\infty}\exp\left[-\left(a-\frac{i\,m}{2\,\hbar\,t}\right)\,x'^2 - \frac{i\,m}{\hbar\,t}\,x\,x'\right]\, dx' \\
&= \sqrt{\frac{m}{2\,\pi\,i\,\hbar\,t}}\left(\frac{2\,a}{\pi}\right)^{1/4}\exp\left[\frac{i\,m}{2\,\hbar\,t}\,x^2\right]\sqrt{\frac{\pi}{a-i\,m/(2\,\hbar\,t)}}\,\exp\left[-\frac{(m\,x/\hbar\,t)^2}{4\,(a-i\,m/(2\,\hbar\,t))}\right]
\end{aligned}$$

where we have again used the general expression for the Gaussian integral. This simplifies to

$$\boxed{\Psi(x,t) = \left(\frac{2\,a}{\pi}\right)^{1/4} \sqrt{\frac{1}{1+i\,2\,a\,\hbar\,t/m}}\ \exp\left[-\frac{a}{1+i\,2\,a\,\hbar\,t/m}\,x^2\right]\,,}$$

exactly as found in Problem 2.21.

Problem 6.31

First we need to compute $\Phi(p)$.

$$\begin{aligned}
\Phi(p) &= \frac{1}{\sqrt{2\,\pi\,\hbar}} \int_{-\infty}^{\infty} e^{-i\,p\,x/\hbar}\,\psi(x)\ dx \\
&= \sqrt{\frac{\lambda}{2\,\pi\,\hbar}} \int_{-\infty}^{\infty} e^{-\lambda\,|x|-i\,p\,x/\hbar}\,dx \\
&= \sqrt{\frac{\lambda}{2\,\pi\,\hbar}} \left[\int_{-\infty}^{0} e^{(\lambda-i\,p/\hbar)\,x}\,dx + \int_{0}^{\infty} e^{-(\lambda+i\,p/\hbar)\,x}\,dx\right] \\
&= \sqrt{\frac{\lambda}{2\,\pi\,\hbar}} \left[\frac{1}{\lambda-i\,p/\hbar} + \frac{1}{\lambda+i\,p/\hbar}\right] \\
&= \sqrt{\frac{2\,\lambda}{\pi\,\hbar}}\,\frac{\lambda}{(p/\hbar)^2+\lambda^2}
\end{aligned}$$

Then we may use Equation 6.81 to compute $\hat{T}(a)\ \psi(x)$.

$$\hat{T}(a)\ \psi(x) = \int_{-\infty}^{\infty} e^{-i\,p\,a/\hbar}\,\frac{e^{i\,p\,x/\hbar}}{\sqrt{2\,\pi\,\hbar}}\,\sqrt{\frac{2\,\lambda}{\pi\,\hbar}}\,\frac{\lambda}{(p/\hbar)^2+\lambda^2}\,dp\,.$$

Let $p = q\,\lambda\,\hbar$ so that

$$\begin{aligned}
\hat{T}(a)\ \psi(x) &= \frac{\sqrt{\lambda}}{\pi} \int_{-\infty}^{\infty} \frac{e^{i\,q\,\lambda(x-a)}}{q^2+1}\,dq = \frac{2\,\sqrt{\lambda^3}}{\pi} \int_{0}^{\infty} \frac{\cos\left[q\,\lambda\,(x-a)\right]}{q^2+1}\,dq \\
&= \frac{2\,\sqrt{\lambda}}{\pi} \int_{0}^{\infty} \frac{\cos(q\,\lambda\,|x-a|)}{q^2+1}\,dq\,.
\end{aligned}$$

The remaining integral can be looked up in any standard table (or computed by contour integration if you're familiar with the technique) and

$$\hat{T}(a)\ \psi(x) = \sqrt{\lambda}\,e^{-\lambda\,|x-a|}\,,$$

exactly as required.

Problem 6.32

(a) We have

$$
\begin{aligned}
(\mathbf{a}\cdot\boldsymbol{\sigma})\,(\mathbf{b}\cdot\boldsymbol{\sigma}) &= \sum_j a_j\,\sigma_j \sum_k b_k\,\sigma_k \\
&= \sum_j \sum_k a_j\,b_k \left(\delta_{jk} + i\sum_n \epsilon_{jkn}\,\sigma_n\right) \\
&= \sum_j a_j\,b_j + i\,\sum_n \sum_j \sum_k \epsilon_{jkn} a_j\,b_k\,\sigma_n \\
&= \mathbf{a}\cdot\mathbf{b} + i\,\sum_n \left[\mathbf{a}\times\mathbf{b}\right]_n\,\sigma_n \\
&= \mathbf{a}\cdot\mathbf{b} + i\,(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}
\end{aligned}
$$

where the critical identity in the second line comes from Problem 4.29.

(b) First note that from part (a), for a unit vector $\mathbf{n}$,

$$
(\mathbf{n}\cdot\boldsymbol{\sigma})^2 = \mathbf{n}\cdot\mathbf{n} + i\,(\mathbf{n}\times\mathbf{n})\cdot\boldsymbol{\sigma} = 1
$$

and therefore

$$
(\mathbf{n}\cdot\boldsymbol{\sigma})^2 = \begin{cases} \mathbf{n}\cdot\boldsymbol{\sigma} & n \text{ odd} \\ 1 & n \text{ even} \end{cases}
$$

We can then write

$$
\begin{aligned}
\exp\left[-i\,\frac{\varphi}{\hbar}\mathbf{n}\cdot\mathsf{S}\right] &= \exp\left[i\,\frac{\varphi}{2}\,\mathbf{n}\cdot\sigma\right] \\
&= \sum_{k=0}^{\infty} \frac{1}{n!}\left(-\frac{i\,\varphi}{2}\right)^k (\mathbf{n}\cdot\sigma)^k \\
&= \sum_{k\,\text{even}} \frac{1}{k!}\left(-\frac{i\,\varphi}{2}\right)^k + \sum_{k\,\text{odd}} \frac{1}{k!}\left(-\frac{i\,\varphi}{2}\right)^k \mathbf{n}\cdot\boldsymbol{\sigma} \\
&= \sum_{k\,\text{even}} \frac{(-1)^{k/2}}{k!}\left(\frac{\varphi}{2}\right)^k - i\sum_{k\,\text{odd}} \frac{(-1)^{(k-1)/2}}{k!}\left(\frac{\varphi}{2}\right)^k \mathbf{n}\cdot\boldsymbol{\sigma} \\
&= \cos\!\left(\frac{\varphi}{2}\right) - i\,\sin\!\left(\frac{\varphi}{2}\right)\,\mathbf{n}\cdot\boldsymbol{\sigma}\,.
\end{aligned}
$$

I've kept everything as sums but it would also be fine to just write out the first half-dozen or so terms in the series.

(c) In polar coordinates

$$
\mathbf{n} = \sin\theta\,\cos\phi\,\hat{\imath} + \sin\theta\,\sin\phi\,\hat{\jmath} + \cos\theta\,\hat{k}
$$

and

$$
\begin{aligned}
\mathsf{R}_n &= \cos\left(\frac{\varphi}{2}\right) - i\,\sin\left(\frac{\varphi}{2}\right)\,[n_x\,\sigma_x + n_y\,\sigma_y + n_z\,\sigma_z] \\
&= \cos\left(\frac{\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\,\sin\left(\frac{\varphi}{2}\right)\left[\sin\theta\,\cos\phi\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right. \\
&\quad \left. + \sin\theta\,\sin\phi\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \cos\theta\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \\
&= \cos\left(\frac{\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\,\sin\left(\frac{\varphi}{2}\right)\begin{pmatrix} \cos\theta & \sin\theta\,e^{-i\,\phi} \\ \sin\theta\,e^{i\,\phi} & -\cos\theta \end{pmatrix} .
\end{aligned}
$$

(d) The Hermitian conjugate of R_n is

$$
\begin{aligned}
\mathsf{R}_n^\dagger &= \cos\left(\frac{\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i\,\sin\left(\frac{\varphi}{2}\right)\begin{pmatrix} \cos\theta & \sin\theta\,e^{i\,\phi} \\ \sin\theta\,e^{-i\,\phi} & -\cos\theta \end{pmatrix}^T \\
&= \cos\left(\frac{\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i\,\sin\left(\frac{\varphi}{2}\right)\begin{pmatrix} \cos\theta & \sin\theta\,e^{-i\,\phi} \\ \sin\theta\,e^{i\,\phi} & -\cos\theta \end{pmatrix}
\end{aligned}
$$

which is clearly a rotation by $-\varphi/2$ about the same axis, so it must be the inverse of R_n. However, lets check it explicitly as well:

$$
\begin{aligned}
\mathsf{R}_n\,\mathsf{R}_n^\dagger &= \cos\left(\frac{\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\,\cos\left(\frac{\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&\quad + i\cos\left(\frac{\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\,\sin\left(\frac{\varphi}{2}\right)\begin{pmatrix} \cos\theta & \sin\theta\,e^{-i\,\phi} \\ \sin\theta\,e^{i\,\phi} & -\cos\theta \end{pmatrix} \\
&\quad - i\sin\left(\frac{\varphi}{2}\right)\begin{pmatrix} \cos\theta & \sin\theta\,e^{-i\,\phi} \\ \sin\theta\,e^{i\,\phi} & -\cos\theta \end{pmatrix}\,\cos\left(\frac{\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&\quad + \sin\left(\frac{\varphi}{2}\right)\begin{pmatrix} \cos\theta & \sin\theta\,e^{-i\,\phi} \\ \sin\theta\,e^{i\,\phi} & -\cos\theta \end{pmatrix} \\
&\quad \times \sin\left(\frac{\varphi}{2}\right)\begin{pmatrix} \cos\theta & \sin\theta\,e^{-i\,\phi} \\ \sin\theta\,e^{i\,\phi} & -\cos\theta \end{pmatrix} \\
&= \cos^2\left(\frac{\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&\quad + \sin^2\left(\frac{\varphi}{2}\right)\begin{pmatrix} \cos^2\theta + \sin^2\theta & 0 \\ 0 & \sin^2\theta + \cos^2\theta \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .
\end{aligned}
$$

(e) For a rotation about the z axis, $\theta = 0$ and

$$
\begin{aligned}
\mathsf{R} &= \begin{pmatrix} \cos(\varphi/2) - i\,\sin(\varphi/2) & 0 \\ 0 & \cos(\varphi/2) + i\,\sin(\varphi/2) \end{pmatrix} \\
&= \begin{pmatrix} e^{-i\,\varphi/2} & 0 \\ 0 & e^{i\,\varphi/2} \end{pmatrix} .
\end{aligned}
$$

Then

$$
\begin{aligned}
\mathsf{S}'_x &= \mathsf{R}^\dagger\, \mathsf{S}_x\, \mathsf{R} \\
&= \begin{pmatrix} e^{i\,\varphi/2} & 0 \\ 0 & e^{-i\,\varphi/2} \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-i\,\varphi/2} & 0 \\ 0 & e^{i\,\varphi/2} \end{pmatrix} \\
&= \frac{\hbar}{2} \begin{pmatrix} 0 & e^{i\,\varphi} \\ e^{-i\,\varphi} & 0 \end{pmatrix} .
\end{aligned}
$$

This can then be written as

$$
\begin{aligned}
\mathsf{S}'_x &= \frac{\hbar}{2} \left[\cos\varphi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \sin\varphi \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right] \\
&= \mathsf{S}_x \, \cos\varphi - \mathsf{S}_y \, \sin\varphi
\end{aligned}
$$

which is precisely what we expect for the rotation of a vector (Equation 6.31).

(f) For a π rotation about the x axis, $\theta = \pi/2$, $\phi = 0$, and $\varphi = \pi$ so that

$$
\mathsf{R} = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} .
$$

and

$$
\mathsf{R} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -i \begin{pmatrix} 0 \\ 1 \end{pmatrix}
$$

which transforms an up spin into a down spin, albeit with a different phase factor.

(g) For a rotation of $2\,\pi$ about any axis, $\varphi = 2\,\pi$ and $\sin(\varphi/2) = 0$ so that

$$
\mathsf{R}(2\,\pi) = -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .
$$

This is surprising because it is *not* simply the identity matrix!

Problem 6.33

(a) In polar coordinates $x = r\,\cos\phi$ and $y = r\,\sin\phi$ the states are

$$
\psi_{ab}(r,\phi) = \frac{2}{L}\, \sin\left[\frac{a\,\pi}{L}\left(r\,\cos\phi - \frac{L}{2}\right)\right] \, \sin\left[\frac{b\,\pi}{L}\left(r\,\sin\phi - \frac{L}{2}\right)\right] .
$$

Rotating the state counter-clockwise produces

$$\begin{aligned}
\hat{R}\,\psi_{ab}(r,\phi) &= \psi_{ab}(r,\phi-\pi/2)\\
&= \frac{2}{L}\,\sin\left\{\frac{a\,\pi}{L}\left[r\,\cos\Big(\phi-\frac{\pi}{2}\Big)-\frac{L}{2}\right]\right\}\,\sin\left\{\frac{b\,\pi}{L}\left[r\,\sin\Big(\phi-\frac{\pi}{2}\Big)-\frac{L}{2}\right]\right\}\\
&= \frac{2}{L}\,\sin\left[\frac{a\,\pi}{L}\left(r\,\sin\phi-\frac{L}{2}\right)\right]\,\sin\left[\frac{b\,\pi}{L}\left(-r\cos\phi-\frac{L}{2}\right)\right]\\
&= \frac{2}{L}\,\sin\left[\frac{a\,\pi}{L}\left(y-\frac{L}{2}\right)\right]\,\sin\left[-\frac{b\,\pi}{L}\left(x-\frac{L}{2}+L\right)\right]\\
&= -\frac{2}{L}\,\sin\left[\frac{b\,\pi}{L}\left(x-\frac{L}{2}\right)+b\,\pi\right]\,\sin\left[\frac{a\,\pi}{L}\left(y-\frac{L}{2}\right)\right]\\
&= (-1)^{b+1}\,\frac{2}{L}\,\sin\left[\frac{b\,\pi}{L}\left(x-\frac{L}{2}\right)\right]\,\sin\left[\frac{a\,\pi}{L}\left(y-\frac{L}{2}\right)\right]
\end{aligned}$$

so that

$$\boxed{\hat{R}\,\psi_{ab} = (-1)^{b+1}\,\psi_{ba}\,.}$$

(b) Using the result from part (a),

$$\begin{aligned}
\hat{R}\,\psi_{\pm} &= \frac{1}{\sqrt{2}}\,\left[\hat{R}\,\psi_{ab}\pm\hat{R}\,\psi_{ba}\right]\\
&= \frac{1}{\sqrt{2}}\,\left[(-1)^{b+1}\,\psi_{ba}\pm(-1)^{a+1}\,\psi_{ab}\right]\\
&= \pm(-1)^{a+1}\,\frac{1}{\sqrt{2}}\,\left[\psi_{ab}\pm(-1)^{a+b}\,\psi_{ba}\right]\,.
\end{aligned}$$

Now if a and b are both even or both odd then $(-1)^{a+b}=1$ and $\psi_{\pm}$ is an eigenstate of $\hat{R}$ with eigenvalue $\mp(-1)^{a}$.

(c) Plot is shown below. All of the listed symmetries are clearly present.

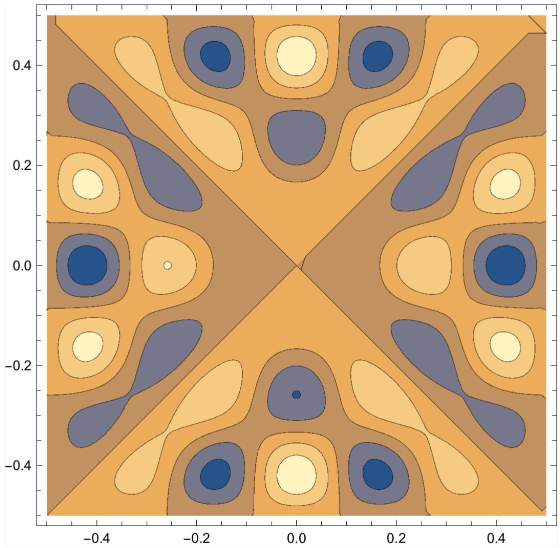
```
In[∘]:= ψ[a_, b_, x_, y_] := 2/L Sin[a π/L (x - L/2)] Sin[b π/L (y - L/2)]

In[∘]:= ψM[x_, y_] := (ψ[5, 7, x, y] - ψ[7, 5, x, y])/√2

In[∘]:= L = 1;

In[∘]:= ContourPlot[ψM[x, y], {x, -1/2, 1/2}, {y, -1/2, 1/2}]
```

Out[∘]=



Problem 6.34

(a) We first write

$$
\begin{aligned}
\mathbf{M}\cdot\mathbf{L} &= M_x\,L_x + M_y\,L_y + M_z\,L_z \\
&= \frac{M_+ + M_-}{2}\,\frac{L_+ + L_-}{2} + \frac{M_+ - M_-}{2\,i}\,\frac{L_+ - L_-}{2\,i} + M_z\,L_z \\
&= \frac{M_+\,L_- + M_-\,L_+}{2} + M_z\,L_z\,.
\end{aligned}
$$

Now we apply this to $\psi_{n\ell\ell}$ to get

$$
\begin{aligned}
\frac{1}{2}\,M_+\,L_-\,\psi_{n\ell\ell} + \frac{1}{2}\,M_-\,L_+\,\psi_{n\ell\ell} + M_z\,L_z\,\psi_{n\ell\ell} &= 0 \\
\frac{1}{2}\left(L_-\,M_+ + [M_+, L_-]\right)\,\psi_{n\ell\ell} + 0 + \ell\,\hbar\,M_z\,\psi_{n\ell\ell} &= 0 \\
\frac{1}{2}\,L_-\,c_{n\ell}\,\psi_{n\ell+1\ell+1} + \frac{1}{2}\,[M_+, L_-]\,\psi_{n\ell\ell} + \ell\,\hbar\,M_z\,\psi_{n\ell\ell} &= 0\,.
\end{aligned}
$$

The commutator (remember **M** is a vector operator) is given in Equation 6.54.

$$\frac{1}{2}\, B^{\ell}_{\ell+1}\, c_{n\ell}\, \psi_{n\ell+1\ell} + \hbar\, M_z\, \psi_{n\ell\ell} + \ell\, \hbar\, M_z\, \psi_{n\ell\ell} = 0$$

$$\sqrt{\frac{\ell+1}{2}}\, \hbar\, c_{n\ell}\, \psi_{n\ell\ell-1} = -(\ell+1)\ \hbar\, M_z\, \psi_{n\ell\ell}$$

so that

$$\boxed{\hat{M}_z\, \psi_{n\ell\ell} = -\frac{1}{\sqrt{2\,(\ell+1)}}\, c_{n\ell}\, \psi_{n\ell+1\ell}\,.}$$

(b) Note that, just as for $\mathbf{M}\cdot\mathbf{L}$ in part (a),

$$\mathbf{M}\cdot\mathbf{M} = \frac{M_+\, M_- + M_-\, M_+}{2} + M_z^2\,.$$

Then from vi,

$$M^2\, \psi_{n\,\ell\,\ell} = \left[\left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2 + \frac{2}{m}\, \hat{H}\, \left(L^2 + \hbar^2\right)\right]\, \psi_{n\,\ell\,\ell}$$

$$\frac{1}{2}\, M_+\, M_-\, \psi_{n\ell\ell} + \frac{1}{2}\, M_-\, M_+\, \psi_{n\ell\ell} + M_z^2\, \psi_{n\,\ell\,\ell} = \left\{\left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2 + \frac{2}{m}\, E_n\, \left[\ell\,(\ell+1)+1\right]\, \hbar^2\right\}\, \psi_{n\ell\ell}$$

$$\frac{1}{2}\, \left[M_+, M_-\right]\, \psi_{n\ell\ell} + M_-\, M_+\, \psi_{n\ell\ell} + M_z^2\, \psi_{n\,\ell\,\ell} = \left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2\, \left[1 - \frac{\ell^2+\ell+1}{n^2}\right]\, \psi_{n\ell\ell}\,.$$

We can work out the commutator from v,

$$\begin{aligned}\left[M_+, M_-\right] &= \left[M_x, M_x\right] + i\, \left[M_y, M_x\right] - i\, \left[M_x, M_y\right] - \left[M_y, M_y\right] \\ &= -2\, i\, \left[M_x, M_y\right] = -2\, \hbar\, L_z\, \frac{2}{m}\, \hat{H}\,.\end{aligned}$$

Therefore we have

$$-\hbar\, L_z\, \frac{2}{m}\, \hat{H}\, \psi_{n\ell\ell} + M_-\, M_+\, \psi_{n\ell\ell} + M_z^2\, \psi_{n\,\ell\,\ell} = \left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2\, \left[1 - \frac{\ell^2+\ell+1}{n^2}\right]\, \psi_{n\ell\ell}$$

$$-\hbar\, \ell\, \hbar\, \frac{2}{m}\, E_n\, \psi_{n\ell\ell} + M_-\, M_+\, \psi_{n\ell\ell} + M_z^2\, \psi_{n\,\ell\,\ell} = \left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2\, \left[1 - \frac{\ell^2+\ell+1}{n^2}\right]\, \psi_{n\ell\ell}$$

so that

$$\boxed{\hat{M}_-\, \hat{M}_+\, \psi_{n\ell\ell} = \left\{\left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2\, \left[1 - \left(\frac{\ell+1}{n}\right)^2\right] - \hat{M}_z^2\right\}\, \psi_{n\ell\ell}\,.}$$

(c) Finally we note that

$$\begin{aligned}|c_{n\ell}|^2 &= \int \left(M_+\, \psi_{n\ell\ell}\right)^*\, \left(M_+\, \psi_{n\ell\ell}\right)\, d^3\mathbf{r} \\ &= \int \psi^*_{n\ell\ell}\, M_-\, M_+\, \psi_{n\ell\ell}\, d^3\mathbf{r}\,.\end{aligned}$$

From part (b) this is

$$
\begin{aligned}
|c_{n\ell}|^2 &= \left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2 \left[1-\left(\frac{\ell+1}{n}\right)^2\right] - \int \psi^*_{n\ell\ell}\, M_z^2\, \psi_{n\ell\ell}\, d^3\mathbf{r} \\
&= \left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2 \left[1-\left(\frac{\ell+1}{n}\right)^2\right] - \int \left(M_z\, \psi_{n\ell\ell}\right)^*\; M_z\, \psi_{n\ell\ell}\, d^3\mathbf{r}
\end{aligned}
$$

and from part (a) this is

$$
|c_{n\ell}|^2 = \left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2 \left[1-\left(\frac{\ell+1}{n}\right)^2\right] - \frac{1}{2\,(\ell+1)}\; |c_{n\ell}|^2\; \underbrace{\int \psi^*_{n\ell+1\ell}\, \psi_{n\ell+1\ell}\, d^3\mathbf{r}}_{1}\;.
$$

Finally, solving for $c_{n\ell}$ gives

$$
\boxed{|c_{n\ell}|^2 = \frac{2\,\ell+3}{2\,\ell+2}\,\left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2 \left[1-\left(\frac{\ell+1}{n}\right)^2\right]\;.}
$$

As we see, this nonzero except when $\ell = n-1$.

Problem 6.35

(a) For an infinitesimal velocity δ

$$
\begin{aligned}
\hat{x}' &\approx \hat{\Gamma}^\dagger\, \hat{x}\, \hat{\Gamma} \\
&\approx \left(1+\frac{i}{\hbar}\,\delta\,(t\,\hat{p}-m\,\hat{x})\right)\, \hat{x}\, \left(1-\frac{i}{\hbar}\,\delta\,(t\,\hat{p}-m\,\hat{x})\right) \\
&\approx \hat{x} + \frac{i}{\hbar}\,\delta\,t\;[\hat{p},\hat{x}] - \frac{i}{\hbar}\,\delta\,m\;[\hat{x},\hat{x}] \\
&\approx \hat{x} - \delta\,t
\end{aligned}
$$

and

$$
\begin{aligned}
\hat{p}' &\approx \left(1+\frac{i}{\hbar}\,\delta\,(t\,\hat{p}-m\,\hat{x})\right)\, \hat{p}\, \left(1-\frac{i}{\hbar}\,\delta\,(t\,\hat{p}-m\,\hat{x})\right) \\
&\approx \hat{x} + \frac{i}{\hbar}\,\delta\,t\;[\hat{p},\hat{p}] - \frac{i}{\hbar}\,\delta\,m\;[\hat{x},\hat{p}] \\
&\approx \hat{p} + m\,\delta\,.
\end{aligned}
$$

The first equation just says that the origins of the two coordinate systems are displaced by an amount δt at time t and the second equation is simply Galilean velocity addition: in the primed frame, the velocity of the particle is greater by δ.

(b) Let the operators be

$$
\hat{A} = \frac{-i\,v\,t}{\hbar}\,\hat{p} \qquad \hat{B} = \frac{i\,m\,v}{\hbar}\,\hat{x}
$$

so that

$$\hat{C} = \left[\hat{A}, \hat{B}\right] = \frac{m\,v^2\,t}{\hbar}\,[\hat{p}, \hat{x}] = -i\,m\,v^2\,t\,.$$

Then, according the the Baker-Campbell-Hausdorff formula,

$$\begin{aligned}\hat{\Gamma} &= e^{\hat{A}+\hat{B}} = e^{\hat{A}}\,e^{\hat{B}}\,e^{-\hat{C}/2} \\ &= \exp\left[-\frac{i}{\hbar}\,v\,t\,\hat{p}\right]\,\exp\left[\frac{i}{\hbar}\,m\,v\,\hat{x}\right]\,\exp\left[\frac{i}{\hbar}\,\frac{m\,v^2}{2}\,t\right]\,.\end{aligned}$$

The first exponential is simply the translation operator and

$$\boxed{\hat{\Gamma} = \hat{T}(v\,t)\,\exp\left[\frac{i}{\hbar}\left(m\,v\,\hat{x} + \frac{m\,v^2}{2}\,t\right)\right]\,.}$$

Now if we simply switch the roles of $\hat{A}$ and $\hat{B}$, that will change the sign of $\hat{C}$ and again applying the Baker-Campbell-Hausdorff gives

$$\hat{\Gamma} = \exp\left[\frac{i}{\hbar}\,m\,v\,\hat{x}\right]\,\exp\left[-\frac{i}{\hbar}\,v\,t\,\hat{p}\right]\,\exp\left[-\frac{i}{\hbar}\,\frac{m\,v^2}{2}\,t\right]$$

or

$$\boxed{\hat{\Gamma} = \exp\left[\frac{i}{\hbar}\left(m\,v\,\hat{x} - \frac{m\,v^2}{2}\,t\right)\right]\,\hat{T}(v\,t)\,.}$$

(c) Consider $\hat{\Psi}' = \Gamma\,\Psi$. We have

$$i\,\hbar\,\frac{\partial}{\partial t}\left(\hat{\Gamma}\,\Psi\right) = i\,\hbar\,\frac{d\Gamma}{dt}\,\Psi + i\,\hbar\,\Gamma\,\frac{\partial\Psi}{\partial t}$$

and by the assumption that Ψ satisfies the time-dependent Schrödinger equation with hamiltonian H we have

$$\begin{aligned}i\,\hbar\,\frac{\partial}{\partial t}\left(\hat{\Gamma}\,\Psi\right) &= i\,\hbar\,\frac{d\Gamma}{dt}\,\Psi + \Gamma\,\hat{H}\,\Psi \\ &= \left[i\,\hbar\,\frac{d\Gamma}{dt}\,\Gamma^\dagger + \Gamma\,\hat{H}\,\hat{\Gamma}^\dagger\right]\,\hat{\Gamma}\,\Psi\,.\end{aligned}$$

Therefore Ψ' satisfies the Schrödinger equation with Hamiltonian

$$\begin{aligned}\hat{H}_\gamma =& \hat{\Gamma}\,\hat{H}\,\hat{\Gamma}^\dagger + i\,\hbar\,\frac{d\hat{\Gamma}}{dt}\,\hat{\Gamma} \\ &= \exp\left[\frac{i}{\hbar}\left(m\,v\,\hat{x} - \frac{m\,v^2}{2}\,t\right)\right]\,\hat{T}(v\,t)\,\hat{H}\,\hat{T}^\dagger(v\,t) \\ &\quad\times\exp\left[-\frac{i}{\hbar}\left(m\,v\,\hat{x} - \frac{m\,v^2}{2}\,t\right)\right] + i\,\hbar\,\frac{d\hat{\Gamma}}{dt}\,\hat{\Gamma}^\dagger \\ &= \exp\left[\frac{i}{\hbar}\,m\,v\,\hat{x}\right]\left(\frac{\hat{p}^2}{2\,m} + V(x - v\,t)\right)\,\exp\left[-\frac{i}{\hbar}\,m\,v\,\hat{x}\right] + i\,\hbar\,\frac{d\hat{\Gamma}}{dt}\,\hat{\Gamma}^\dagger\,.\end{aligned}$$

First we compute

$$\begin{aligned}
\frac{d\hat{\Gamma}}{dt} &= \left(\frac{d}{dt}\,\hat{T}(v\,t)\right)\,\exp\left[\frac{i}{\hbar}\left(m\,v\,\hat{x} + \frac{m\,v^2}{2}\,t\right)\right] \\
&\quad + \hat{T}(v\,t)\,\frac{d}{dt}\,\exp\left[\frac{i}{\hbar}\left(m\,v\,\hat{x} + \frac{m\,v^2}{2}\,t\right)\right] \\
&= -\,\frac{i}{\hbar}\,v\,\hat{p}\,\hat{T}(v\,t)\,\exp\left[\frac{i}{\hbar}\left(m\,v\,\hat{x} + \frac{m\,v^2}{2}\,t\right)\right] \\
&\quad + \hat{T}(v\,t)\,\frac{i}{\hbar}\left(\frac{m\,v^2}{2}\right)\,\exp\left[\frac{i}{\hbar}\left(m\,v\,\hat{x} + \frac{m\,v^2}{2}\,t\right)\right] \\
&= -\,\frac{i}{\hbar}\left(v\,\hat{p} - \frac{m\,v^2}{2}\right)\,\hat{\Gamma}
\end{aligned}$$

and therefore

$$i\,\hbar\,\frac{\partial\hat{\Gamma}}{\partial t}\,\hat{\Gamma}^\dagger = v\,\hat{p} - \frac{m\,v^2}{2}\,.$$

Finally we need to compute

$$\begin{aligned}
&e^{i\,m\,v\,\hat{x}/\hbar}\left(\frac{\hat{p}^2}{2\,m} + V(x - v\,t)\right)\,e^{-i\,m\,v\,\hat{x}/\hbar} \\
&= \frac{1}{2\,m}\,e^{i\,m\,v\,\hat{x}/\hbar}\,p^2\,e^{-i\,m\,v\,\hat{x}/\hbar} + V(x - v\,t) \\
&= \frac{1}{2\,m}\,e^{i\,m\,v\,\hat{x}/\hbar}\,p\,e^{-i\,m\,v\,\hat{x}/\hbar}\,e^{i\,m\,v\,\hat{x}/\hbar}\,p\,e^{-i\,m\,v\,\hat{x}/\hbar} + V(x - v\,t)
\end{aligned}$$

where

$$\begin{aligned}
\left[e^{i\,m\,v\,\hat{x}/\hbar}, \hat{p}\right] &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\,m\,v}{\hbar}\right)^n\,[\hat{x}^n, \hat{p}] \\
&= \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{i\,m\,v}{\hbar}\right)^n\,i\,\hbar\,n\,\hat{x}^{n-1} \\
&= -m\,v\,\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(\frac{i\,m\,v}{\hbar}\,\hat{x}\right)^{n-1} \\
&= -m\,v\,e^{i\,m\,v\,x/\hbar}\,.
\end{aligned}$$

That means that

$$e^{i\,m\,v\,\hat{x}/\hbar}\,\hat{p}\,e^{-i\,m\,v\,\hat{x}/\hbar} = \hat{p} - m\,v$$

and putting all of this together we get

$$\begin{aligned}
\hat{H}_\gamma &= \frac{1}{2\,m}\,(\hat{p} - m\,v)^2 + V(x - v\,t) + v\,\hat{p} - \frac{m\,v^2}{2} \\
&= \frac{1}{2\,m}\,\hat{p}^2 + V(x - v\,t)\,\,.
\end{aligned}$$

(d) Finally, we want to compare to Problem 2.50. In that case, the solution in the frame with the stationary potential is

$$\Psi(x,t) = \psi_0(x)\,\,e^{-i\,E\,t/\hbar}$$

where E is the bound-state energy and the solution in the frame with the moving potential is

$$\begin{aligned}
\Psi'(x,t) &= \hat{\Gamma}\,\Psi \\
&= \exp\left[\frac{i}{\hbar}\left(m\,v\,\hat{x} - \frac{m\,v^2}{2}\,t\right)\right]\,\hat{T}(v\,t)\,\frac{\sqrt{m\,\alpha}}{\hbar}\,e^{-m\,\alpha\,|x|^2/\hbar^2}\,e^{-i\,E\,t/\hbar} \\
&= \exp\left[\frac{i}{\hbar}\left(m\,v\,\hat{x} - \frac{m\,v^2}{2}\,t\right)\right]\,\frac{\sqrt{m\,\alpha}}{\hbar}\,e^{-m\,\alpha\,|x-v\,t|^2/\hbar^2}\,e^{-i\,E\,t/\hbar} \\
&= \frac{\sqrt{m\,\alpha}}{\hbar}\,e^{-m\,\alpha\,|x-v\,t|^2/\hbar^2}\,e^{-i\left[\left(E+m\,v^2/2\right)\,t-m\,v\,x\right]/\hbar}
\end{aligned}$$

as shown in Problem 2.50.

Problem 6.36

(a) On a test function $f(x)$,

$$\hat{x}'\,f = \hat{\Theta}^{-1}\,\hat{x}\,\hat{\Theta}\,f(x) = \hat{\Theta}^{-1}\,\hat{x}\,f^*(x) = \hat{\Theta}^{-1}\,x\,f^*(x) = x\,f(x)\ ,$$

since x is a real number. And

$$\begin{aligned}
\hat{p}'\,f &= \hat{\Theta}^{-1}\,\hat{p}\,\hat{\Theta}\,f(x) = \hat{\Theta}^{-1}\,\hat{p}\,f^*(x) = \hat{\Theta}^{-1}\left(-i\,\hbar\,\frac{d}{dx}\right)\,f^*(x) \\
&= i\,\hbar\,\frac{d}{dx}\,f(x) = -\hat{p}\,f(x)\ .
\end{aligned}$$

(b) We have

$$\begin{aligned}
\hat{U}(\delta)\;\hat{\Theta}\,\hat{U}(\delta) &= \hat{\Theta} \\
\left(1 - i\,\frac{\delta}{\hbar}\,\hat{H}\right)\;\hat{\Theta}\,\left(1 - i\,\frac{\delta}{\hbar}\,\hat{H}\right) &\approx \hat{\Theta} \\
\hat{\Theta} - i\,\frac{\delta}{\hbar}\,\hat{H}\,\hat{\Theta} + \hat{\Theta}\left(-i\,\frac{\delta}{\hbar}\,\hat{H}\right) &\approx \hat{\Theta} \\
-i\,\frac{\delta}{\hbar}\,\hat{H}\,\hat{\Theta} + i\,\frac{\delta}{\hbar}\,\hat{\Theta}\,\hat{H} &\approx 0
\end{aligned}$$

where you have to remember to conjugate the i in the second term when you interchange it with $\hat{\Theta}$. Therefore the statement is equivalent to $\left[\hat{H},\hat{\Theta}\right] = 0$.

(c) If $\hat{H}\,\psi_n = E_n\,\psi_n$ and $\hat{H}$ commutes with $\hat{\Theta}$, then

$$\hat{H}\,\psi_n^* = \hat{H}\,\hat{\Theta}\,\psi_n = \hat{\Theta}\,\hat{H}\,\psi_n = \hat{\Theta}\,E_n\,\psi_n = E_n\,\psi_n^* \qquad \bigstar$$

since E_n is of course real. If the energy is non-degenerate, then ψ_n^* must be a constant (of magnitude 1 since the functions have the same norm) times ψ_n: $\psi_n^* = c\,\psi_n$. One can then simply multiply ψ_n by an appropriate factor to make it real; $\sqrt{c}\,\psi_n$ will do the job.

(d) i. For a momentum eigenfunction

$$\hat{\Theta}\,f_p(x) = \hat{\Theta}\,\frac{1}{\sqrt{2\,\pi\,\hbar}}\,e^{i\,p\,x/\hbar} = \frac{1}{\sqrt{2\,\pi\,\hbar}}\,e^{-i\,p\,x/\hbar} = f_{-p}(x)\ .$$

ii. For a hydrogen wave function (see Equation 4.32 for the Y_ℓ^m)

$$\begin{aligned}\hat{\Theta}\,\psi_{n\ell m}(\mathbf{r}) &= \hat{\Theta}\,R_{n\ell}(r)\;Y_\ell^m(\theta,\phi) = R_{n\ell}(r)\,(-1)^m\;Y_\ell^{-m}(\theta,\phi)\\ &= (-1)^m\;\psi_{n\ell -m}(\mathbf{r})\;.\end{aligned}$$

Both states are clearly degenerate with the corresponding untransformed state and describe particle moving in the opposite direction (flipped p or L_z respectively).

Problem 6.37

(a) Acting on a generic spinor

$$\begin{aligned}\hat{\Theta}^2\begin{pmatrix} a \\ b\end{pmatrix} &= \hat{\Theta}\begin{pmatrix} -b^* \\ a^*\end{pmatrix} \equiv \hat{\Theta}\begin{pmatrix} a' \\ b'\end{pmatrix} = \begin{pmatrix} -(b')^* \\ (a')^*\end{pmatrix}\\ &= \begin{pmatrix} -(a^*)^* \\ (-b^*)^*\end{pmatrix} = -\begin{pmatrix} a \\ b\end{pmatrix}\end{aligned}$$

where I defined a' and b' to make it easier to follow the manipulations.

(b) Lets assume that they are the same state. Then

$$\begin{aligned}\hat{\Theta}^2\;|\psi_n\rangle &= \hat{\Theta}\;|\psi_n'\rangle = \hat{\Theta}\,c\;|\psi_n\rangle = c^*\,\hat{\Theta}\;|\psi_n\rangle = c^*\;|\psi_n'\rangle\\ &= c^*\,c\;|\psi_n\rangle = |c|^2\;|\psi_n\rangle\end{aligned}$$

but we know from part (a) that $\Theta^2 = -1$ and this is a contradiction since, of course, $|c|^2 > 0$.

Chapter 7

Time-Independent Perturbation Theory

Problem 7.1

(a)

$$\psi_n^0(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right), \text{ so } E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle = \frac{2}{a}\alpha\int_0^a \sin^2\left(\frac{n\pi}{a}x\right)\delta\left(x-\frac{a}{2}\right)\,dx.$$

$$E_n^1 = \frac{2\alpha}{a}\sin^2\left(\frac{n\pi}{a}\frac{a}{2}\right) = \frac{2\alpha}{a}\sin^2\left(\frac{n\pi}{2}\right) = \boxed{\left\{\begin{array}{ll} 0, & \text{if } n \text{ is even,} \\ 2\alpha/a, & \text{if } n \text{ is odd.}\end{array}\right\}}$$

For even n the wave function is zero at the location of the perturbation ($x = a/2$), so it never "feels" H'.

(b) Here $n = 1$, so we need

$$\langle\psi_m^0|H'|\psi_1^0\rangle = \frac{2\alpha}{a}\int \sin\left(\frac{m\pi}{a}x\right)\delta\left(x-\frac{a}{2}\right)\sin\left(\frac{\pi}{a}x\right)\,dx = \frac{2\alpha}{a}\sin\left(\frac{m\pi}{2}\right)\sin\left(\frac{\pi}{2}\right) = \frac{2\alpha}{a}\sin\left(\frac{m\pi}{2}\right).$$

This is zero for even m, so the first three nonzero terms will be $m = 3$, $m = 5$, and $m = 7$. Meanwhile, $E_1^0 - E_m^0 = \dfrac{\pi^2\hbar^2}{2ma^2}(1-m^2)$, so

$$\begin{aligned}
\psi_1^1 &= \sum_{m=3,5,7,\dots}\frac{(2\alpha/a)\sin(m\pi/2)}{E_1^0 - E_m^0}\psi_m^0 = \frac{2\alpha}{a}\frac{2ma^2}{\pi^2\hbar^2}\left[\frac{-1}{1-9}\psi_3^0 + \frac{1}{1-25}\psi_5^0 + \frac{-1}{1-49}\psi_7^0 + \dots\right] \\
&= \frac{4ma\alpha}{\pi^2\hbar^2}\sqrt{\frac{2}{a}}\left[\frac{1}{8}\sin\left(\frac{3\pi}{a}x\right) - \frac{1}{24}\sin\left(\frac{5\pi}{a}x\right) + \frac{1}{48}\sin\left(\frac{7\pi}{a}x\right) + \dots\right] \\
&= \boxed{\frac{m\alpha}{\pi^2\hbar^2}\sqrt{\frac{a}{2}}\left[\sin\left(\frac{3\pi}{a}x\right) - \frac{1}{3}\sin\left(\frac{5\pi}{a}x\right) + \frac{1}{6}\sin\left(\frac{7\pi}{a}x\right) + \dots\right]}.
\end{aligned}$$

Problem 7.2

(a) $E_n = (n + \frac{1}{2})\hbar\omega'$, where $\omega' \equiv \sqrt{k(1+\epsilon)/m} = \omega\sqrt{1+\epsilon} = \omega(1 + \frac{1}{2}\epsilon - \frac{1}{8}\epsilon^2 + \frac{1}{16}\epsilon^3 \cdots)$, so

$$\boxed{E_n = (n + \tfrac{1}{2})\hbar\omega\sqrt{1+\epsilon} = (n + \tfrac{1}{2})\hbar\omega(1 + \tfrac{1}{2}\epsilon - \tfrac{1}{8}\epsilon^2 + \cdots).}$$

(b) $H' = \frac{1}{2}k'x^2 - \frac{1}{2}kx^2 = \frac{1}{2}kx^2(1+\epsilon-1) = \epsilon(\frac{1}{2}kx^2) = \epsilon V$, where V is the unperturbed potential energy. So $E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle = \epsilon\langle n|V|n\rangle$, with $\langle n|V|n\rangle$ the expectation value of the (unperturbed) potential energy in the n^{th} unperturbed state. This is most easily obtained from the virial theorem (Problem 3.37), but it can also be derived algebraically. In this case the virial theorem says $\langle T\rangle = \langle V\rangle$. But $\langle T\rangle + \langle V\rangle = E_n^0$. So $\langle V\rangle = \frac{1}{2}E_n^0 = \frac{1}{2}(n+\frac{1}{2})\hbar\omega$; $\boxed{E_n^1 = \frac{\epsilon}{2}(n+\frac{1}{2})\hbar\omega,}$ which is precisely the ϵ^1 term in the power series from part (a).

Problem 7.3

(a) In terms of the one-particle states (Eq. 2.31) and energies (Eq. 2.30):

Ground state: $\psi_1^0(x_1,x_2) = \psi_1(x_1)\psi_1(x_2) = \boxed{\frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right);}$ $E_1^0 = 2E_1 = \boxed{\frac{\pi^2\hbar^2}{ma^2}.}$

First excited state: $\psi_2^0(x_1,x_2) = \frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_2) + \psi_2(x_1)\psi_1(x_2)]$

$$= \boxed{\frac{\sqrt{2}}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) + \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right];} \quad E_2^0 = E_1 + E_2 = \boxed{\frac{5}{2}\frac{\pi^2\hbar^2}{ma^2}.}$$

(b)

$$E_1^1 = \langle\psi_1^0|H'|\psi_1^0\rangle = (-aV_0)\left(\frac{2}{a}\right)^2\int_0^a\int_0^a \sin^2\left(\frac{\pi x_1}{a}\right)\sin^2\left(\frac{\pi x_2}{a}\right)\delta(x_1-x_2)\,dx_1\,dx_2$$

$$= -\frac{4V_0}{a}\int_0^a \sin^4\left(\frac{\pi x}{a}\right)dx = -\frac{4V_0}{a}\frac{a}{\pi}\int_0^\pi \sin^4 y\,dy = -\frac{4V_0}{\pi}\cdot\frac{3\pi}{8} = \boxed{-\frac{3}{2}V_0.}$$

$$E_2^1 = \langle\psi_2^0|H'|\psi_2^0\rangle$$

$$= (-aV_0)\left(\frac{2}{a^2}\right)\iint_0^a \left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) + \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]^2 \delta(x_1-x_2)\,dx_1\,dx_2$$

$$= -\frac{2V_0}{a}\int_0^a \left[\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right)\right]^2 dx$$

$$= -\frac{8V_0}{a}\int_0^a \sin^2\left(\frac{\pi x}{a}\right)\sin^2\left(\frac{2\pi x}{a}\right)dx = -\frac{8V_0}{a}\cdot\frac{a}{\pi}\int_0^\pi \sin^2 y\sin^2(2y)\,dy$$

$$= -\frac{8V_0}{\pi}\cdot 4\int_0^\pi \sin^2 y\sin^2 y\cos^2 y\,dy = -\frac{32V_0}{\pi}\int_0^\pi (\sin^4 y - \sin^6 y)\,dy$$

$$= -\frac{32V_0}{\pi}\left(\frac{3\pi}{8} - \frac{5\pi}{16}\right) = \boxed{-2V_0.}$$

Problem 7.4

(a) To get the eigenvalues of

$$\mathsf{H} = \mathsf{H}_0 + \mathsf{H}' = \begin{pmatrix} E_a^0 + \lambda V_{aa} & \lambda V_{ab} \\ \lambda V_{ba} & E_b^0 + \lambda V_{bb} \end{pmatrix} = \begin{pmatrix} A & \lambda V_{ab} \\ \lambda V_{ab}^* & B \end{pmatrix}$$

we solve the characteristic equation:

$$\begin{vmatrix} (A-E) & \lambda V_{ab} \\ \lambda V_{ab}^* & (B-E) \end{vmatrix} = (A-E)(B-E) - \lambda^2 |V_{ab}|^2 = E^2 - E(A+B) + AB - C = 0$$

(for short, $A \equiv E_a^0 + \lambda V_{aa},\ B \equiv E_b^0 + \lambda V_{bb},\ C \equiv \lambda^2 |V_{ab}|^2$). Thus

$$E_\pm = \frac{1}{2}\left[A + B \pm \sqrt{(A+B)^2 - 4(AB - C)}\right] = \boxed{\frac{1}{2}\left[A + B \pm \sqrt{(A-B)^2 + 4C}\right].}$$

(b) $E_\pm = \dfrac{1}{2}\left[(A+B) \pm (B-A)\sqrt{1 + \dfrac{4C}{(B-A)^2}}\right]$. To order λ^2,

$$\frac{4C}{(B-A)^2} \approx \frac{4\lambda^2 |V_{ab}|^2}{(E_b^0 - E_a^0)^2}; \quad \sqrt{1 + \frac{4C}{(B-A)^2}} \approx 1 + \frac{1}{2}\frac{4\lambda^2 |V_{ab}|^2}{(E_b^0 - E_a^0)^2}$$

$$E_\pm \approx \left\{(E_a^0 + E_b^0) + \lambda(V_{aa} + V_{bb}) \pm \left[(E_b^0 - E_a^0) + \lambda(V_{bb} - V_{aa}) + \lambda^2 \frac{2|V_{ab}|^2}{(E_b^0 - E_a^0)}\right]\right\}.$$

$$E_+ \approx \frac{1}{2}\left[E_a^0 + E_b^0 + \lambda(V_{aa} + V_{bb}) + E_b^0 - E_a^0 + \lambda(V_{bb} - V_{aa}) + \lambda^2 \frac{2|V_{ab}|^2}{(E_b^0 - E_a^0)}\right]$$

$$= E_b^0 + \lambda V_{bb} + \lambda^2 \frac{|V_{ab}|^2}{(E_b^0 - E_a^0} \to \boxed{E_+ \approx E_b^0 + V_{bb} + \frac{|V_{ab}|^2}{(E_b^0 - E_a^0)}.}$$

Similarly, $\boxed{E_- \approx E_a^0 + V_{aa} - \dfrac{|V_{ab}|^2}{(E_b^0 - E_a^0)}.}$ First-order perturbation theory (Equation 7.9) says

$$E_a^1 = \langle \psi_a^0 | H' | \psi_a^0 \rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} V_{aa} & V_{ab} \\ V_{ba} & V_{bb} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = V_{aa},$$

$$E_b^1 = \langle \psi_b^0 | H' | \psi_b^0 \rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} V_{aa} & V_{ab} \\ V_{ba} & V_{bb} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = V_{bb},$$

confirming the middle terms in the boxed equations. Second-order perturbation theory (Equation 7.15) says

$$E_a^2 = \frac{|\langle \psi_b^0 | H' | \psi_a^0 \rangle|^2}{(E_a^0 - E_b^0)}; \quad \langle \psi_b^0 | H' | \psi_a^0 \rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} V_{aa} & V_{ab} \\ V_{ba} & V_{bb} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = V_{ba}; \quad E_a^2 = -\frac{|V_{ab}|^2}{(E_b^0 - E_a^0)},$$

$$E_b^2 = \frac{|\langle \psi_a^0 | H' | \psi_b^0 \rangle|^2}{(E_b^0 - E_a^0)}; \quad \langle \psi_a^0 | H' | \psi_b^0 \rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} V_{aa} & V_{ab} \\ V_{ba} & V_{bb} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = V_{ab}; \quad E_b^2 = \frac{|V_{ab}|^2}{(E_b^0 - E_a^0)},$$

confirming the third terms in the boxed equations.

(c) Returning to the boxed equation in (a),

$$E_{\pm} = \frac{1}{2}\left[(E_a^0 + E_b^0) \pm (E_b^0 - E_a^0)\sqrt{1 + \frac{4|V_{ab}|^2}{(E_b^0 - E_a^0)^2}}\right].$$

But the power series expansion for $\sqrt{1+\epsilon}$ converges only for $|\epsilon| < 1$, which means that the perturbation series converges (in this case) only for

$$\frac{4|V_{ab}|^2}{(E_b^0 - E_a^0)^2} < 1, \quad \text{or} \quad \left|\frac{V_{ab}}{E_b^0 - E_z^0}\right| < \frac{1}{2}. \quad \checkmark$$

Problem 7.5

(a)

$$\langle\psi_m^0|H|\psi_n^0\rangle = \frac{2}{a}\alpha \int_0^a \sin\left(\frac{m\pi}{a}x\right)\delta\left(x - \frac{a}{2}\right)\sin\left(\frac{n\pi}{a}x\right)\, dx = \frac{2\alpha}{a}\sin\left(\frac{m\pi}{2}\right)\sin\left(\frac{n\pi}{2}\right),$$

which is zero unless both m and n are odd—in which case it is $\pm 2\alpha/a$. So Eq. 7.15 says

$$E_n^2 = \sum_{m\neq n,\,\text{odd}} \left(\frac{2\alpha}{a}\right)^2 \frac{1}{(E_n^0 - E_m^0)}. \quad \text{But Eq. 2.30 says} \quad E_n^0 = \frac{\pi^2\hbar^2}{2ma^2}n^2, \text{ so}$$

$$\boxed{E_n^2 = \begin{cases} 0, & \text{if } n \text{ is even;} \\ 2m\left(\dfrac{2\alpha}{\pi\hbar}\right)^2 \displaystyle\sum_{m\neq n,\,\text{odd}} \frac{1}{(n^2 - m^2)}, & \text{if } n \text{ is odd.}\end{cases}}$$

To sum the series, note that $\dfrac{1}{(n^2 - m^2)} = \dfrac{1}{2n}\left(\dfrac{1}{m+n} - \dfrac{1}{m-n}\right)$. Thus,

<u>for $n = 1$</u>: $\displaystyle\sum = \frac{1}{2}\sum_{3,5,7,\ldots}\left(\frac{1}{m+1} - \frac{1}{m-1}\right)$

$$= \frac{1}{2}\left(\frac{1}{4} + \frac{1}{6} + \frac{1}{8} + \cdots - \frac{1}{2} - \frac{1}{4} - \frac{1}{6} - \frac{1}{8}\cdots\right) = \frac{1}{2}\left(-\frac{1}{2}\right) = -\frac{1}{4};$$

<u>for $n = 3$</u>: $\displaystyle\sum = \frac{1}{6}\sum_{1,5,7,\ldots}\left(\frac{1}{m+3} - \frac{1}{m-3}\right)$

$$= \frac{1}{6}\left(\frac{1}{4} + \frac{1}{8} + \frac{1}{10} + \cdots + \frac{1}{2} - \frac{1}{2} - \frac{1}{4} - \frac{1}{6} - \frac{1}{8} - \frac{1}{10}\cdots\right) = \frac{1}{6}\left(-\frac{1}{6}\right) = -\frac{1}{36}.$$

In general, there is perfect cancellation except for the "missing" term $1/2n$ in the first sum, so the total is $\dfrac{1}{2n}\left(-\dfrac{1}{2n}\right) = -\dfrac{1}{(2n)^2}$. Therefore: $\boxed{E_n^2 = \begin{cases} 0, & \text{if } n \text{ is even;} \\ -2m\left(\alpha/\pi\hbar n\right)^2, & \text{if } n \text{ is odd.}\end{cases}}$

(b)

$$H' = \frac{1}{2}\epsilon k x^2; \quad \langle\psi_m^0|H'|\psi_n^0\rangle = \frac{1}{2}\epsilon k\langle m|x^2|n\rangle. \quad \text{Using Eqs. 2.67 and 2.70:}$$

$$\langle m|x^2|n\rangle = \frac{\hbar}{2m\omega}\langle m|(a_+^2 + a_+a_- + a_-a_+ + a_-^2)|n\rangle$$

$$= \frac{\hbar}{2m\omega}\left[\sqrt{(n+1)(n+2)}\langle m|n+2\rangle + n\langle m|n\rangle + (n+1)\langle m|n\rangle + \sqrt{n(n-1)}\langle m|n-2\rangle\right].$$

So, for $m \neq n$, $\langle\psi_m^0|H'|\psi_n^0\rangle = \left(\frac{1}{2}k\epsilon\right)\left(\frac{\hbar}{2m\omega}\right)\left[\sqrt{(n+1)(n+2)}\,\delta_{m,n+2} + \sqrt{n(n-1)}\,\delta_{m,n-2}\right].$

$$E_n^2 = \left(\frac{\epsilon\hbar\omega}{4}\right)^2 \sum_{m\neq n} \frac{\left[\sqrt{(n+1)(n+2)}\,\delta_{m,n+2} + \sqrt{n(n-1)}\,\delta_{m,n-2}\right]^2}{(n+\frac{1}{2})\hbar\omega - (m+\frac{1}{2})\hbar\omega}$$

$$= \frac{\epsilon^2\hbar\omega}{16}\sum_{m\neq n}\frac{[(n+1)(n+2)\,\delta_{m,n+2} + n(n-1)\,\delta_{m,n-2}]}{(n-m)}$$

$$= \frac{\epsilon^2\hbar\omega}{16}\left[\frac{(n+1)(n+2)}{n-(n+2)} + \frac{n(n-1)}{n-(n-2)}\right] = \frac{\epsilon^2\hbar\omega}{16}\left[-\frac{1}{2}(n+1)(n+2) + \frac{1}{2}n(n-1)\right]$$

$$= \frac{\epsilon^2\hbar\omega}{32}\left(-n^2 - 3n - 2 + n^2 - n\right) = \frac{\epsilon^2\hbar\omega}{32}(-4n-2) = \boxed{-\epsilon^2\frac{1}{8}\hbar\omega\left(n+\frac{1}{2}\right)}$$

(which agrees with the ϵ^2 term in the exact solution—Problem 7.2(a)).

Problem 7.6

(a)

$$E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle = -qE\langle n|x|n\rangle = \boxed{0} \text{ (Problem 2.12).}$$

From Eq. 7.15 and Problem 3.39: $E_n^2 = (qE)^2\sum_{m\neq n}\frac{|\langle m|x|n\rangle|^2}{(n-m)\hbar\omega}$

$$= \frac{(qE)^2}{\hbar\omega}\frac{\hbar}{2m\omega}\sum_{m\neq n}\frac{[\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{n},\delta_{m,n-1}]^2}{(n-m)} = \frac{(qE)^2}{2m\omega^2}\sum_{m\neq n}\frac{[(n+1)\,\delta_{m,n+1} + n\,\delta_{m,n-1}]}{(n-m)}$$

$$= \frac{(qE)^2}{2m\omega^2}\left[\frac{(n+1)}{n-(n+1)} + \frac{n}{n-(n-1)}\right] = \frac{(qE)^2}{2m\omega^2}[-(n+1)+n] = \boxed{-\frac{(qE)^2}{2m\omega^2}.}$$

(b) $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \left(\frac{1}{2}m\omega^2x^2 - qEx\right)\psi = E\psi.$ With the suggested change of variables,

$$\left(\frac{1}{2}m\omega^2x^2 - qEx\right) = \frac{1}{2}m\omega^2\left[x' + \left(\frac{qE}{m\omega^2}\right)\right]^2 - qE\left[x' + \left(\frac{qE}{m\omega^2}\right)\right]$$

$$= \frac{1}{2}m\omega^2x'^2 + m\omega^2x'\frac{qE}{m\omega^2} + \frac{1}{2}m\omega^2\frac{(qE)^2}{m^2\omega^4} - qEx' - \frac{(qE)^2}{m\omega^2} = \frac{1}{2}m\omega^2x'^2 - \frac{1}{2}\frac{(qE)^2}{m\omega^2}.$$

So the Schrödinger equation says

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx'^2}+\frac{1}{2}m\omega^2 x'^2\psi=\left[E+\frac{1}{2}\frac{(qE)^2}{m\omega^2}\right]\psi,$$

which is the Schrödinger equation for a simple harmonic oscillator, in the variable x'. The constant on the right must therefore be $(n+\frac{1}{2})\hbar\omega$, and we conclude that

$$\boxed{E_n=(n+\frac{1}{2})\hbar\omega-\frac{1}{2}\frac{(qE)^2}{m\omega^2}.}$$

The subtracted term is exactly what we got in part (a) using perturbation theory. Evidently all the higher corrections (like the first-order correction) are zero, in this case.

Problem 7.7

(a)

$$\begin{aligned}
\langle\psi_m^0|H'|\psi_1^0\rangle &= \int_0^{a/2}\sqrt{\frac{2}{a}}\sin\left(\frac{m\pi x}{a}\right)V_0\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)dx\\
&=\frac{2V_0}{a}\int_0^{a/2}\frac{1}{2}\left[\cos\left(\frac{(m-1)\pi x}{a}\right)-\cos\left(\frac{(m+1)\pi x}{a}\right)\right]dx\\
&=\frac{V_0}{a}\left[\frac{a}{(m-1)\pi}\sin\left(\frac{(m-1)\pi x}{a}\right)-\frac{a}{(m+1)\pi}\sin\left(\frac{(m+1)\pi x}{a}\right)\right]\Bigg|_0^{a/2}\\
&=\frac{V_0}{\pi}\left[\frac{1}{(m-1)}\sin\left(\frac{(m-1)\pi}{2}\right)-\frac{1}{(m+1)}\sin\left(\frac{(m+1)\pi}{2}\right)\right].
\end{aligned}$$

If m is odd, the result is zero. So the first three nonzero terms are $m=2$, $m=4$, and $m=6$.

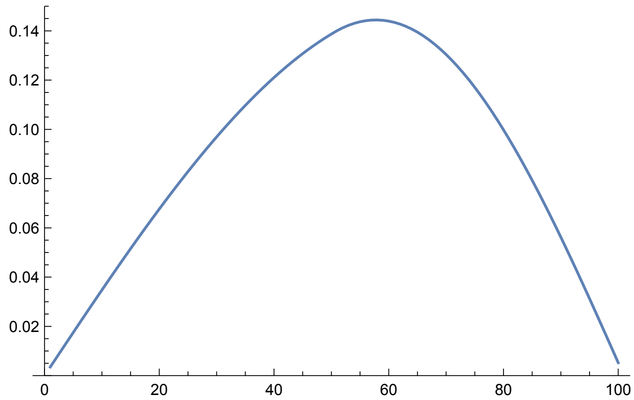
$$\begin{aligned}
\langle\psi_2^0|H'|\psi_1^0\rangle &= \frac{V_0}{\pi}\left[\sin\left(\frac{\pi}{2}\right)-\frac{1}{3}\sin\left(\frac{3\pi}{2}\right)\right]=\frac{V_0}{\pi}\left(1+\frac{1}{3}\right)=\frac{4V_0}{3\pi},\\
\langle\psi_4^0|H'|\psi_1^0\rangle &= \frac{V_0}{\pi}\left[\frac{1}{3}\sin\left(\frac{3\pi}{2}\right)-\frac{1}{5}\sin\left(\frac{5\pi}{2}\right)\right]=\frac{V_0}{\pi}\left(-\frac{1}{3}-\frac{1}{5}\right)=-\frac{8V_0}{15\pi},\\
\langle\psi_6^0|H'|\psi_1^0\rangle &= \frac{V_0}{\pi}\left[\frac{1}{5}\sin\left(\frac{5\pi}{2}\right)-\frac{1}{7}\sin\left(\frac{7\pi}{2}\right)\right]=\frac{V_0}{\pi}\left(\frac{1}{5}+\frac{1}{7}\right)=\frac{12V_0}{35\pi}.
\end{aligned}$$

Plugging this into Equation 7.13:

$$\begin{aligned}
\psi_1^1 &= \frac{4V_0}{\pi}\frac{2ma^2}{\pi^2\hbar^2}\sqrt{\frac{2}{a}}\left[\frac{1}{3(1-4)}\sin\left(\frac{2\pi x}{a}\right)-\frac{2}{15(1-16)}\sin\left(\frac{4\pi x}{a}\right)+\frac{3}{35(1-36)}\sin\left(\frac{6\pi x}{a}\right)+\cdots\right]\\
&=\boxed{\frac{8V_0ma^2}{\pi^3\hbar^2}\sqrt{\frac{2}{a}}\left[-\frac{1}{(3)^2}\sin\left(\frac{2\pi x}{a}\right)+\frac{2}{(15)^2}\sin\left(\frac{4\pi x}{a}\right)-\frac{3}{(35)^2}\sin\left(\frac{6\pi x}{a}\right)+\cdots\right].}
\end{aligned}$$

(b) $V_0=\dfrac{4\hbar^2}{ma^2}$, $\lambda=\dfrac{\hbar^2}{2m(\Delta x)^2}=\dfrac{(N+1)^2}{8}V_0$. In the left half ($j\le 50$), $v_j=\dfrac{V_0}{\lambda}=\dfrac{8}{(101)^2}$; in the right half $v_j=0$. Here is the Mathematica code:

```
h = Table[If[i == j, 2 + If[i < 51, (8 / 10201), 0], 0], {i, 100}, {j, 100}]
k = Table[If[i == j + 1, -1, 0], {i, 100}, {j, 100}]
m = Table[If[i == j - 1, -1, 0], {i, 100}, {j, 100}]
p = Table[h[[i, j]] + k[[i, j]] + m[[i, j]], {i, 100}, {j, 100}]
EVE = Eigenvectors[N[p]]
ListLinePlot[EVE[[100]], PlotRange → {0, 0.15}]
```

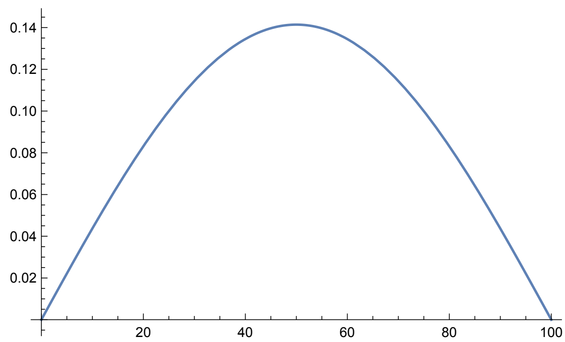



```
EIG = Eigenvalues[N[p]]
EIG[[100]]
0.00132025
```

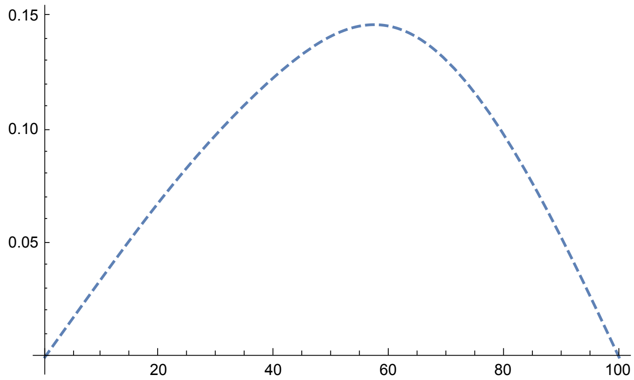
The lowest eigenvalue is $0.00132025\,\lambda = (10201/8)(0.00132025)\,V_0 = \boxed{1.6835\,V_0.}$ First-order perturbation theory (Example 7.1) says it is approximately $\dfrac{\pi^2\hbar^2}{2ma^2} + \dfrac{V_0}{2} = \left(\dfrac{\pi^2}{8} + \dfrac{1}{2}\right)V_0 = 1.7337\,V_0$. The agreement is not too bad, considering that this is a relatively large perturbation.

(c) In the figures below, the centered graph is the unperturbed ground state, the dashed graph is the perturbation theory wave function, and the solid line is the numerical solution. (The latter is automatically normalized by Mathematica.) The agreement between the latter two is remarkably good.

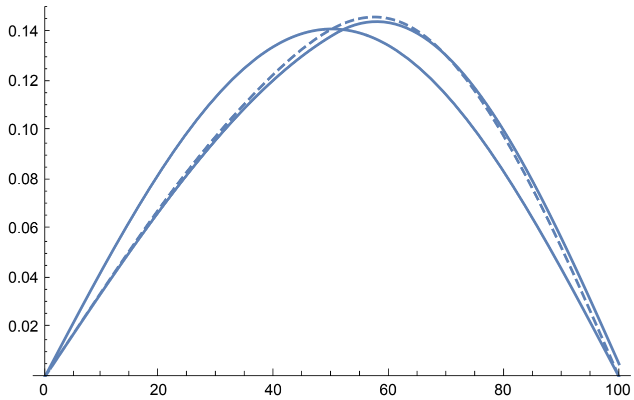
```
Plot[√(2 / 100) Sin[π x / 100], {x, 0, 100}]
```



```
Plot[√(2 / 100)
  (Sin[π x / 100] + 32/π^3 (- 1/3^2 Sin[2 π x / 100] + 2/15^2 Sin[4 π x / 100] - 3/35^2 Sin[6 π x / 100])
  {x, 0, 100}, PlotStyle → Dashed]
```




```
Show[%14, %27, %28]
```




```
T = EVE[[100]]
```

$$\sum_{i=1}^{100} (\texttt{T[[i]]})\texttt{^}2$$

```
1.
```

Problem 7.8

(a)

$$\langle\psi_+^0|\psi_-^0\rangle = \langle(\alpha_+\psi_a^0 + \beta_+\psi_b^0)|(\alpha_-\psi_a^0 + \beta_-\psi_b^0)\rangle$$

$$= \alpha_+^*\alpha_-\langle\psi_a^0|\psi_a^0\rangle + \alpha_+^*\beta_-\langle\psi_a^0|\psi_b^0\rangle + \beta_+^*\alpha_-\langle\psi_b^0|\psi_a^0\rangle + \beta_+^*\beta_-\langle\psi_b^0|\psi_b^0\rangle$$

$$= \alpha_+^*\alpha_- + \beta_+^*\beta_-. \quad \text{But Eq. 7.27} \;\Rightarrow \beta_\pm = \alpha_\pm(E_\pm^1 - W_{aa})/W_{ab}, \quad \text{so}$$

$$\langle\psi_+^0|\psi_-^0\rangle = \alpha_+^*\alpha_-\left[1+\frac{(E_+^1-W_{aa})(E_-^1-W_{aa})}{W_{ab}{}^*W_{ab}}\right] = \frac{\alpha_+^*\alpha_-}{|W_{ab}|^2}\left[|W_{ab}|^2+(E_+^1-W_{aa})(E_-^1-W_{aa})\right].$$

The term in square brackets is:

$[\ ] = E_+^1E_-^1 - W_{aa}(E_+^1+E_-^1)+|W_{ab}|^2+W_{aa}^2$. But Eq. 7.33 $\Rightarrow$ $E_\pm^1 = \frac{1}{2}[(W_{aa}+W_{bb})\pm\surd]$, where $\surd$ is shorthand for the square root term. So $E_+^1+E_-^1 = W_{aa}+W_{bb}$, and

$$E_+^1E_-^1 = \frac{1}{4}\left[(W_{aa}+W_{bb})^2-(\surd)^2\right] = \frac{1}{4}\left[(W_{aa}+W_{bb})^2-(W_{aa}-W_{bb})^2-4|W_{ab}|^2\right] = W_{aa}W_{bb}-|W_{ab}|^2.$$

Thus $[\ ] = W_{aa}W_{bb}-|W_{ab}|^2-W_{aa}(W_{aa}+W_{bb})+|W_{ab}|^2+W_{aa}^2 = 0$, so $\langle\psi_+^0|\psi_-^0\rangle = 0$. QED

(b)

$$\begin{aligned}\langle\psi_+^0|H'|\psi_-^0\rangle &= \alpha_+^*\alpha_-\langle\psi_a^0|H'|\psi_a^0\rangle+\alpha_+^*\beta_-\langle\psi_a^0|H'|\psi_b^0\rangle+\beta_+^*\alpha_-\langle\psi_b^0|H'|\psi_a^0\rangle+\beta_+^*\beta_-\langle\psi_b^0|H'|\psi_b^0\rangle\\ &= \alpha_+^*\alpha_-W_{aa}+\alpha_+^*\beta_-W_{ab}+\beta_+^*\alpha_-W_{ba}+\beta_+^*\beta_-W_{bb}\\ &= \alpha_+^*\alpha_-\left[W_{aa}+W_{ab}\frac{(E_-^1-W_{aa})}{W_{ab}}+W_{ba}\frac{(E_+^1-W_{aa})}{W_{ab}^*}+W_{bb}\frac{(E_+^1-W_{aa})}{W_{ab}^*}\frac{(E_-^1-W_{aa})}{W_{ab}}\right]\\ &= \alpha_+^*\alpha_-\left[W_{aa}+E_-^1-W_{aa}+E_+^1-W_{aa}+W_{bb}\frac{(E_+^1-W_{aa})(E_-^1-W_{aa})}{|W_{ab}|^2}\right].\end{aligned}$$

But we know from (a) that $\dfrac{(E_+^1-W_{aa})(E_-^1-W_{aa})}{|W_{ab}|^2} = -1$, so

$$\langle\psi_+^0|H'|\psi_-^0\rangle = \alpha_+^*\alpha_-[E_-^1+E_+^1-W_{aa}-W_{bb}] = 0.\quad \text{QED}$$

(c)

$$\begin{aligned}\langle\psi_\pm^0|H'|\psi_\pm^0\rangle &= \alpha_\pm^*\alpha_\pm\langle\psi_a^0|H'|\psi_a^0\rangle+\alpha_\pm^*\beta_\pm\langle\psi_a^0|H'|\psi_b^0\rangle+\beta_\pm^*\alpha_\pm\langle\psi_b^0|H'|\psi_a^0\rangle+\beta_\pm^*\beta_\pm\langle\psi_b^0|H'|\psi_b^0\rangle\\ &= |\alpha_\pm|^2\left[W_{aa}+W_{ab}\frac{(E_\pm^1-W_{aa})}{W_{ab}}\right]+|\beta_\pm|^2\left[W_{ba}\frac{(E_\pm^1-W_{bb})}{W_{ba}}+W_{bb}\right]\end{aligned}$$

(this time I used Eq. 7.29 to express α in terms of β, in the third term).

$$\therefore \langle\psi_\pm^0|H'|\psi_\pm^0\rangle = |\alpha_\pm|^2(E_\pm^1)+|\beta_\pm|^2(E_\pm^1) = \left(|\alpha_\pm|^2+|\beta_\pm|^2\right)E_\pm^1 = E_\pm^1.\quad \text{QED}$$

Problem 7.9

(a) See Problem 2.46.

(b) With $a\to n, b\to -n$, we have:

$$W_{aa} = W_{bb} = -\frac{V_0}{L}\int_{-L/2}^{L/2}e^{-x^2/a^2}dx \approx -\frac{V_0}{L}\int_{-\infty}^{\infty}e^{-x^2/a^2}dx = -\frac{V_0}{L}a\sqrt{\pi}.$$

$$W_{ab} = -\frac{V_0}{L}\int_{-L/2}^{L/2}e^{-x^2/a^2}e^{-4\pi nix/L}dx \approx -\frac{V_0}{L}\int_{-\infty}^{\infty}e^{-(x^2/a^2+4\pi nix/L)}dx = -\frac{V_0}{L}a\sqrt{\pi}e^{-(2\pi na/L)^2}.$$

(We did this integral in Problem 2.21.) In this case $W_{aa} = W_{bb}$, and W_{ab} is real, so Eq. 7.33 $\Rightarrow$

$$E_\pm^1 = W_{aa}\pm|W_{ab}|,\quad \text{or}\quad E_\pm^1 = \boxed{-\sqrt{\pi}\frac{V_0a}{L}\left(1\mp e^{-(2\pi na/L)^2}\right).}$$

(c) Equation 7.27 $\Rightarrow \beta = \alpha \dfrac{(E^1 - W_{aa})}{W_{ab}} = \alpha \left[\dfrac{\pm\sqrt{\pi}(V_0 a/L)e^{-(2\pi na/L)^2}}{-\sqrt{\pi}(V_0 a/L)e^{-(2\pi na/L)^2}}\right] = \mp\alpha$. Evidently, the "good" linear combinations are:

$$\psi_+ = \alpha\psi_n - \alpha\psi_{-n} = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{L}}\left[e^{i2\pi nx/L} - e^{-i2\pi nx/L}\right] = \boxed{i\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi nx}{L}\right)} \quad \text{and}$$

$$\psi_- = \alpha\psi_n + \alpha\psi_{-n} = \boxed{\sqrt{\frac{2}{L}}\cos\left(\frac{2\pi nx}{L}\right).} \quad \text{Using Eq. 7.9, we have :}$$

$$E^1_+ = \langle\psi_+|H'|\psi_+\rangle = \frac{2}{L}(-V_0)\int_{-L/2}^{L/2} e^{-x^2/a^2}\sin^2\left(\frac{2\pi nx}{L}\right)dx,$$

$$E^1_- = \langle\psi_-|H'|\psi_-\rangle = \frac{2}{L}(-V_0)\int_{-L/2}^{L/2} e^{-x^2/a^2}\cos^2\left(\frac{2\pi nx}{L}\right)dx.$$

But $\sin^2\theta = (1-\cos 2\theta)/2$, and $\cos^2\theta = (1+\cos 2\theta)/2$, so

$$E^1_\pm \approx -\frac{V_0}{L}\int_{-\infty}^{\infty} e^{-x^2/a^2}\left[1 \mp \cos\left(\frac{4\pi nx}{L}\right)\right]dx = -\frac{V_0}{L}\left[\int_{-\infty}^{\infty} e^{-x^2/a^2}dx \mp \int_{-\infty}^{\infty} e^{-x^2/a^2}\cos\left(\frac{4\pi nx}{L}\right)dx\right]$$

$$= -\frac{V_0}{L}\left[\sqrt{\pi}\,a \mp a\sqrt{\pi}e^{-(2\pi na/L)^2}\right] = -\sqrt{\pi}\frac{V_0 a}{L}\left[1 \mp e^{-(2\pi na/L)^2}\right], \quad \text{same as (b).}$$

(d) $Af(x) = f(-x)$ (the parity operator). The eigenstates are *even* functions (with eigenvalue $+1$) and *odd* functions (with eigenvalue -1). The linear combinations we found in (c) are precisely the odd and even linear combinations of ψ_n and ψ_{-n}.

Problem 7.10

Expanding the exact energies (Equation 7.21) to first order in ϵ:

$$E_{mn} = \left(m+\frac{1}{2}\right)\hbar\omega_+ + \left(n+\frac{1}{2}\right)\hbar\omega_- = \left(m+\frac{1}{2}\right)\hbar\omega\sqrt{1+\epsilon} + \left(n+\frac{1}{2}\right)\hbar\omega\sqrt{1-\epsilon}$$

$$\approx \left(m+\frac{1}{2}\right)\hbar\omega\left(1+\frac{\epsilon}{2}\right) + \left(n+\frac{1}{2}\right)\hbar\omega\left(1-\frac{\epsilon}{2}\right) = (m+n+1)\hbar\omega + \frac{\epsilon}{2}(m-n)\hbar\omega.$$

So for $m=1,\ n=0$ the first-order correction is $+\epsilon(\hbar\omega/2)$, and for $n=1,\ m=0$ it is $-\epsilon(\hbar\omega/2)$, confirming Equation 7.34.

Problem 7.11

Ground state is nondegenerate; Eqs. 7.9 $\Rightarrow$

$$E^1 = \left(\frac{2}{a}\right)^3 a^3 V_0 \iiint_0^a \sin^2\left(\frac{\pi}{a}x\right)\sin^2\left(\frac{\pi}{a}y\right)\sin^2\left(\frac{\pi}{a}z\right)\delta(x-\frac{a}{4})\delta(y-\frac{a}{2})\delta(z-\frac{3a}{4})\,dx\,dy\,dz$$

$$= 8V_0\sin^2\left(\frac{\pi}{4}\right)\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{3\pi}{4}\right) = 8V_0\left(\frac{1}{2}\right)(1)\left(\frac{1}{2}\right) = \boxed{2V_0.}$$

First excited states:

$$W_{aa} = 8V_0 \iiint \sin^2\left(\frac{\pi}{a}x\right)\sin^2\left(\frac{\pi}{a}y\right)\sin^2\left(\frac{2\pi}{a}z\right)\delta(x-\frac{a}{4})\delta(y-\frac{a}{2})\delta(z-\frac{3a}{4})\,dx\,dy\,dz$$
$$= 8V_0\left(\frac{1}{2}\right)(1)(1) = 4V_0.$$

$$W_{bb} = 8V_0 \iiint \sin^2\left(\frac{\pi}{a}x\right)\sin^2\left(\frac{2\pi}{a}y\right)\sin^2\left(\frac{\pi}{a}z\right)\delta(x-\frac{a}{4})\delta(y-\frac{a}{2})\delta(z-\frac{3a}{4})\,dx\,dy\,dz$$
$$= 8V_0\left(\frac{1}{2}\right)(0)\left(\frac{1}{2}\right) = 0.$$

$$W_{cc} = 8V_0 \iiint \sin^2\left(\frac{2\pi}{a}x\right)\sin^2\left(\frac{\pi}{a}y\right)\sin^2\left(\frac{\pi}{a}z\right)\delta(x-\frac{a}{4})\delta(y-\frac{a}{2})\delta(z-\frac{3a}{4})\,dx\,dy\,dz$$
$$= 8V_0(1)(1)\left(\frac{1}{2}\right) = 4V_0.$$

$$W_{ab} = 8V_0\sin^2\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin(\pi)\sin\left(\frac{3\pi}{2}\right)\sin\left(\frac{3\pi}{4}\right) = 0.$$
$$W_{ac} = 8V_0\sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin^2\left(\frac{\pi}{2}\right)\sin\left(\frac{3\pi}{2}\right)\sin\left(\frac{3\pi}{4}\right) = 8V_0\left(\frac{1}{\sqrt{2}}\right)(1)(1)(-1)\left(\frac{1}{\sqrt{2}}\right) = -4V_0.$$
$$W_{bc} = 8V_0\sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin(\pi)\sin\left(\frac{\pi}{2}\right)\sin^2\left(\frac{3\pi}{4}\right) = 0.$$
$$\mathsf{W} = 4V_0\begin{pmatrix}1 & 0 & -1\\ 0 & 0 & 0\\ -1 & 0 & 1\end{pmatrix} = 4V_0\mathsf{D};\quad \det(\mathsf{D}-\lambda) = \begin{vmatrix}(1-\lambda) & 0 & -1\\ 0 & -\lambda & 0\\ -1 & 0 & (1-\lambda)\end{vmatrix} = -\lambda(1-\lambda)^2 + \lambda = 0 \quad \Rightarrow$$
$$\lambda = 0, \quad \text{or} \quad (1-\lambda)^2 = 1 \Rightarrow 1-\lambda = \pm 1 \Rightarrow \lambda = 0 \quad \text{or} \quad \lambda = 2.$$

So the first-order corrections to the energies are $\boxed{0,\ 0,\ 8V_0.}$

Problem 7.12

(a) $\boxed{\chi_1 = \begin{pmatrix}1\\0\\0\end{pmatrix},\ \text{eigenvalue } \boxed{V_0;}}$ $\boxed{\chi_2 = \begin{pmatrix}0\\1\\0\end{pmatrix},\ \text{eigenvalue } \boxed{V_0;}}$ $\boxed{\chi_3 = \begin{pmatrix}0\\0\\1\end{pmatrix},\ \text{eigenvalue } \boxed{2V_0.}}$

(b) Characteristic equation: $\det(\mathsf{H}-\lambda) = \begin{vmatrix}[V_0(1-\epsilon)-\lambda] & 0 & 0\\ 0 & [V_0-\lambda] & \epsilon V_0\\ 0 & \epsilon V_0 & [2V_0-\lambda]\end{vmatrix} = 0;$

$$[V_0(1-\epsilon)-\lambda][(V_0-\lambda)(2V_0-\lambda)-(\epsilon V_0)^2] = 0 \Rightarrow \boxed{\lambda_1 = V_0(1-\epsilon).}$$
$$(V_0-\lambda)(2V_0-\lambda)-(\epsilon V_0)^2 = 0 \Rightarrow \lambda^2 - 3V_0\lambda + (2V_0^2 - \epsilon^2V_0^2) = 0 \Rightarrow$$
$$\lambda = \frac{3V_0 \pm \sqrt{9V_0^2 - 4(2V_0^2-\epsilon^2V_0^2)}}{2} = \frac{V_0}{2}\left[3 \pm \sqrt{1+4\epsilon^2}\right] \approx \frac{V_0}{2}\left[3 \pm (1+2\epsilon^2)\right].$$
$$\boxed{\lambda_2 = \frac{V_0}{2}\left(3 - \sqrt{1+4\epsilon^2}\right) \approx V_0(1-\epsilon^2); \quad \lambda_3 = \frac{V_0}{2}\left(3 + \sqrt{1+4\epsilon^2}\right) \approx V_0(2+\epsilon^2).}$$

(c)

$$\mathsf{H}' = \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \quad E_3^1 = \langle \chi_3 | H' | \chi_3 \rangle = \epsilon V_0 \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= \epsilon V_0 \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \boxed{0} \text{ (no first-order correction).}$$

$$E_3^2 = \sum_{m=1,2} \frac{|\langle \chi_m | H' | \chi_3 \rangle|^2}{E_3^0 - E_m^0}; \quad \langle \chi_1 | H' | \chi_3 \rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0,$$

$$\langle \chi_2 | H' | \chi_3 \rangle = \epsilon V_0 \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \epsilon V_0.$$

$E_3^0 - E_2^0 = 2V_0 - V_0 = V_0$. So $E_3^2 = (\epsilon V_0)^2 / V_0 = \boxed{\epsilon^2 V_0.}$ Through second-order, then,

$$E_3 = E_3^0 + E_3^1 + E_3^2 = 2V_0 + 0 + \epsilon^2 V_0 = V_0(2 + \epsilon^2) \quad \text{(same as we got for } \lambda_3 \text{ in (b)).}$$

(d)

$$W_{aa} = \langle \chi_1 | H' | \chi_1 \rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix} = -\epsilon V_0.$$

$$W_{bb} = \langle \chi_2 | H' | \chi_2 \rangle = \epsilon V_0 \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0.$$

$$W_{ab} = \langle \chi_1 | H' | \chi_2 \rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0.$$

Plug the expressions for W_{aa}, W_{bb}, and W_{ab} into Eq. 7.33:

$$E_{\pm}^1 = \frac{1}{2} \left[-\epsilon V_0 + 0 \pm \sqrt{\epsilon^2 V_0^2 + 0} \right] = \frac{1}{2}(-\epsilon V_0 \pm \epsilon V_0) = \{0, -\epsilon V_0\}.$$

To first-order, then, $\boxed{E_1 = V_0 - \epsilon V_0, \quad E_2 = V_0,}$ and these are consistent (to first order in ϵ) with what we got in (b).

Problem 7.13

Given a set of orthonormal states $\{\psi_j^0\}$ that are degenerate eigenfunctions of the unperturbed Hamiltonian:

$$H\psi_j^0 = E^0 \psi_j^0, \quad \langle \psi_j^0 | \psi_l^0 \rangle = \delta_{jl},$$

construct the general linear combination,

$$\psi^0 = \sum_{j=1}^{n} \alpha_j \psi_j^0.$$

It too is an eigenfunction of the unperturbed Hamiltonian, with the same eigenvalue:

$$H^0\psi^0 = \sum_{j=1}^{n} \alpha_j H^0 \psi_j^0 = E^0 \sum_{j=1}^{n} \alpha_j \psi_j^0 = E^0\psi^0.$$

We want to solve the Schrödinger equation $H\psi = E\psi$ for the perturbed Hamiltonian $H = H^0 + \lambda H'$. Expand the eigenvalues and eigenfunctions as power series in λ:

$$E = E^0 + \lambda E^1 + \lambda^2 E^2 + \dots, \quad \psi = \psi^0 + \lambda\psi^1 + \lambda^2\psi^2 + \dots.$$

Plug these into the Schrödinger equation and collect like powers:

$$(H^0 + \lambda H')(\psi^0 + \lambda\psi^1 + \lambda^2\psi^2 + \dots) = (E^0 + \lambda E^1 + \lambda^2 E^2 + \dots)(\psi^0 + \lambda\psi^1 + \lambda^2\psi^2 + \dots) \quad \Rightarrow$$

$$H^0\psi^0 + \lambda(H^0\psi^1 + H'\psi^0) + \dots = E^0\psi^0 + \lambda(E^0\psi^1 + E^1\psi^0) + \dots$$

The zeroth-order terms cancel; to first order

$$H^0\psi^1 + H'\psi^0 = E^0\psi^1 + E^1\psi^0.$$

Take the inner product with ψ_j^0:

$$\langle\psi_j^0|H^0\psi^1\rangle + \langle\psi_j^0|H'\psi^0\rangle = E^0\langle\psi_j^0|\psi^1\rangle + E^1\langle\psi_j^0|\psi^0\rangle.$$

But $\langle\psi_j^0|H^0\psi^1\rangle = \langle H^0\psi_j^0|\psi^1\rangle = E^0\langle\psi_j^0|\psi^1\rangle$, so the first terms cancel, leaving

$$\langle\psi_j^0|H'\psi^0\rangle = E^1\langle\psi_j^0|\psi^0\rangle.$$

Now use $\psi^0 = \sum_{l=1}^{n} \alpha_l \psi_l^0$, and exploit the orthonormality of $\{\psi_l^0\}$:

$$\sum_{l=1}^{n} \alpha_l \langle\psi_j^0|H'|\psi_l^0\rangle = E^1 \sum_{l=1}^{n} \alpha_l \langle\psi_j^0|\psi_l^0\rangle = E^1\alpha_j,$$

or, defining

$$W_{jl} \equiv \langle\psi_j^0|H'|\psi_l^0\rangle, \quad \boxed{\sum_{l=1}^{n} W_{jl}\alpha_l = E^1\alpha_l.}$$

This (the generalization of Eq. 7.27 for the case of n-fold degeneracy) is the eigenvalue equation for the matrix W (whose jl^{th} element, in the $\{\psi_j^0\}$ basis, is W_{jl}); E^1 is the eigenvalue, and the eigenvector (in the $\{\psi_j^0\}$ basis) is $\chi_j = \alpha_j$. *Conclusion:* The first-order corrections to the energy are the eigenvalues of W. QED

Problem 7.14

(a) From Eq. 4.70: $E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = -\frac{1}{2}mc^2\left(\frac{1}{\hbar c}\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{1}{n^2} = \boxed{-\frac{\alpha^2 mc^2}{2n^2}.}$

(b) I have found a wonderful solution—unfortunately, there isn't enough room on this page for the proof.

Problem 7.15

Equation 4.218 $\Rightarrow \langle V\rangle = 2E_n$, for hydrogen. $V = -\dfrac{e^2}{4\pi\epsilon_0}\dfrac{1}{r}$; $E_n = -\left[\dfrac{m}{2\hbar^2}\left(\dfrac{e^2}{4\pi\epsilon_0}\right)^2\right]\dfrac{1}{n^2}$. So

$$-\frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{r}\right\rangle = -2\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} \quad\Rightarrow\quad \left\langle\frac{1}{r}\right\rangle = \left(\frac{me^2}{4\pi\epsilon_0\hbar^2}\right)\frac{1}{n^2} = \frac{1}{an^2} \quad \text{(Eq. 4.72). QED}$$

Problem 7.16

In Problem 4.52 we found (for $n = 3$, $\ell = 2$, $m = 1$) that $\langle r^s\rangle = \dfrac{(s+6)!}{6!}\left(\dfrac{3a}{2}\right)^s$.

$$\underline{s=0}:\ \langle 1\rangle = \frac{6!}{6!}(1) = \boxed{1} \quad \text{(of course).} \quad \checkmark$$

$$\underline{s=-1}:\ \left\langle\frac{1}{r}\right\rangle = \frac{5!}{6!}\left(\frac{3a}{2}\right)^{-1} = \frac{1}{6}\cdot\frac{2}{3a} = \boxed{\frac{1}{9a}} \quad \left(\text{Eq. 7.56 says } \frac{1}{3^2a} = \frac{1}{9a}\right). \quad \checkmark$$

$$\underline{s=-2}:\ \left\langle\frac{1}{r^2}\right\rangle = \frac{4!}{6!}\left(\frac{3a}{2}\right)^{-2} = \frac{1}{6\cdot 5}\cdot\frac{4}{9a^2} = \boxed{\frac{2}{135a^2}} \quad \left(\text{Eq. 7.57 says } \frac{1}{(5/2)\cdot 27\cdot a^2} = \frac{2}{135a^2}\right). \quad \checkmark$$

$$\underline{s=-3}:\ \left\langle\frac{1}{r^3}\right\rangle = \frac{3!}{6!}\left(\frac{3a}{2}\right)^{-3} = \frac{1}{6\cdot 5\cdot 4}\cdot\frac{8}{27a^3} = \boxed{\frac{1}{405a^3}} \quad \left(\text{Eq. 7.66 says } \frac{1}{2(5/2)3\cdot 27\cdot a^3} = \frac{1}{405a^3}\right). \checkmark$$

For $s = -7$ (or smaller) the integral does not converge: $\langle 1/r^7\rangle = \infty$ in this state; this is reflected in the fact that $(-1)! = \infty$.

Problem 7.17

Equation 7.55 $\Rightarrow E_r^1 = -\dfrac{1}{2mc^2}\left[E^2 - 2E\langle V\rangle + \langle V^2\rangle\right]$. Here $E = (n+\frac{1}{2})\hbar\omega$, $V = \frac{1}{2}m\omega^2x^2 \Rightarrow$

$$E_r^1 = -\frac{1}{2mc^2}\left[\left(n+\frac{1}{2}\right)^2\hbar^2\omega^2 - 2\left(n+\frac{1}{2}\right)\hbar\omega\frac{1}{2}m\omega^2\langle x^2\rangle + \frac{1}{4}m^2\omega^4\langle x^4\rangle\right].$$

But Problem 2.12 $\Rightarrow$ $\langle x^2\rangle = (n+\frac{1}{2})\dfrac{\hbar}{m\omega}$, so

$$E_r^1 = -\frac{1}{2mc^2}\left[\left(n+\frac{1}{2}\right)^2\hbar^2\omega^2 - \left(n+\frac{1}{2}\right)^2\hbar^2\omega^2 + \frac{1}{4}m^2\omega^4\langle x^4\rangle\right] = -\frac{m\omega^4}{8c^2}\langle x^4\rangle.$$

From Eq. 2.70: $x^4 = \dfrac{\hbar^2}{4m^2\omega^2}\left(a_+^2 + a_+a_- + a_-a_+ + a_-^2\right)\left(a_+^2 + a_+a_- + a_-a_+ + a_-^2\right)$,

$$\langle x^4\rangle = \frac{\hbar^2}{4m^2\omega^2}\langle n|\left(a_+^2a_-^2 + a_+a_-a_+a_- + a_+a_-a_-a_+ + a_-a_+a_+a_- + a_-a_+a_-a_+ + a_-^2a_+^2\right)|n\rangle.$$

(Note that only terms with equal numbers of raising and lowering operators will survive). Using Eq. 2.67,

$$\langle x^4\rangle = \frac{\hbar^2}{4m^2\omega^2}\langle n|\left[a_+^2\left(\sqrt{n(n-1)}\,|n-2\rangle\right) + a_+a_-(n\,|n\rangle) + a_+a_-\big((n+1)\,|n\rangle\big)\right.$$

$$
\begin{aligned}
&\quad +a_-a_+\,(n\,|n\rangle) + a_-a_+\big((n+1)\,|n\rangle\big) + a_-^2\left(\sqrt{(n+1)(n+2)}\,|n+2\rangle\right)\Big] \\
&= \frac{\hbar^2}{4m^2\omega^2}\langle n|\Big[\sqrt{n(n-1)}\left(\sqrt{n(n-1)}\,|n\rangle\right) + n\,(n\,|n\rangle) + (n+1)\,(n\,|n\rangle) \\
&\quad +n\big((n+1)\,|n\rangle\big) + (n+1)\big((n+1)\,|n\rangle\big) + \sqrt{(n+1)(n+2)}\left(\sqrt{(n+1)(n+2)}\,|n\rangle\right)\Big] \\
&= \frac{\hbar^2}{4m^2\omega^2}\left[n(n-1) + n^2 + (n+1)n + n(n+1) + (n+1)^2 + (n+1)(n+2)\right] \\
&= \left(\frac{\hbar}{2m\omega}\right)^2 (n^2 - n + n^2 + n^2 + n + n^2 + n + n^2 + 2n + 1 + n^2 + 3n + 2) = \left(\frac{\hbar}{2m\omega}\right)^2 (6n^2 + 6n + 3).
\end{aligned}
$$

$$
E_r^1 = -\frac{m\omega^4}{8c^2}\cdot\frac{\hbar^2}{4m^2\omega^2}\cdot 3(2n^2+2n+1) = \boxed{-\frac{3}{32}\left(\frac{\hbar^2\omega^2}{mc^2}\right)(2n^2+2n+1).}
$$

Problem 7.18

Quoting the Laplacian in spherical coordinates (Eq. 4.13), we have, for states with no dependence on θ or ϕ:

$$
p^2 = -\hbar^2\nabla^2 = -\frac{\hbar^2}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right).
$$

Question: Is it Hermitian?

Using integration by parts (twice), and test functions $f(r)$ and $g(r)$:

$$
\begin{aligned}
\langle f|p^2 g\rangle &= -\hbar^2\int_0^\infty f\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dg}{dr}\right)4\pi r^2\,dr = -4\pi\hbar^2\int_0^\infty f\frac{d}{dr}\left(r^2\frac{dg}{dr}\right)dr \\
&= -4\pi\hbar^2\left\{r^2 f\frac{dg}{dr}\Big|_0^\infty - \int_0^\infty r^2\frac{df}{dr}\frac{dg}{dr}\,dr\right\} \\
&= -4\pi\hbar^2\left\{r^2 f\frac{dg}{dr}\Big|_0^\infty - r^2 g\frac{df}{dr}\Big|_0^\infty + \int_0^\infty \frac{d}{dr}\left(r^2\frac{df}{dr}\right)g\,dr\right\} \\
&= -4\pi\hbar^2\left(r^2 f\frac{dg}{dr} - r^2 g\frac{df}{dr}\right)\Big|_0^\infty + \langle p^2 f|g\rangle.
\end{aligned}
$$

The boundary term at infinity vanishes for functions $f(r)$ and $g(r)$ that go to zero exponentially; the boundary term at zero is killed by the factor r^2, as long as the functions (and their derivatives) are finite. So

$$
\langle f|p^2 g\rangle = \langle p^2 f|g\rangle,
$$

and hence p^2 is Hermitian.

As for p^4, first note that

$$
\begin{aligned}
\nabla^2\left[e^{-kr}\right] &= \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}e^{-kr}\right) = \frac{1}{r^2}\frac{d}{dr}\left(-kr^2e^{-kr}\right) \\
&= -\frac{k}{r^2}\left(2re^{-kr} - kr^2e^{-kr}\right) = \left(k^2 - \frac{2k}{r}\right)e^{-kr}.
\end{aligned}
$$

So

$$
\nabla^4\left[e^{-kr}\right] = \nabla^2\left[\left(k^2 - \frac{2k}{r}\right)e^{-kr}\right] = k^2\nabla^2\left[e^{-kr}\right] - 2k\nabla^2\left(\frac{1}{r}e^{-kr}\right).
$$

Now, for any functions f and g,

$$\nabla^2(fg) = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}(fg) = \boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}g + g\boldsymbol{\nabla}f) = 2\boldsymbol{\nabla}f\cdot\boldsymbol{\nabla}g + f\nabla^2 g + g\nabla^2 f,$$

so (using $\nabla^2(1/r) = -4\pi\,\delta^3(\mathbf{r})$)

$$\begin{aligned}
\nabla^2\left(\frac{1}{r}e^{-kr}\right) &= 2\boldsymbol{\nabla}\left(\frac{1}{r}\right)\cdot\boldsymbol{\nabla}\left(e^{-kr}\right) + \frac{1}{r}\nabla^2\left(e^{-kr}\right) + e^{-kr}\nabla^2\left(\frac{1}{r}\right)\\
&= 2\left(-\frac{1}{r^2}\hat{\mathbf{r}}\right)\cdot\left(-ke^{-kr}\hat{\mathbf{r}}\right) + \frac{1}{r}\left[\left(k^2 - \frac{2k}{r}\right)e^{-kr}\right] + e^{-kr}\left[-4\pi\delta^3(\mathbf{r})\right]\\
&= \frac{2k}{r^2}e^{-kr} + \frac{k^2}{r}e^{-kr} - \frac{2k}{r^2}e^{-kr} - 4\pi\delta^3(\mathbf{r}) = \frac{k^2}{r}e^{-kr} - 4\pi\delta^3(\mathbf{r}).
\end{aligned}$$

Therefore

$$\begin{aligned}
\nabla^4\left[e^{-kr}\right] &= k^2\left(k^2 - \frac{2k}{r}\right)e^{-kr} - 2k\left[\frac{k^2}{r}e^{-kr} - 4\pi\delta^3(\mathbf{r})\right]\\
&= \left(k^4 - \frac{4k^3}{r}\right)e^{-kr} + 8\pi k\delta^3(\mathbf{r}).
\end{aligned}$$

Then

$$\begin{aligned}
\langle e^{-jr}|\nabla^4 e^{-kr}\rangle &= \int e^{-jr}\left[\left(k^4 - \frac{4k^3}{r}\right)e^{-kr} + 8\pi k\delta^3(\mathbf{r})\right]d^3\mathbf{r}\\
&= 4\pi\int_0^\infty\left(k^4 - \frac{4k^3}{r}\right)e^{-(j+k)r}r^2\,dr + 8\pi k\\
&= 4\pi k\left[k^3\int_0^\infty r^2e^{-(j+k)r}\,dr - 4k^2\int_0^\infty re^{-(j+k)r}\,dr + 2\right]\\
&= 4\pi k\left[k^3\frac{2}{(j+k)^3} - 4k^2\frac{1}{(j+k)^2} + 2\right]\\
&= 8\pi k\left[\frac{k^3 - 2k^2(j+k) + (j+k)^3}{(j+k)^3}\right]\\
&= \frac{8\pi k}{(j+k)^3}\left(k^3 - 2k^2j - 2k^3 + j^3 + 3j^2k + 3jk^2 + k^3\right)\\
&= \frac{8\pi jk}{(j+k)^3}\left(j^2 + 3jk + k^2\right) = \langle\nabla^4 e^{-jr}|e^{-kr}\rangle.
\end{aligned}$$

(The final step follows immediately, because the penultimate expression is symmetric under $j \leftrightarrow k$.) Thus $p^4 = (\hbar^4/4m^4)\nabla^4$ is hermitian for functions of the form ψ_{n00}. [Actually, I've only proved it for functions of the form e^{-kr}, whereas $\psi_{n00} = f_n(r)e^{-r/na}$ (the exponential is multiplied by a polynomial of degree $n-1$). But remember, the potential problems come from boundary terms at $r \to 0$, and higher powers of r are only going to make such terms go to zero even more rapidly. It's e^{-kr} with *no* factor of r that's going to cause trouble if anything does. So we're safe.]

Problem 7.19

(a)

$$[\mathbf{L}\cdot\mathbf{S}, L_x] = [L_xS_x + L_yS_y + L_zS_z, L_x] = S_x\left[L_x, L_x\right] + S_y\left[L_y, L_x\right] + S_z\left[L_z, L_x\right]$$

$$= S_x(0) + S_y(-i\hbar L_z) + S_z(i\hbar L_y) = i\hbar(L_y S_z - L_z S_y) = i\hbar(\mathbf{L}\times\mathbf{S})_x.$$

Same goes for the other two components, so $\boxed{[\mathbf{L}\cdot\mathbf{S},\mathbf{L}] = i\hbar(\mathbf{L}\times\mathbf{S}).}$

(b) $[\mathbf{L}\cdot\mathbf{S},\mathbf{S}]$ is identical, only with $\mathbf{L}\leftrightarrow\mathbf{S}$: $\boxed{[\mathbf{L}\cdot\mathbf{S},\mathbf{S}] = i\hbar(\mathbf{S}\times\mathbf{L}).}$

(c) $[\mathbf{L}\cdot\mathbf{S},\mathbf{J}] = [\mathbf{L}\cdot\mathbf{S},\mathbf{L}] + [\mathbf{L}\cdot\mathbf{S},\mathbf{S}] = i\hbar(\mathbf{L}\times\mathbf{S}+\mathbf{S}\times\mathbf{L}) = \boxed{0.}$

(d) L^2 commutes with all components of $\mathbf{L}$ (and $\mathbf{S}$) , so $\boxed{\left[\mathbf{L}\cdot\mathbf{S},L^2\right] = 0.}$

(e) Likewise, $\boxed{\left[\mathbf{L}\cdot\mathbf{S},S^2\right] = 0.}$

(f) $\left[\mathbf{L}\cdot\mathbf{S},J^2\right] = \left[\mathbf{L}\cdot\mathbf{S},L^2\right] + \left[\mathbf{L}\cdot\mathbf{S},S^2\right] + 2\left[\mathbf{L}\cdot\mathbf{S},\mathbf{L}\cdot\mathbf{S}\right] = 0+0+0 \Longrightarrow \boxed{\left[\mathbf{L}\cdot\mathbf{S},J^2\right] = 0.}$

Problem 7.20

With the plus sign, $j = \ell + 1/2$ $(\ell = j - 1/2)$: Eq. 7.58 $\Rightarrow E_r^1 = -\dfrac{(E_n)^2}{2mc^2}\left(\dfrac{4n}{j} - 3\right)$.

$$\text{Equation 7.67} \Rightarrow E_{\rm so}^1 = \frac{(E_n)^2}{mc^2}\frac{n\left[j(j+1) - (j-\frac{1}{2})(j+\frac{1}{2}) - \frac{3}{4}\right]}{(j-\frac{1}{2})j(j+\frac{1}{2})}$$
$$= \frac{(E_n)^2}{mc^2}\frac{n(j^2+j-j^2+\frac{1}{4}-\frac{3}{4})}{(j-\frac{1}{2})j(j+\frac{1}{2})} = \frac{(E_n)^2}{mc^2}\frac{n}{j(j+\frac{1}{2})}.$$

$$E_{\rm fs}^1 = E_r^1 + E_{\rm so}^1 = \frac{(E_n)^2}{2mc^2}\left(-\frac{4n}{j} + 3 + \frac{2n}{j(j+\frac{1}{2})}\right)$$
$$= \frac{(E_n)^2}{2mc^2}\left\{3 + \frac{2n}{j(j+\frac{1}{2})}\left[1 - 2\left(j+\frac{1}{2}\right)\right]\right\} = \frac{(E_n)^2}{2mc^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right).$$

With the minus sign, $j = \ell - 1/2$ $(\ell = j + 1/2)$: Eq. 6.57 $\Rightarrow E_r^1 = -\dfrac{(E_n)^2}{2mc^2}\left(\dfrac{4n}{j+1} - 3\right)$.

$$\text{Equation 7.67} \Rightarrow E_{\rm so}^1 = \frac{(E_n)^2}{mc^2}\frac{n\left[j(j+1) - (j+\frac{1}{2})(j+\frac{3}{2}) - \frac{3}{4}\right]}{(j+\frac{1}{2})(j+1)(j+\frac{3}{2})}$$
$$= \frac{(E_n)^2}{mc^2}\frac{n(j^2+j-j^2-2j-\frac{3}{4}-\frac{3}{4})}{(j+\frac{1}{2})(j+1)(j+\frac{3}{2})} = \frac{(E_n)^2}{mc^2}\frac{-n}{(j+1)(j+\frac{1}{2})}.$$

$$E_{\rm fs}^1 = \frac{(E_n)^2}{2mc^2}\left[-\frac{4n}{j+1} + 3 - \frac{2n}{(j+1)(j+\frac{1}{2})}\right] = \frac{(E_n)^2}{2mc^2}\left\{3 - \frac{2n}{(j+1)(j+\frac{1}{2})}\left[1 + 2\left(j+\frac{1}{2}\right)\right]\right\}$$

$= \dfrac{(E_n)^2}{2mc^2}\left(3 - \dfrac{4n}{j+\frac{1}{2}}\right)$. For both signs, then, $E_{\rm fs}^1 = \dfrac{(E_n)^2}{2mc^2}\left(3 - \dfrac{4n}{j+\frac{1}{2}}\right)$. QED

Problem 7.21

$E_3^0 - E_2^0 = h\nu = \dfrac{2\pi\hbar c}{\lambda} = E_1\left(\dfrac{1}{9} - \dfrac{1}{4}\right) = -\dfrac{5}{36}E_1 \Rightarrow \lambda = -\dfrac{36}{5}\dfrac{2\pi\hbar c}{E_1};\quad E_1 = -13.6\,\text{eV};$

$\hbar c = 1.97\times 10^{-11}$ MeV·cm; $\quad \lambda = \dfrac{36}{5}\dfrac{(2\pi)(1.97\times 10^{-11}\times 10^6\ \text{eV}\cdot\text{cm})}{(13.6\ \text{eV})} = 6.55\times 10^{-5}\ \text{cm} = \boxed{655\ \text{nm.}}$

$\nu = \dfrac{c}{\lambda} = \dfrac{3.00\times 10^8\,\text{m/s}}{6.55\times 10^{-7}\,\text{m}} = \boxed{4.58\times 10^{14}\ \text{Hz.}}$ Equation 7.68 $\Rightarrow E_{fs}^1 = \dfrac{(E_n)^2}{2mc^2}\left(3 - \dfrac{4n}{j+\frac{1}{2}}\right)$:

<u>For $n=2$</u>: $\ell = 0$ or $\ell = 1$, so $j = 1/2$ or $3/2$. Thus $n = 2$ splits into *two* levels :

$$\underline{j=1/2}:\ E_2^1 = \frac{(E_2)^2}{2mc^2}\left(3-\frac{8}{1}\right) = -\frac{5}{2}\frac{(E_2)^2}{mc^2} = -\frac{5}{2}\left(\frac{1}{4}\right)^2\frac{(E_1)^2}{mc^2} = -\frac{5}{32}\frac{(13.6\,\text{eV})^2}{(.511\times 10^6\,\text{eV})} = -5.66\times 10^{-5}\text{eV}.$$

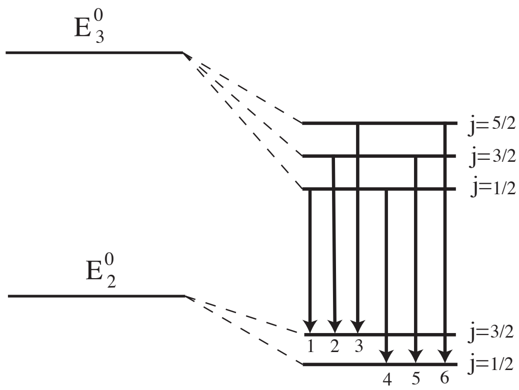
$$\underline{j=3/2}:\ E_2^1 = \frac{(E_2)^2}{2mc^2}\left(3-\frac{8}{2}\right) = -\frac{1}{2}\frac{(E_2)^2}{mc^2} = -\frac{1}{32}(3.62\times 10^{-4}\,\text{eV}) = -1.13\times 10^{-5}\text{eV}.$$

<u>For $n=3$</u>: $\ell = 0, 1$ or 2, so $j = 1/2, 3/2$ or $5/2$. Thus $n = 3$ splits into *three* levels :

$$\underline{j=1/2}:\ E_3^1 = \frac{(E_3)^2}{2mc^2}\left(3-\frac{12}{1}\right) = -\frac{9}{2}\frac{(E_3)^2}{mc^2} = -\frac{9}{2}\left(\frac{1}{9^2}\right)\frac{(E_1)^2}{mc^2} = -\frac{1}{18}(3.62\times 10^{-4}\text{eV}) = -2.01\times 10^{-5}\text{eV}.$$

$$\underline{j=3/2}:\ E_3^1 = \frac{(E_3)^2}{2mc^2}\left(3-\frac{12}{2}\right) = -\frac{3}{2}\frac{(E_3)^2}{mc^2} = -\frac{1}{54}(3.62\times 10^{-4}\,\text{eV}) = -0.67\times 10^{-5}\ \text{eV}.$$

$$\underline{j=5/2}:\ E_3^1 = \frac{(E_3)^2}{2mc^2}\left(3-\frac{12}{3}\right) = -\frac{1}{2}\frac{(E_3)^2}{mc^2} = -\frac{1}{162}(3.62\times 10^{-4}\,\text{eV}) = -0.22\times 10^{-5}\ \text{eV}.$$



There are *six* transitions here; their energies are $(E_3^0 + E_3^1) - (E_2^0 + E_2^1) = (E_3^0 - E_2^0) + \Delta E$, where $\Delta E \equiv E_3^1 - E_2^1$. Let $\beta \equiv (E_1)^2/mc^2 = 3.62\times 10^{-4}\,\text{eV}$. Then:

$$\underline{(\tfrac{1}{2}\to\tfrac{3}{2})}:\quad \Delta E = \left[\left(-\frac{1}{18}\right) - \left(-\frac{1}{32}\right)\right]\beta = -\frac{7}{288}\beta = -8.80\times 10^{-6}\ \text{eV}.$$

$$\underline{(\tfrac{3}{2}\to\tfrac{3}{2})}:\quad \Delta E = \left[\left(-\frac{1}{54}\right) - \left(-\frac{1}{32}\right)\right]\beta = \frac{11}{864}\beta = 4.61\times 10^{-6}\ \text{eV}.$$

$$\underline{(\tfrac{5}{2}\to\tfrac{3}{2})}:\quad \Delta E = \left[\left(-\frac{1}{162}\right) + \left(\frac{1}{32}\right)\right]\beta = \frac{65}{2592}\beta = 9.08\times 10^{-6}\ \text{eV}.$$

$$\underline{(\tfrac{1}{2}\to\tfrac{1}{2})}:\quad \Delta E = \left[\left(\frac{5}{32}\right) - \left(\frac{1}{18}\right)\right]\beta = \frac{29}{288}\beta = 36.45\times 10^{-6}\ \text{eV}.$$

$$\underline{(\frac{3}{2} \to \frac{1}{2})}: \quad \Delta E = \left[\left(-\frac{1}{54}\right) + \left(\frac{5}{32}\right)\right]\beta = \frac{119}{864}\beta = 49.86 \times 10^{-6}\,\text{eV}.$$

$$\underline{(\frac{5}{2} \to \frac{1}{2})}: \quad \Delta E = \left[\left(-\frac{1}{162}\right) + \left(\frac{5}{32}\right)\right]\beta = \frac{389}{2592}\beta = 54.33 \times 10^{-6}\,\text{eV}.$$

Conclusion: There are *six* lines; one of them ($\frac{1}{2} \to \frac{3}{2}$) has a frequency *less* than the unperturbed line, the other five have (slightly) *higher* frequencies. In order they are: $\frac{3}{2} \to \frac{3}{2}$; $\frac{5}{2} \to \frac{3}{2}$; $\frac{1}{2} \to \frac{1}{2}$; $\frac{3}{2} \to \frac{1}{2}$; $\frac{5}{2} \to \frac{1}{2}$. The frequency spacings are:

$\nu_2 - \nu_1$	$=$	$(\Delta E_2 - \Delta E_1)/2\pi\hbar$	$=$	3.23×10^9 Hz
$\nu_3 - \nu_2$	$=$	$(\Delta E_3 - \Delta E_2)/2\pi\hbar$	$=$	1.08×10^9 Hz
$\nu_4 - \nu_3$	$=$	$(\Delta E_4 - \Delta E_3)/2\pi\hbar$	$=$	6.60×10^9 Hz
$\nu_5 - \nu_4$	$=$	$(\Delta E_5 - \Delta E_4)/2\pi\hbar$	$=$	3.23×10^9 Hz
$\nu_6 - \nu_5$	$=$	$(\Delta E_6 - \Delta E_5)/2\pi\hbar$	$=$	1.08×10^9 Hz

Problem 7.22

$$\sqrt{\left(j+\frac{1}{2}\right)^2 - \alpha^2} = \left(j+\frac{1}{2}\right)\sqrt{1-\left(\frac{\alpha}{j+\frac{1}{2}}\right)^2} \approx \left(j+\frac{1}{2}\right)\left[1-\frac{1}{2}\left(\frac{\alpha}{j+\frac{1}{2}}\right)^2\right] = (j+\frac{1}{2}) - \frac{\alpha^2}{2(j+\frac{1}{2})}.$$

$$\frac{\alpha}{n-(j+\frac{1}{2})+\sqrt{(j+\frac{1}{2})^2-\alpha^2}} \approx \frac{\alpha}{n-(j+\frac{1}{2})+(j+\frac{1}{2})-\frac{\alpha^2}{2(j+\frac{1}{2})}} = \frac{\alpha}{n-\frac{\alpha^2}{2(j+\frac{1}{2})}}$$

$$= \frac{\alpha}{n\left[1-\frac{\alpha^2}{2n(j+\frac{1}{2})}\right]} \approx \frac{\alpha}{n}\left[1+\frac{\alpha^2}{2n(j+\frac{1}{2})}\right].$$

$$\left[1+\left(\frac{\alpha}{n-(j+\frac{1}{2})+\sqrt{(j+\frac{1}{2})^2-\alpha^2}}\right)^2\right]^{-1/2} \approx \left[1+\frac{\alpha^2}{n^2}\left(1+\frac{\alpha^2}{n(j+\frac{1}{2})}\right)\right]^{-1/2}$$

$$\approx 1-\frac{1}{2}\frac{\alpha^2}{n^2}\left(1+\frac{\alpha^2}{n(j+\frac{1}{2})}\right)+\frac{3}{8}\frac{\alpha^4}{n^4} = 1-\frac{\alpha^2}{2n^2}+\frac{\alpha^4}{2n^4}\left(\frac{-n}{j+\frac{1}{2}}+\frac{3}{4}\right).$$

$$E_{nj} \approx mc^2\left[1-\frac{\alpha^2}{2n^2}+\frac{\alpha^4}{2n^4}\left(\frac{-n}{j+\frac{1}{2}}+\frac{3}{4}\right)-1\right] = -\frac{\alpha^2 mc^2}{2n^2}\left[1+\frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}}-\frac{3}{4}\right)\right]$$

$$= -\frac{13.6\,\text{eV}}{n^2}\left[1+\frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}}-\frac{3}{4}\right)\right], \quad \text{confirming Eq. 7.69.}$$

Problem 7.23

Equation 7.60 $\Rightarrow \mathbf{B} = \frac{1}{4\pi\epsilon_0}\frac{e}{mc^2r^3}\mathbf{L}$. Say $L = \hbar$, $r = a$; then

$$B = \frac{1}{4\pi\epsilon_0}\frac{e\hbar}{mc^2a^3}$$

$$= \frac{(1.60\times10^{-19}\,\text{C})(1.05\times10^{-34}\,\text{J}\cdot\text{s})}{4\pi\left(8.9\times10^{-12}\,\text{C}^2/\text{N}\cdot\text{m}^2\right)\left(9.1\times10^{-31}\,\text{kg}\right)\left(3\times10^8\,\text{m/s}\right)^2\left(0.53\times10^{-10}\,\text{m}\right)^3} = \boxed{12\ \text{T}.}$$

So a "strong" Zeeman field is $B_{\text{ext}} \gg 10$ T, and a "weak" one is $B_{\text{ext}} \ll 10$ T. Incidentally, the earth's field (10^{-4} T) is definitely *weak*.

Problem 7.24

For $n = 2$, $\ell = 0$ ($j = 1/2$) or $\ell = 1$ ($j = 1/2$ or $3/2$). The eight states are:

$$\left.\begin{aligned} |1\rangle &= |2\ 0\ \tfrac{1}{2}\ \tfrac{1}{2}\rangle \\ |2\rangle &= |2\ 0\ \tfrac{1}{2}\ -\tfrac{1}{2}\rangle \end{aligned}\right\} g_J = \left[1 + \frac{(1/2)(3/2) + (3/4)}{2(1/2)(3/2)}\right] = 1 + \frac{3/2}{3/2} = 2.$$

$$\left.\begin{aligned} |3\rangle &= |2\ 1\ \tfrac{1}{2}\ \tfrac{1}{2}\rangle \\ |4\rangle &= |2\ 1\ \tfrac{1}{2}\ -\tfrac{1}{2}\rangle \end{aligned}\right\} g_J = \left[1 + \frac{(1/2)(3/2) - (1)(2) + (3/4)}{2(1/2)(3/2)}\right] = 1 + \frac{-1/2}{3/2} = 2/3.$$

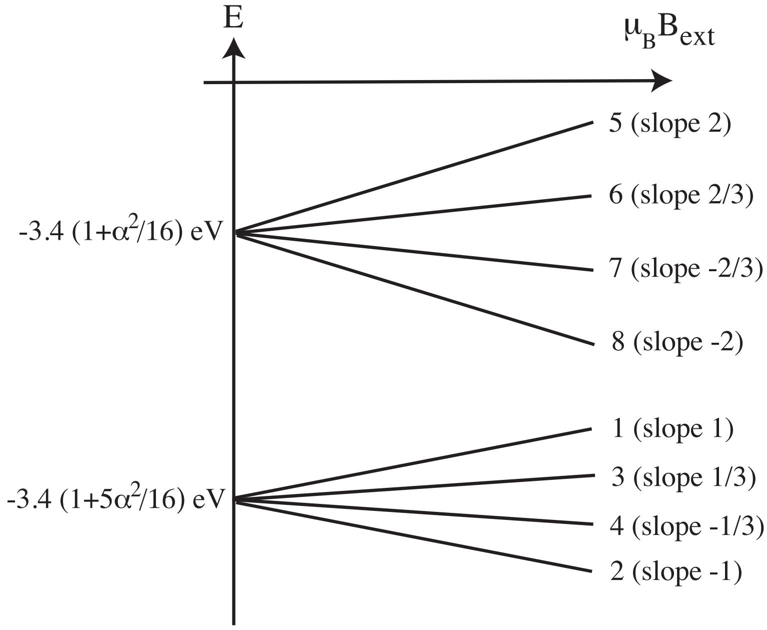
In these four cases, $E_{nj} = -\dfrac{13.6 \text{ eV}}{4}\left[1 + \dfrac{\alpha^2}{4}\left(\dfrac{2}{1} - \dfrac{3}{4}\right)\right] = -3.4 \text{ eV}\left(1 + \dfrac{5}{16}\alpha^2\right).$

$$\left.\begin{aligned} |5\rangle &= |2\ 1\ \tfrac{3}{2}\ \tfrac{3}{2}\rangle \\ |6\rangle &= |2\ 1\ \tfrac{3}{2}\ \tfrac{1}{2}\rangle \\ |7\rangle &= |2\ 1\ \tfrac{3}{2}\ -\tfrac{1}{2}\rangle \\ |8\rangle &= |2\ 1\ \tfrac{3}{2}\ -\tfrac{3}{2}\rangle \end{aligned}\right\} g_J = \left[1 + \frac{(3/2)(5/2) - (1)(2) + (3/4)}{2(3/2)(5/2)}\right] = 1 + \frac{5/2}{15/2} = 4/3.$$

In these four cases, $E_{nj} = -3.4 \text{ eV}\left[1 + \dfrac{\alpha^2}{4}\left(\dfrac{2}{2} - \dfrac{3}{4}\right)\right] = -3.4 \text{ eV}\left(1 + \dfrac{1}{16}\alpha^2\right).$

The energies are:

$$\boxed{\begin{aligned} E_1 &= -3.4 \text{ eV } \left(1 + \tfrac{5}{16}\alpha^2\right) + \mu_B B_{\text{ext}}. \\ E_2 &= -3.4 \text{ eV } \left(1 + \tfrac{5}{16}\alpha^2\right) - \mu_B B_{\text{ext}}. \\ E_3 &= -3.4 \text{ eV } \left(1 + \tfrac{5}{16}\alpha^2\right) + \tfrac{1}{3}\mu_B B_{\text{ext}}. \\ E_4 &= -3.4 \text{ eV } \left(1 + \tfrac{5}{16}\alpha^2\right) - \tfrac{1}{3}\mu_B B_{\text{ext}}. \\ E_5 &= -3.4 \text{ eV } \left(1 + \tfrac{1}{16}\alpha^2\right) + 2\mu_B B_{\text{ext}}. \\ E_6 &= -3.4 \text{ eV } \left(1 + \tfrac{1}{16}\alpha^2\right) + \tfrac{2}{3}\mu_B B_{\text{ext}}. \\ E_7 &= -3.4 \text{ eV } \left(1 + \tfrac{1}{16}\alpha^2\right) - \tfrac{2}{3}\mu_B B_{\text{ext}}. \\ E_8 &= -3.4 \text{ eV } \left(1 + \tfrac{1}{16}\alpha^2\right) - 2\mu_B B_{\text{ext}}. \end{aligned}}$$



Problem 7.25

The Wigner-Eckart theorem tells us that

$$\langle n'\,\ell'\,m'|\mathbf{V}|n\,\ell\,m\rangle = \left\{\begin{array}{c} \frac{1}{\sqrt{2}}C^{\ell\ 1\ \ell'}_{m-1\,m'} - \frac{1}{\sqrt{2}}C^{\ell\ 1\ \ell'}_{m\,0\,m'} \\ \frac{i}{\sqrt{2}}C^{\ell\ 1\ \ell'}_{m-1\,m'} + \frac{i}{\sqrt{2}}C^{\ell\ 1\ \ell'}_{m\,1\,m'} \\ C^{\ell\ 1\ \ell'}_{m\,0\,m'} \end{array}\right\} \langle n'\,\ell'||V||n\,\ell\rangle = \mathbf{M}\langle n'\,\ell'||V||n\,\ell\rangle,$$

where $\mathbf{M}$ stands for the coefficient in the curly brackets. By the same token,
$\langle n'\,\ell'\,m'|\mathbf{W}|n\,\ell\,m\rangle = \mathbf{M}\langle n'\,\ell'||W||n\,\ell\rangle$, with the *same* coefficients $\mathbf{M}$. So the two vectors are proportional.

Problem 7.26

$$E^1_{\text{fs}} = \langle n\ell m_\ell m_s|(H'_r + H'_{\text{so}})|n\ell m_\ell m_s\rangle = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{\ell+1/2} - 3\right] + \frac{e^2}{8\pi\epsilon_0 m^2c^2}\frac{\hbar^2 m_\ell m_s}{\ell(\ell+1/2)(\ell+1)n^3a^3}.$$

$$\text{Now}\left\{\begin{array}{lcl} \dfrac{2E_n^2}{mc^2} & = & \left(-\dfrac{2E_1}{mc^2}\right)\left(-\dfrac{E_1}{n^4}\right) = \dfrac{\alpha^2}{n^4}(13.6\text{ eV}). \quad \text{(Problem 7.14.)} \\ \dfrac{e^2\hbar^2}{8\pi\epsilon_0 m^2c^2a^3} & = & \dfrac{e^2\hbar^2(me^2)^3}{2\cdot 4\pi\epsilon_0 m^2c^2(4\pi\epsilon_0\hbar^2)^3} = \left[\dfrac{m}{2\hbar^2}\left(\dfrac{e^2}{4\pi\epsilon_0}\right)^2\right]\left(\dfrac{e^2}{4\pi\epsilon_0\hbar c}\right)^2 = \alpha^2(13.6\text{ eV}). \end{array}\right.$$

$$E^1_{\text{fs}} = \frac{13.6\text{ eV}}{n^3}\alpha^2\left\{-\frac{1}{(\ell+1/2)} + \frac{3}{4n} + \frac{m_\ell m_s}{\ell(\ell+1/2)(\ell+1)}\right\} = \frac{13.6\text{ eV}}{n^3}\alpha^2\left\{\frac{3}{4n} - \frac{\ell(\ell+1) - m_\ell m_s}{\ell(\ell+1/2)(l+1)}\right\}. \quad \text{QED}$$

Problem 7.27

The Bohr energy is the same for all of them: $E_2 = -13.6\text{ eV}/2^2 = -3.4$ eV. The Zeeman contribution is the second term in Eq. 7.83: $\mu_B B_{\text{ext}}(m_\ell + 2m_s)$. The fine structure is given by Eq. 7.86: $E^1_{\text{fs}} = (13.6\text{ eV}/8)\alpha^2\{\cdots\} = (1.7\text{ eV})\alpha^2\{\cdots\}$. In the table below I record the 8 states, the value of $(m_\ell + 2m_s)$, the value of $\{\cdots\} \equiv \frac{3}{8} - \left[\frac{\ell(\ell+1) - m_\ell m_s}{\ell(\ell+1/2)(\ell+1)}\right]$, and (in the last column) the total energy, $-3.4\text{ eV}\,[1 - (\alpha^2/2)\{\cdots\}] + (m_\ell + 2m_s)\mu_B B_{\text{ext}}$.

State $= \lvert n\ell m_\ell m_s\rangle$	$(m_\ell + 2m_s)$	$\{\cdots\}$	Total Energy
$\lvert 1\rangle = \lvert 2\ 0\ 0\ \frac{1}{2}\rangle$	1	$-5/8$	-3.4 eV $[1 + (5/16)\alpha^2] + \mu_B B_{\text{ext}}$
$\lvert 2\rangle = \lvert 2\ 0\ 0 - \frac{1}{2}\rangle$	-1	$-5/8$	-3.4 eV $[1 + (5/16)\alpha^2] - \mu_B B_{\text{ext}}$
$\lvert 3\rangle = \lvert 2\ 1\ 1\ \frac{1}{2}\rangle$	2	$-1/8$	-3.4 eV $[1 + (1/16)\alpha^2] + 2\mu_B B_{\text{ext}}$
$\lvert 4\rangle = \lvert 2\ 1 - 1 - \frac{1}{2}\rangle$	-2	$-1/8$	-3.4 eV $[1 + (1/16)\alpha^2] - 2\mu_B B_{\text{ext}}$
$\lvert 5\rangle = \lvert 2\ 1\ 0\ \frac{1}{2}\rangle$	1	$-7/24$	-3.4 eV $[1 + (7/48)\alpha^2] + \mu_B B_{\text{ext}}$
$\lvert 6\rangle = \lvert 2\ 1\ 0 - \frac{1}{2}\rangle$	-1	$-7/24$	-3.4 eV $[1 + (7/48)\alpha^2] - \mu_B B_{\text{ext}}$
$\lvert 7\rangle = \lvert 2\ 1\ 1 - \frac{1}{2}\rangle$	0	$-11/24$	-3.4 eV $[1 + (11/48)\alpha^2]$
$\lvert 8\rangle = \lvert 2\ 1 - 1\ \frac{1}{2}\rangle$	0	$-11/24$	-3.4 eV $[1 + (11/48)\alpha^2]$

Ignoring fine structure there are $\boxed{\text{five}}$ distinct levels—corresponding to the possible values of $(m_\ell + 2m_s)$:

$$\boxed{2 \quad (d=1);\ 1 \quad (d=2);\ 0 \quad (d=2);\ -1 \quad (d=2);\ -2 \quad (d=1).}$$

Problem 7.28

Equation 7.74 $\Rightarrow E^1_z = \frac{e}{2m}\mathbf{B}_{\text{ext}}\cdot\langle\mathbf{L} + 2\mathbf{S}\rangle = \frac{e}{2m}B_{\text{ext}}2m_s\hbar = 2m_s\mu_B B_{\text{ext}}$ (same as the Zeeman term in Eq. 7.83, with $m_l = 0$). Equation 7.69 $\Rightarrow E_{nj} = -\frac{13.6\text{ eV}}{n^2}\left[1 + \frac{\alpha^2}{n^2}\left(n - \frac{3}{4}\right)\right]$ (since $j = 1/2$). So the total energy is

$$\boxed{E = -\frac{13.6\text{ eV}}{n^2}\left[1 + \frac{\alpha^2}{n^2}\left(n - \frac{3}{4}\right)\right] + 2m_s\mu_B B_{\text{ext}}.}$$

Fine structure is the α^2 term: $E^1_{\text{fs}} = -\frac{13.6\text{ eV}}{n^4}\alpha^2\left(n - \frac{3}{4}\right) = \frac{13.6\text{ eV}}{n^3}\alpha^2\left(\frac{3}{4n} - 1\right)$, which is the same as Eq. 7.86, with the term in square brackets set equal to 1. QED

Problem 7.29

Equation 7.68 $\Rightarrow E^1_{\text{fs}} = \frac{E_2^2}{2mc^2}\left(3 - \frac{8}{j+1/2}\right) = \frac{E_1^2}{32mc^2}\left(3 - \frac{8}{j+1/2}\right)$; $\frac{E_1}{mc^2} = -\frac{\alpha^2}{2}$ (Problem 7.14), so

$$E^1_{\text{fs}} = -\frac{E_1}{32}\left(\frac{\alpha^2}{2}\right)\left(3 - \frac{8}{j+1/2}\right) = \frac{13.6\text{ eV}}{64}\alpha^2\left(3 - \frac{8}{j+1/2}\right) = \gamma\left(3 - \frac{8}{j+1/2}\right).$$

For $j = 1/2$ $(\psi_1, \psi_2, \psi_6, \psi_8)$, $H^1_{\text{fs}} = \gamma(3 - 8) = -5\gamma$. For $j = 3/2$ $(\psi_3, \psi_4, \psi_5, \psi_7)$, $H^1_{\text{fs}} = \gamma(3 - \frac{8}{2}) = -\gamma$.

This confirms all the γ terms in $-\mathsf{W}$ (p. 309). Meanwhile, $H'_z = (e/2m)B_{\text{ext}}(L_z + 2S_z)$ (Eq. 7.73); $\psi_1, \psi_2, \psi_3, \psi_4$ are eigenstates of L_z and S_z; for these there are only diagonal elements:

$$\langle H'_z\rangle = \frac{e\hbar}{2m}B_{\text{ext}}(m_l + 2m_s) = (m_l + 2m_s)\beta;\quad \langle H'_z\rangle_{11} = \beta;\quad \langle H'_z\rangle_{22} = -\beta;\quad \langle H'_z\rangle_{33} = 2\beta;\quad \langle H'_z\rangle_{44} = -2\beta.$$

This confirms the upper left corner of $-\mathsf{W}$. Finally:

$$\left.\begin{aligned}
(L_z+2S_z)|\psi_5\rangle &= +\hbar\sqrt{\tfrac{2}{3}}|1\ 0\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\\
(L_z+2S_z)|\psi_6\rangle &= -\hbar\sqrt{\tfrac{1}{3}}|1\ 0\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\\
(L_z+2S_z)|\psi_7\rangle &= -\hbar\sqrt{\tfrac{2}{3}}|1\ 0\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle\\
(L_z+2S_z)|\psi_8\rangle &= -\hbar\sqrt{\tfrac{1}{3}}|1\ 0\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle
\end{aligned}\right\}\ \text{so}\
\begin{aligned}
\langle H_z'\rangle_{55} &= (2/3)\beta,\\
\langle H_z'\rangle_{66} &= (1/3)\beta,\\
\langle H_z'\rangle_{77} &= -(2/3)\beta,\\
\langle H_z'\rangle_{88} &= -(1/3)\beta,\\
\langle H_z'\rangle_{56} &= \langle H_z'\rangle_{65} = -(\sqrt{2}/3)\beta,\\
\langle H_z'\rangle_{78} &= \langle H_z'\rangle_{87} = -(\sqrt{2}/3)\beta,
\end{aligned}$$

which confirms the remaining elements.

Problem 7.30

There are eighteen $n=3$ states (in general, $2n^2$).

WEAK FIELD

Equation 7.69 $\Rightarrow E_{3j} = -\dfrac{13.6\text{ eV}}{9}\left[1+\dfrac{\alpha^2}{9}\left(\dfrac{3}{j+1/2}-\dfrac{3}{4}\right)\right] = -1.51\text{ eV}\left[1+\dfrac{\alpha^2}{3}\left(\dfrac{1}{j+1/2}-\dfrac{1}{4}\right)\right].$

Equation 7.79 $\Rightarrow E_z^1 = g_J m_j \mu_B B_{\text{ext}}$.

State $\|3\ \ell\ j\ m_j\rangle$		g_J(Eq. 6.75)	$\frac{1}{3}\left(\frac{1}{j+1/2}-\frac{1}{4}\right)$	Total Energy
$\ell=0,\ j=1/2$	$\|3\ 0\ \frac{1}{2}\ \frac{1}{2}\rangle$	2	1/4	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{4}\right)+\mu_B B_{\text{ext}}$
$\ell=0,\ j=1/2$	$\|3\ 0\ \frac{1}{2}\ -\frac{1}{2}\rangle$	2	1/4	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{4}\right)-\mu_B B_{\text{ext}}$
$\ell=1,\ j=1/2$	$\|3\ 1\ \frac{1}{2}\ \frac{1}{2}\rangle$	2/3	1/4	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{4}\right)+\frac{1}{3}\mu_B B_{\text{ext}}$
$\ell=1,\ j=1/2$	$\|3\ 1\ \frac{1}{2}\ -\frac{1}{2}\rangle$	2/3	1/4	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{4}\right)-\frac{1}{3}\mu_B B_{\text{ext}}$
$\ell=1,\ j=3/2$	$\|3\ 1\ \frac{3}{2}\ \frac{3}{2}\rangle$	4/3	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right)+2\mu_B B_{\text{ext}}$
$\ell=1,\ j=3/2$	$\|3\ 1\ \frac{3}{2}\ \frac{1}{2}\rangle$	4/3	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right)+\frac{2}{3}\mu_B B_{\text{ext}}$
$\ell=1,\ j=3/2$	$\|3\ 1\ \frac{3}{2}\ -\frac{1}{2}\rangle$	4/3	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right)-\frac{2}{3}\mu_B B_{\text{ext}}$
$\ell=1,\ j=3/2$	$\|3\ 1\ \frac{3}{2}\ -\frac{3}{2}\rangle$	4/3	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right)-2\mu_B B_{\text{ext}}$
$\ell=2,\ j=3/2$	$\|3\ 2\ \frac{3}{2}\ \frac{3}{2}\rangle$	4/5	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right)+\frac{6}{5}\mu_B B_{\text{ext}}$
$\ell=2,\ j=3/2$	$\|3\ 2\ \frac{3}{2}\ \frac{1}{2}\rangle$	4/5	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right)+\frac{2}{5}\mu_B B_{\text{ext}}$
$\ell=2,\ j=3/2$	$\|3\ 2\ \frac{3}{2}\ -\frac{1}{2}\rangle$	4/5	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right)-\frac{2}{5}\mu_B B_{\text{ext}}$
$\ell=2,\ j=3/2$	$\|3\ 2\ \frac{3}{2}\ -\frac{3}{2}\rangle$	4/5	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right)-\frac{6}{5}\mu_B B_{\text{ext}}$
$\ell=2,\ j=5/2$	$\|3\ 2\ \frac{5}{2}\ \frac{5}{2}\rangle$	6/5	1/36	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{36}\right)+3\mu_B B_{\text{ext}}$
$\ell=2,\ j=5/2$	$\|3\ 2\ \frac{5}{2}\ \frac{3}{2}\rangle$	6/5	1/36	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{36}\right)+\frac{9}{5}\mu_B B_{\text{ext}}$
$\ell=2,\ j=5/2$	$\|3\ 2\ \frac{5}{2}\ \frac{1}{2}\rangle$	6/5	1/36	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{36}\right)+\frac{3}{5}\mu_B B_{\text{ext}}$
$\ell=2,\ j=5/2$	$\|3\ 2\ \frac{5}{2}\ -\frac{1}{2}\rangle$	6/5	1/36	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{36}\right)-\frac{3}{5}\mu_B B_{\text{ext}}$
$\ell=2,\ j=5/2$	$\|3\ 2\ \frac{5}{2}\ -\frac{3}{2}\rangle$	6/5	1/36	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{36}\right)-\frac{9}{5}\mu_B B_{\text{ext}}$
$\ell=2,\ j=5/2$	$\|3\ 2\ \frac{5}{2}\ -\frac{5}{2}\rangle$	6/5	1/36	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{36}\right)-3\mu_B B_{\text{ext}}$

STRONG FIELD

Equation 7.83 $\Rightarrow -1.51\,\text{eV} + (m_\ell + 2m_s)\mu_B B_{\text{ext}}$;

$$\text{Equation 7.86} \Rightarrow \frac{13.6\,\text{eV}}{27}\alpha^2\left\{\frac{1}{4} - \left[\frac{\ell(\ell+1) - m_\ell m_s}{\ell(\ell+1/2)(\ell+1)}\right]\right\} = -1.51\text{ eV}\frac{\alpha^2}{3}\left\{\left[\frac{\ell(\ell+1) - m_\ell m_s}{\ell(\ell+1/2)(\ell+1)} - \frac{1}{4}\right]\right\}.$$

$$E_{\text{tot}} = -1.51\text{ eV}(1+\alpha^2 A) + (m_\ell + 2m_s)\mu_B B_{\text{ext}}, \text{ where } A \equiv \frac{1}{3}\left\{\left[\frac{\ell(\ell+1) - m_\ell m_s}{\ell(\ell+1/2)(\ell+1)} - \frac{1}{4}\right]\right\}.$$

These terms are given in the table below:

State	$\vert n\ \ell\ m_\ell\ m_s\rangle$	$(m_\ell + 2m_s)$	A	Total Energy
$\ell = 0$	$\vert 3\ 0\ 0\ \frac{1}{2}\rangle$	1	1/4	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{4}\right) + \mu_B B_{\text{ext}}$
$\ell = 0$	$\vert 3\ 0\ 0 -\frac{1}{2}\rangle$	-1	1/4	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{4}\right) - \mu_B B_{\text{ext}}$
$\ell = 1$	$\vert 3\ 1\ 1\ \frac{1}{2}\rangle$	2	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right) + 2\mu_B B_{\text{ext}}$
$\ell = 1$	$\vert 3\ 1 -1 -\frac{1}{2}\rangle$	-2	1/12	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{12}\right) - 2\mu_B B_{\text{ext}}$
$\ell = 1$	$\vert 3\ 1\ 0\ \frac{1}{2}\rangle$	1	5/36	$-1.51\text{ eV}\left(1+\frac{5\alpha^2}{36}\right) + \mu_B B_{\text{ext}}$
$\ell = 1$	$\vert 3\ 1\ 0 -\frac{1}{2}\rangle$	-1	5/36	$-1.51\text{ eV}\left(1+\frac{5\alpha^2}{36}\right) - \mu_B B_{\text{ext}}$
$\ell = 1$	$\vert 3\ 1 -1\ \frac{1}{2}\rangle$	0	7/36	$-1.51\text{ eV}\left(1+\frac{7\alpha^2}{36}\right)$
$\ell = 1$	$\vert 3\ 1\ 1 -\frac{1}{2}\rangle$	0	7/36	$-1.51\text{ eV}\left(1+\frac{7\alpha^2}{36}\right)$
$\ell = 2$	$\vert 3\ 2\ 2\ \frac{1}{2}\rangle$	3	1/36	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{36}\right) + 3\mu_B B_{\text{ext}}$
$\ell = 2$	$\vert 3\ 2 -2 -\frac{1}{2}\rangle$	-3	1/36	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{36}\right) - 3\mu_B B_{\text{ext}}$
$\ell = 2$	$\vert 3\ 2\ 1\ \frac{1}{2}\rangle$	2	7/180	$-1.51\text{ eV}\left(1+\frac{7\alpha^2}{180}\right) + 2\mu_B B_{\text{ext}}$
$\ell = 2$	$\vert 3\ 2 -1 -\frac{1}{2}\rangle$	-2	7/180	$-1.51\text{ eV}\left(1+\frac{7\alpha^2}{180}\right) - 2\mu_B B_{\text{ext}}$
$\ell = 2$	$\vert 3\ 2\ 0\ \frac{1}{2}\rangle$	1	1/20	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{20}\right) + \mu_B B_{\text{ext}}$
$\ell = 2$	$\vert 3\ 2\ 0 -\frac{1}{2}\rangle$	-1	1/20	$-1.51\text{ eV}\left(1+\frac{\alpha^2}{20}\right) - \mu_B B_{\text{ext}}$
$\ell = 2$	$\vert 3\ 2 -1\ \frac{1}{2}\rangle$	0	11/180	$-1.51\text{ eV}\left(1+\frac{11\alpha^2}{180}\right)$
$\ell = 2$	$\vert 3\ 2\ 1 -\frac{1}{2}\rangle$	0	11/180	$-1.51\text{ eV}\left(1+\frac{11\alpha^2}{180}\right)$
$\ell = 2$	$\vert 3\ 2 -2\ \frac{1}{2}\rangle$	-1	13/180	$-1.51\text{ eV}\left(1+\frac{13\alpha^2}{180}\right) - \mu_B B_{\text{ext}}$
$\ell = 2$	$\vert 3\ 2\ 2 -\frac{1}{2}\rangle$	1	13/180	$-1.51\text{ eV}\left(1+\frac{13\alpha^2}{180}\right) + \mu_B B_{\text{ext}}$

INTERMEDIATE FIELD

As in the book, I'll use the basis $|n\ \ell\ j\ m_j\rangle$ (same as for weak field); then the fine structure matrix elements are diagonal: Eq. 7.68 $\Rightarrow$

$$E^1_{\text{fs}} = \frac{E_3^2}{2mc^2}\left(3 - \frac{12}{j+1/2}\right) = \frac{E_1^2}{54mc^2}\left(1 - \frac{4}{j+1/2}\right) = -\frac{E_1\alpha^2}{108}\left(1 - \frac{4}{j+1/2}\right) = 3\gamma\left(1 - \frac{4}{j+1/2}\right),$$

$\gamma \equiv \dfrac{13.6\text{ eV}}{324}\alpha^2$. For $j = 1/2$, $E^1_{\text{fs}} = -9\gamma$; for $j = 3/2, E^1_{\text{fs}} = -3\gamma$; for $j = 5/2, E^1_{\text{fs}} = -\gamma$.

The Zeeman Hamiltonian is Eq. 7.73: $H_z' = \frac{1}{\hbar}(L_z + 2S_z)\mu_B B_{\text{ext}}$. The first eight states ($\ell = 0$ and $\ell = 1$) are the same as before (p. 309), so the β terms in W are unchanged; recording just the non-zero blocks of $-$W:

$$(9\gamma-\beta),(9\gamma+\beta),(3\gamma-2\beta),(3\gamma+2\beta),\begin{pmatrix}(3\gamma-\frac{2}{3}\beta) & \frac{\sqrt{2}}{3}\beta\\ \frac{\sqrt{2}}{3}\beta & (9\gamma-\frac{1}{3}\beta)\end{pmatrix},\begin{pmatrix}(3\gamma+\frac{2}{3}\beta) & \frac{\sqrt{2}}{3}\beta\\ \frac{\sqrt{2}}{3}\beta & (9\gamma+\frac{1}{3}\beta)\end{pmatrix}.$$

The other 10 states ($\ell = 2$) must first be decomposed into eigenstates of L_z and S_z:

$$|\tfrac{5}{2}\ \tfrac{5}{2}\rangle = |2\ 2\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle \implies (\gamma-3\beta)$$

$$|\tfrac{5}{2}-\tfrac{5}{2}\rangle = |2-2\rangle|\tfrac{1}{2}-\tfrac{1}{2}\rangle \implies (\gamma+3\beta)$$

$$\left.\begin{aligned}|\tfrac{5}{2}\ \tfrac{3}{2}\rangle &= \sqrt{\tfrac{1}{5}}|2\ 2\rangle|\tfrac{1}{2}-\tfrac{1}{2}\rangle + \sqrt{\tfrac{4}{5}}|2\ 1\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\\ |\tfrac{3}{2}\ \tfrac{3}{2}\rangle &= \sqrt{\tfrac{4}{5}}|2\ 2\rangle|\tfrac{1}{2}-\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{5}}|2\ 1\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\end{aligned}\right\}\implies\begin{pmatrix}(\gamma-\frac{9}{5}\beta) & \frac{2}{5}\beta\\ \frac{2}{5}\beta & (3\gamma-\frac{6}{5}\beta)\end{pmatrix}$$

$$\left.\begin{aligned}|\tfrac{5}{2}\ \tfrac{1}{2}\rangle &= \sqrt{\tfrac{2}{5}}|2\ 1\rangle|\tfrac{1}{2}-\tfrac{1}{2}\rangle + \sqrt{\tfrac{3}{5}}|2\ 0\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\\ |\tfrac{3}{2}\ \tfrac{1}{2}\rangle &= \sqrt{\tfrac{3}{5}}|2\ 1\rangle|\tfrac{1}{2}-\tfrac{1}{2}\rangle - \sqrt{\tfrac{2}{5}}|2\ 0\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\end{aligned}\right\}\implies\begin{pmatrix}(\gamma-\frac{3}{5}\beta) & \frac{\sqrt{6}}{5}\beta\\ \frac{\sqrt{6}}{5}\beta & (3\gamma-\frac{2}{5}\beta)\end{pmatrix}$$

$$\left.\begin{aligned}|\tfrac{5}{2}-\tfrac{1}{2}\rangle &= \sqrt{\tfrac{3}{5}}|2\ 0\rangle|\tfrac{1}{2}-\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{5}}|2-1\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\\ |\tfrac{3}{2}-\tfrac{1}{2}\rangle &= \sqrt{\tfrac{2}{5}}|2\ 0\rangle|\tfrac{1}{2}-\tfrac{1}{2}\rangle - \sqrt{\tfrac{3}{5}}|2-1\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\end{aligned}\right\}\implies\begin{pmatrix}(\gamma+\frac{3}{5}\beta) & \frac{\sqrt{6}}{5}\beta\\ \frac{\sqrt{6}}{5}\beta & (3\gamma+\frac{2}{5}\beta)\end{pmatrix}$$

$$\left.\begin{aligned}|\tfrac{5}{2}-\tfrac{3}{2}\rangle &= \sqrt{\tfrac{4}{5}}|2-1\rangle|\tfrac{1}{2}-\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{5}}|2-2\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\\ |\tfrac{3}{2}-\tfrac{3}{2}\rangle &= \sqrt{\tfrac{1}{5}}|2-1\rangle|\tfrac{1}{2}-\tfrac{1}{2}\rangle - \sqrt{\tfrac{4}{5}}|2-2\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\end{aligned}\right\}\implies\begin{pmatrix}(\gamma+\frac{9}{5}\beta) & \frac{2}{5}\beta\\ \frac{2}{5}\beta & (3\gamma+\frac{6}{5}\beta)\end{pmatrix}$$

[*Sample Calculation:* For the last two, letting $Q \equiv \frac{1}{\hbar}(L_z + 2S_z)$, we have
$Q|\frac{5}{2}-\frac{3}{2}\rangle = -2\sqrt{\frac{4}{5}}|2-1\rangle|\frac{1}{2}-\frac{1}{2}\rangle - \sqrt{\frac{1}{5}}|2-2\rangle|\frac{1}{2}\ \frac{1}{2}\rangle$;
$Q|\frac{3}{2}-\frac{3}{2}\rangle = -2\sqrt{\frac{1}{5}}|2-1\rangle|\frac{1}{2}-\frac{1}{2}\rangle + \sqrt{\frac{4}{5}}|2-2\rangle|\frac{1}{2}\ \frac{1}{2}\rangle$.
$\langle\frac{5}{2}-\frac{3}{2}|Q|\frac{5}{2}-\frac{3}{2}\rangle = (-2)\frac{4}{5} - \frac{1}{5} = -\frac{9}{5}$; $\langle\frac{3}{2}-\frac{3}{2}|Q|\frac{3}{2}-\frac{3}{2}\rangle = (-2)\frac{1}{5} - \frac{4}{5} = -\frac{6}{5}$;
$\langle\frac{5}{2}-\frac{3}{2}|Q|\frac{3}{2}-\frac{3}{2}\rangle = -2\sqrt{\frac{4}{5}}\sqrt{\frac{1}{5}} + \sqrt{\frac{1}{5}}\sqrt{\frac{4}{5}} = -\frac{4}{5} + \frac{2}{5} = -\frac{2}{5} = \langle\frac{3}{2}-\frac{3}{2}|Q|\frac{5}{2}-\frac{3}{2}\rangle$.]

So the 18×18 matrix $-$W splits into six 1×1 blocks and six 2×2 blocks. We need the eigenvalues of the 2×2 blocks. This means solving 3 characteristic equations (the other 3 are obtained trivially by changing the sign of β):

$$\left(3\gamma - \frac{2}{3}\beta - \lambda\right)\left(9\gamma - \frac{1}{3}\beta - \lambda\right) - \frac{2}{9}\beta^2 = 0 \implies \lambda^2 + \lambda(\beta - 12\gamma) + \gamma(27\gamma - 7\beta) = 0.$$

$$\left(\gamma - \frac{9}{5}\beta - \lambda\right)\left(3\gamma - \frac{6}{5}\beta - \lambda\right) - \frac{4}{25}\beta^2 = 0 \implies \lambda^2 + \lambda(3\beta - 4\gamma) + \left(3\gamma^2 - \frac{33}{5}\gamma\beta + 2\beta^2\right) = 0.$$

$$\left(\gamma - \frac{3}{5}\beta - \lambda\right)\left(3\gamma - \frac{2}{5}\beta - \lambda\right) - \frac{6}{25}\beta^2 = 0 \implies \lambda^2 + \lambda(\beta - 4\gamma) + \gamma\left(3\gamma - \frac{11}{5}\beta\right) = 0.$$

The solutions are:

$$\begin{aligned}\lambda &= -\beta/2 + 6\gamma \pm \sqrt{(\beta/2)^2 + \beta\gamma + 9\gamma^2} \\ \lambda &= -3\beta/2 + 2\gamma \pm \sqrt{(\beta/2)^2 + \tfrac{3}{5}\beta\gamma + \gamma^2} \\ \lambda &= -\beta/2 + 2\gamma \pm \sqrt{(\beta/2)^2 + \tfrac{1}{5}\beta\gamma + \gamma^2}\end{aligned} \quad \Rightarrow \quad \boxed{\begin{aligned}\epsilon_1 &= E_3 - 9\gamma + \beta \\ \epsilon_2 &= E_3 - 3\gamma + 2\beta \\ \epsilon_3 &= E_3 - \gamma + 3\beta \\ \epsilon_4 &= E_3 - 6\gamma + \beta/2 + \sqrt{9\gamma^2 + \beta\gamma + \beta^2/4} \\ \epsilon_5 &= E_3 - 6\gamma + \beta/2 - \sqrt{9\gamma^2 + \beta\gamma + \beta^2/4} \\ \epsilon_6 &= E_3 - 2\gamma + 3\beta/2 + \sqrt{\gamma^2 + \tfrac{3}{5}\beta\gamma + \beta^2/4} \\ \epsilon_7 &= E_3 - 2\gamma + 3\beta/2 - \sqrt{\gamma^2 + \tfrac{3}{5}\beta\gamma + \beta^2/4} \\ \epsilon_8 &= E_3 - 2\gamma + \beta/2 + \sqrt{\gamma^2 + \tfrac{1}{5}\beta\gamma + \beta^2/4} \\ \epsilon_9 &= E_3 - 2\gamma + \beta/2 - \sqrt{\gamma^2 + \tfrac{1}{5}\beta\gamma + \beta^2/4}\end{aligned}}$$

(The other 9 ϵ's are the same, but with $\beta \to -\beta$.) Here $\gamma = \frac{13.6\text{ eV}}{324}\alpha^2$, and $\beta = \mu_B B_{\text{ext}}$.

In the weak-field limit ($\beta \ll \gamma$):

$$\epsilon_4 \approx E_3 - 6\gamma + \beta/2 + 3\gamma\sqrt{1 + \beta/9\gamma} \approx E_3 - 6\gamma + \beta/2 + 3\gamma(1 + \beta/18\gamma) = E_3 - 3\gamma + \frac{2}{3}\beta.$$

$$\epsilon_5 \approx E_3 - 6\gamma + \beta/2 - 3\gamma(1 + \beta/18\gamma) = E_3 - 9\gamma + \frac{1}{3}\beta.$$

$$\epsilon_6 \approx E_3 - 2\gamma + 3\beta/2 + \gamma(1 + 3\beta/10\gamma) = E_3 - \gamma + \frac{9}{5}\beta.$$

$$\epsilon_7 \approx E_3 - 2\gamma + 3\beta/2 - \gamma(1 + 3\beta/10\gamma) = E_3 - 3\gamma + \frac{6}{5}\beta.$$

$$\epsilon_8 \approx E_3 - 2\gamma + \beta/2 + \gamma(1 + \beta/10\gamma) = E_3 - \gamma + \frac{3}{5}\beta.$$

$$\epsilon_9 \approx E_3 - 2\gamma + \beta/2 - \gamma(1 + \beta/10\gamma) = E_3 - 3\gamma + \frac{2}{5}\beta.$$

Noting that $\gamma = -(E_3/36)\alpha^2 = \frac{1.51\text{ eV}}{36}\alpha^2$, we see that the weak field energies are recovered as in the first table.

In the strong-field limit ($\beta \gg \gamma$):

$$\epsilon_4 \approx E_3 - 6\gamma + \beta/2 + \beta/2\sqrt{1 + 4\gamma/\beta} \approx E_3 - 6\gamma + \beta/2 + \beta/2(1 + 2\gamma/\beta) = E_3 - 5\gamma + \beta.$$

$$\epsilon_5 \approx E_3 - 6\gamma + \beta/2 - \beta/2(1 + 2\gamma/\beta) = E_3 - 7\gamma.$$

$$\epsilon_6 \approx E_3 - 2\gamma + 3\beta/2 + \beta/2(1 + 6\gamma/5\beta) = E_3 - \frac{7}{5}\gamma + 2\beta.$$

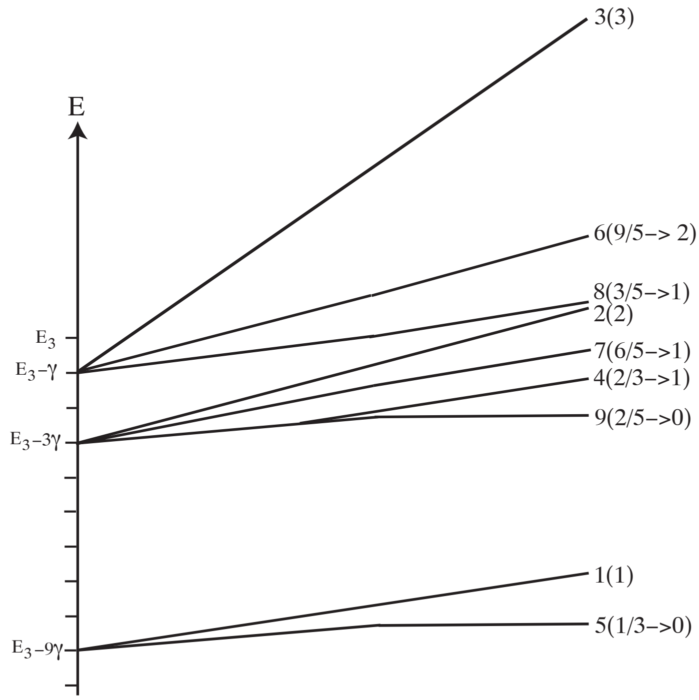
$$\epsilon_7 \approx E_3 - 2\gamma + 3\beta/2 - \beta/2(1 + 6\gamma/5\beta) = E_3 - \frac{13}{5}\gamma + \beta.$$

$$\epsilon_8 \approx E_3 - 2\gamma + \beta/2 + \beta/2(1 + 2\gamma/5\beta) = E_3 - \frac{9}{5}\gamma + \beta.$$

$$\epsilon_9 \approx E_3 - 2\gamma + \beta/2 - \beta/2(1 + 2\gamma/5\beta) = E_3 - \frac{11}{5}\gamma.$$

Again, these reproduce the strong-field results in the second table.

In the figure below each line is labeled by the level number and (in parentheses) the starting and ending slope; for each line there is a corresponding one starting from the same point but sloping *down*.



Problem 7.31

$I \equiv \int (\mathbf{a}\cdot\hat{r})(\mathbf{b}\cdot\hat{r})\sin\theta\, d\theta\, d\phi$

$= \int (a_x \sin\theta\cos\phi + a_y \sin\theta\sin\phi + a_z\cos\theta)(b_x \sin\theta\cos\phi + b_y\sin\theta\sin\phi + b_z\cos\theta)\sin\theta\, d\theta\, d\phi.$

But $\displaystyle\int_0^{2\pi}\sin\phi\, d\phi = \int_0^{2\pi}\cos\phi\, d\phi = \int_0^{2\pi}\sin\phi\cos\phi\, d\phi = 0,$ so only three terms survive :

$$I = \int (a_x b_x \sin^2\theta\cos^2\phi + a_y b_y \sin^2\theta\sin^2\phi + a_z b_z\cos^2\theta)\sin\theta\, d\theta\, d\phi.$$

But $\displaystyle\int_0^{2\pi}\sin^2\phi\, d\phi = \int_0^{2\pi}\cos^2\phi\, d\phi = \pi, \quad \int_0^{2\pi} d\phi = 2\pi,$ so

$$I = \int_0^{\pi}\left[\pi(a_x b_x + a_y b_y)\sin^2\theta + 2\pi a_z b_z\cos^2\theta\right]\sin\theta\, d\theta. \quad \text{But} \int_0^{\pi}\sin^3\theta\, d\theta = \frac{4}{3}, \int_0^{\pi}\cos^2\theta\sin\theta\, d\theta = \frac{2}{3},$$

so $\displaystyle I = \pi(a_x b_x + a_y b_y)\frac{4}{3} + 2\pi a_z b_z\frac{2}{3} = \frac{4\pi}{3}(a_x b_x + a_y b_y + a_z b_z) = \frac{4\pi}{3}(\mathbf{a}\cdot\mathbf{b}).$ QED

[Alternatively, noting that I has to be a *scalar* bilinear in $\mathbf{a}$ and $\mathbf{b}$, we know immediately that $I = A(\mathbf{a}\cdot\mathbf{b})$, where A is some constant (same for all $\mathbf{a}$ and $\mathbf{b}$). To determine A, pick $\mathbf{a} = \mathbf{b} = \hat{k}$; then $I = A = \int\cos^2\theta\sin\theta\, d\theta\, d\phi = 4\pi/3$.]

For states with $\ell = 0$, the wave function is independent of θ and ϕ ($Y_0^0 = 1/\sqrt{4\pi}$), so

$$\left\langle \frac{3(\mathbf{S}_p\cdot\hat{r})(\mathbf{S}_e\cdot\hat{r}) - \mathbf{S}_p\cdot\mathbf{S}_e}{r^3}\right\rangle = \left\{\int_0^{\infty}\frac{1}{r^3}|\psi(r)|^2 r^2 dr\right\}\int\left[3(\mathbf{S}_p\cdot\hat{r})(\mathbf{S}_e\cdot\hat{r}) - \mathbf{S}_p\cdot\mathbf{S}_e\right]\sin\theta\, d\theta\, d\phi.$$

The first angular integral is $3(4\pi/3)(\mathbf{S}_p\cdot\mathbf{S}_e) = 4\pi(\mathbf{S}_p\cdot\mathbf{S}_e)$, while the second is $-(\mathbf{S}_p\cdot\mathbf{S}_e)\int\sin\theta\,d\theta\,d\phi = -4\pi(\mathbf{S}_p\cdot\mathbf{S}_e)$, so the two cancel, and the result is zero. QED [Actually, there is a little sleight-of-hand here, since for $\ell = 0$, $\psi \to$ constant as $r \to 0$, and hence the radial integral diverges logarithmically at the origin. Technically, the first term in Eq. 7.90 is the field outside an infinitesimal *sphere*; the delta-function gives the field *inside*. For this reason it is correct to do the angular integral first (getting zero) and not worry about the radial integral.]

Problem 7.32

From Eq. 7.93 we see that $\Delta E \propto \left(\dfrac{g}{m_p m_e a^3}\right)$; we want reduced mass in a, but *not* in $m_p m_e$ (which come from Eq. 7.89); the notation in Eq. 7.97 obscures this point.

(a) g and m_p are unchanged; $m_e \to m_\mu = 207 m_e$, and $a \to a_\mu$. From Eq. 4.72, $a \propto 1/m$, so

$$\frac{a}{a_\mu} = \frac{m_\mu(\text{reduced})}{m_e} = \frac{m_\mu m_p}{m_\mu + m_p}\cdot\frac{1}{m_e} = \frac{207}{1+207(m_e/m_p)} = \frac{207}{1+207\frac{(9.11\times10^{-31})}{1.67\times10^{-27})}} = \frac{207}{1.11} = 186.$$

$$\Delta E = (5.88\times10^{-6}\text{ eV})\,(1/207)\,(186)^3 = \boxed{0.183\text{ eV.}}$$

(b) $g: 5.59 \to 2;\quad m_p \to m_e;\quad \dfrac{a}{a_p} = \dfrac{m_p(\text{reduced})}{m_e} = \dfrac{m_e^2}{m_e+m_e}\cdot\dfrac{1}{m_e} = \dfrac{1}{2}.$

$$\Delta E = (5.88\times10^{-6}\text{ eV})\left(\frac{2}{5.59}\right)\left(\frac{1.67\times10^{-27}}{9.11\times10^{-31}}\right)\left(\frac{1}{2}\right)^3 = \boxed{4.82\times10^{-4}\text{ eV.}}$$

(c) $g: 5.59 \to 2;\quad m_p \to m_\mu;\quad \dfrac{a}{a_m} = \dfrac{m_m(\text{reduced})}{m_e} = \dfrac{m_e m_\mu}{m_e+m_\mu}\cdot\dfrac{1}{m_e} = \dfrac{207}{208}.$

$$\Delta E = (5.88\times10^{-6})\left(\frac{2}{5.59}\right)\left(\frac{1.67\times10^{-27}}{(207)(9.11\times10^{-31})}\right)\left(\frac{207}{208}\right)^3 = \boxed{1.84\times10^{-5}\text{ eV.}}$$

Problem 7.33

Use perturbation theory:

$$H' = -\frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{b}-\frac{1}{r}\right),\quad \text{for}\quad 0<r<b.\quad \Delta E = \langle\psi|H'|\psi\rangle,\quad \text{with}\quad \psi \equiv \frac{1}{\sqrt{\pi a^3}}e^{-r/a}.$$

$$\begin{aligned}
\Delta E &= -\frac{e^2}{4\pi\epsilon_0}\frac{1}{\pi a^3}4\pi\int_0^b\left(\frac{1}{b}-\frac{1}{r}\right)e^{-2r/a}r^2dr = -\frac{e^2}{\pi\epsilon_0 a^3}\left(\frac{1}{b}\int_0^b r^2e^{-2r/a}dr - \int_0^b re^{-2r/a}dr\right)\\
&= -\frac{e^2}{\pi\epsilon_0 a^3}\left\{\frac{1}{b}\left[-\frac{a}{2}r^2e^{-2r/a} + a\left(\frac{a}{2}\right)^2e^{-2r/a}\left(-\frac{2r}{a}-1\right)\right] - \left[\left(\frac{a}{2}\right)^2e^{-2r/a}\left(-\frac{2r}{a}-1\right)\right]\right\}\Bigg|_0^b\\
&= -\frac{e^2}{\pi\epsilon_0 a^3}\left[-\frac{a}{2b}b^2e^{-2b/a} + \frac{a^3}{4b}e^{-2b/a}\left(-\frac{2b}{a}-1\right) - \frac{a^2}{4}e^{-2b/a}\left(-\frac{2b}{a}-1\right) + \frac{a^3}{4b} - \frac{a^2}{4}\right]\\
&= -\frac{e^2}{\pi\epsilon_0 a^3}\left[e^{-2b/a}\left(-\frac{ab}{2}-\frac{a^2}{2}-\frac{a^3}{4b}+\frac{ab}{2}+\frac{a^2}{4}\right)+\frac{a^2}{4}\left(\frac{a}{b}-1\right)\right]\\
&= -\frac{e^2}{\pi\epsilon_0 a^3}\left[e^{-2b/a}\left(-\frac{a^2}{4}\right)\left(\frac{a}{b}+1\right)+\frac{a^2}{4}\left(\frac{a}{b}-1\right)\right] = \frac{e^2}{4\pi\epsilon_0 a}\left[\left(1-\frac{a}{b}\right)+\left(1+\frac{a}{b}\right)e^{-2b/a}\right].
\end{aligned}$$

Let $+2b/a = \epsilon$ (very small). Then the term in square brackets is:

$$\left(1-\frac{2}{\epsilon}\right)+\left(1+\frac{2}{\epsilon}\right)\left(1-\epsilon+\frac{\epsilon^2}{2}-\frac{\epsilon^3}{6}+\cdots\right)$$
$$=\cancel{1}-\cancel{\frac{2}{\epsilon}}+\cancel{1}+\cancel{\frac{2}{\epsilon}}-\cancel{\epsilon}-\cancel{2}+\frac{\epsilon^2}{2}+\cancel{\epsilon}-\frac{\epsilon^3}{6}-\frac{\epsilon^2}{3}+(\,)\epsilon^3+\cdots=\frac{\epsilon^2}{6}+(\,)\epsilon^3+(\,)\epsilon^4\cdots$$

To leading order, then, $\Delta E = \frac{e^2}{4\pi\epsilon_0}\frac{1}{a}\frac{4b^2}{6a^2}$.

$$E = E_1 = -\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2}; \quad a = \frac{4\pi\epsilon_0\hbar^2}{me^2}; \quad \text{so} \quad Ea = -\frac{e^2}{2(4\pi\epsilon_0)}.$$

$$\frac{\Delta E}{E} = \frac{e^2}{4\pi\epsilon_0}\left(-\frac{2(4\pi\epsilon_0)}{e^2}\right)\frac{2b^2}{3a^2} = \boxed{-\frac{4}{3}\left(\frac{b}{a}\right)^2.}$$

Putting in $a = 5\times 10^{-11}$ m:

$$\frac{\Delta E}{E} = -\frac{4}{3}\left(\frac{10^{-15}}{5\times 10^{-11}}\right)^2 = -\frac{16}{3}\times 10^{-10} \approx \boxed{-5\times 10^{-10}.}$$

$$\text{By contrast,}\ \begin{cases}\text{fine structure:} & \Delta E/E \approx \alpha^2 = (1/137)^2 = 5\times 10^{-5},\\ \text{hyperfine structure:} & \Delta E/E \approx (m_e/m_p)\alpha^2 = (1/1800)(1/137)^2 = 3\times 10^{-8}.\end{cases}$$

So the correction for the finite size of the nucleus is *much* smaller (about 1% of hyperfine).

Problem 7.34

(a) $\tilde{H}_0|\psi_n^0\rangle = H_0|\psi_n^0\rangle + P_D H' P_D|\psi_n^0\rangle$. But $P_D|\psi_n^0\rangle = |\psi_a^0\rangle\langle\psi_a^0|\psi_n^0\rangle + |\psi_b^0\rangle\langle\psi_b^0|\psi_n^0\rangle = 0$, because eigenstates of H_0 belonging to different eigenvalues are orthogonal. And $H_0|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle$, so $\tilde{H}_0|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle$. ✓

$$\begin{aligned}\tilde{H}_0|\psi^0\rangle &= H_0|\psi^0\rangle + P_D H' P_D|\psi^0\rangle. \quad \text{But } H_0|\psi^0\rangle = E^0|\psi^0\rangle, \text{ and } P_D|\psi^0\rangle = |\psi^0\rangle, \text{ so}\\
&= E^0\left(\alpha|\psi_a^0\rangle+\beta|\psi_b^0\rangle\right) + \left(|\psi_a^0\rangle\langle\psi_a^0| + |\psi_b^0\rangle\langle\psi_b^0|\right)H'\left(\alpha|\psi_a^0\rangle+\beta|\psi_b^0\rangle\right)\\
&= E^0\left(\alpha|\psi_a^0\rangle+\beta|\psi_b^0\rangle\right) + \alpha\left(W_{aa}|\psi_a^0\rangle + W_{ba}|\psi_b^0\rangle\right) + \beta\left(W_{ab}|\psi_a^0\rangle + W_{bb}|\psi_b^0\rangle\right)\\
&= \left(\alpha E^0 + \alpha W_{aa} + \beta W_{ab}\right)|\psi_a^0\rangle + \left(\beta E^0 + \alpha W_{ba} + \beta W_{bb}\right)|\psi_b^0\rangle\\
&= (\alpha E^0 + \alpha E^1)|\psi_a^0\rangle + (\beta E^0 + \beta E^1)|\psi_b^0\rangle = (E^0 + E^1)|\psi^0\rangle. \quad ✓\end{aligned}$$

In the last line I used Equations 7.27 and 7.29; E^1 can be either E_+^1 or E_-^1 from Equation 7.33.

(b) Using nondegenerate perturbation theory, to second order (Equations 7.9 and 7.15), for ψ_+:

$$E_+ = (E^0 + E_+^1) + \langle\psi_+^0|\tilde{H}'|\psi_+^0\rangle + \sum_{m\neq +}\frac{|\langle\psi_m^0|\tilde{H}'|\psi_+^0\rangle|^2}{E^0 + E_+^1 - E_m^0}.$$

But

$$\langle\psi_+^0|\tilde{H}'|\psi_+^0\rangle = \langle\psi_+^0|H'|\psi_+^0\rangle - \langle\psi_+^0|P_D H' P_D|\psi_+^0\rangle = 0,$$

because $P_D|\psi_+^0\rangle = |\psi_+^0\rangle$ and $\langle\psi_+^0|P_D = \langle\psi_+^0|$, while

$$\langle\psi_m^0|\tilde{H}'|\psi_+^0\rangle = \langle\psi_m^0|H'|\psi_+^0\rangle - \langle\psi_m^0|P_D H' P_D|\psi_+^0\rangle = \begin{cases}\langle\psi_m^0|H'|\psi_+^0\rangle, & (m \neq \pm)\\ 0, & (m = \pm)\end{cases}$$

(note that $P_D|\psi_m^0\rangle = 0$ if $m \neq \pm$). So

$$E_+ = E^0 + E_+^1 + \sum_{m\neq\pm} \frac{|\langle\psi_m^0|H'|\psi_+^0\rangle|^2}{E^0 + E_+^1 - E_m^0}.$$

(Change the subscripts $+$ to $-$ for E_-.) Typically one drops the E^1 term in the denominator, since it is really a third-order correction.

Problem 7.35

(a)

$$\mathsf{P}_D = \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}1 & 0 & 0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0 & 1 & 0\end{pmatrix} = \begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix} + \begin{pmatrix}0&0&0\\0&1&0\\0&0&0\end{pmatrix} = \begin{pmatrix}1&0&0\\0&1&0\\0&0&0\end{pmatrix}.$$

$$\tilde{\mathsf{H}}_0 = \mathsf{H}_0 + \mathsf{P}_D\mathsf{H}'\mathsf{P}_D = \begin{pmatrix}\epsilon&0&0\\0&\epsilon&0\\0&0&\epsilon'\end{pmatrix} + \begin{pmatrix}1&0&0\\0&1&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&a&b\\a^*&0&c\\b^*&c^*&0\end{pmatrix}\begin{pmatrix}1&0&0\\0&1&0\\0&0&0\end{pmatrix} = \begin{pmatrix}\epsilon&0&0\\0&\epsilon&0\\0&0&\epsilon'\end{pmatrix} + \begin{pmatrix}0&a&0\\a^*&0&0\\0&0&0\end{pmatrix}$$

$$= \begin{pmatrix}\epsilon&a&0\\a^*&\epsilon&0\\0&0&\epsilon'\end{pmatrix}$$

$$\tilde{\mathsf{H}}' = \mathsf{H}' - \mathsf{P}_D\mathsf{H}'\mathsf{P}_D = \begin{pmatrix}0&a&b\\a^*&0&c\\b^*&c^*&0\end{pmatrix} - \begin{pmatrix}0&a&0\\a^*&0&0\\0&0&0\end{pmatrix} = \begin{pmatrix}0&0&b\\0&0&c\\b^*&c^*&0\end{pmatrix}.$$

(b) Eigenvalues of $\tilde{H}_0$:

$$\begin{vmatrix}\epsilon-\lambda & a & 0\\ a^* & \epsilon-\lambda & 0\\ 0 & 0 & \epsilon'-\lambda\end{vmatrix} = (\epsilon-\lambda)^2(\epsilon'-\lambda) - (\epsilon'-\lambda)a^*a = 0 \Rightarrow \boxed{\lambda_1 = \epsilon + |a|,\ \lambda_2 = \epsilon - |a|,\ \lambda_3 = \epsilon'.}$$

The spectrum is nondegenerate (provided that $a \neq 0$ and $\epsilon' \neq \epsilon \pm |a|$). To get the eigenvectors:

$$\underline{\lambda_1}\quad \begin{pmatrix}\epsilon&a&0\\a^*&\epsilon&0\\0&0&\epsilon'\end{pmatrix}\begin{pmatrix}x\\y\\z\end{pmatrix} = (\epsilon+|a|)\begin{pmatrix}x\\y\\z\end{pmatrix} \Rightarrow \left\{\begin{matrix}\epsilon x + ay = (\epsilon+|a|)x\\ a^*x + \epsilon y = (\epsilon+|a|)y\\ \epsilon' z = (\epsilon+|a|)z\end{matrix}\right\} \Rightarrow y = \sqrt{\frac{a^*}{a}}\,x,\ z = 0.$$

$$\underline{\lambda_2}\quad \begin{pmatrix}\epsilon&a&0\\a^*&\epsilon&0\\0&0&\epsilon'\end{pmatrix}\begin{pmatrix}x\\y\\z\end{pmatrix} = (\epsilon-|a|)\begin{pmatrix}x\\y\\z\end{pmatrix} \Rightarrow \left\{\begin{matrix}\epsilon x + ay = (\epsilon-|a|)x\\ a^*x + \epsilon y = (\epsilon-|a|)y\\ \epsilon' z = (\epsilon-|a|)z\end{matrix}\right\} \Rightarrow y = -\sqrt{\frac{a^*}{a}}\,x,\ z = 0.$$

$$\underline{\lambda_3}\quad \begin{pmatrix}\epsilon&a&0\\a^*&\epsilon&0\\0&0&\epsilon'\end{pmatrix}\begin{pmatrix}x\\y\\z\end{pmatrix} = \epsilon'\begin{pmatrix}x\\y\\z\end{pmatrix} \Rightarrow \left\{\begin{matrix}\epsilon x + ay = \epsilon' x\\ a^*x + \epsilon y = \epsilon' y\\ \epsilon' z = \epsilon' z\end{matrix}\right\} \Rightarrow x = y = 0.$$

So the (normalized) eigenvectors are $\boxed{|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \sqrt{a^*/a}\\ 0\end{pmatrix}.}$ $\boxed{|\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -\sqrt{a^*/a}\\ 0\end{pmatrix}.}$ $\boxed{|\psi_3\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}.}$

(c) The "good" states are the eigenstates of $\tilde{\mathsf{H}}_0$: $|\psi_1\rangle$, $|\psi_2\rangle$, and $|\psi_3\rangle$ from part (b). To first order, the energies are the eigenvalues, $\epsilon \pm |a|$ and ϵ'.

Problem 7.36

(a) In terms of the one-dimensional harmonic oscillator states $\{\psi_n(x)\}$, the unperturbed ground state is

$$|0\rangle = \psi_0(x)\psi_0(y)\psi_0(z).$$

$$E_0^1 = \langle 0|H'|0\rangle = \langle \psi_0(x)\psi_0(y)\psi_0(z)|\lambda x^2yz|\psi_0(x)\psi_0(y)\psi_0(z)\rangle = \lambda\langle x^2\rangle_0\langle y\rangle_0\langle z\rangle_0.$$

But $\langle y\rangle_0 = \langle z\rangle_0 = 0.$ So there is *no* change, in first order.

(b) The (triply degenerate) first excited states are

$$\begin{cases} |1\rangle = \psi_0(x)\psi_0(y)\psi_1(z)\\ |2\rangle = \psi_0(x)\psi_1(y)\psi_0(z)\\ |3\rangle = \psi_1(x)\psi_0(y)\psi_0(z)\end{cases}$$

In this basis the perturbation matrix is $W_{ij} = \langle i|H'|j\rangle, \quad i = 1, 2, 3.$

$$\begin{aligned}
\langle 1|H'|1\rangle &= \langle \psi_0(x)\psi_0(y)\psi_1(z)|\lambda x^2yz|\psi_0(x)\psi_0(y)\psi_1(z)\rangle = \lambda\langle x^2\rangle_0\langle y\rangle_0\langle z\rangle_1 = 0,\\
\langle 2|H'|2\rangle &= \langle \psi_0(x)\psi_1(y)\psi_0(z)|\lambda x^2yz|\psi_0(x)\psi_1(y)\psi_0(z)\rangle = \lambda\langle x^2\rangle_0\langle y\rangle_1\langle z\rangle_0 = 0,\\
\langle 3|H'|3\rangle &= \langle \psi_1(x)\psi_0(y)\psi_0(z)|\lambda x^2yz|\psi_1(x)\psi_0(y)\psi_0(z)\rangle = \lambda\langle x^2\rangle_1\langle y\rangle_0\langle z\rangle_0 = 0,\\
\langle 1|H'|2\rangle &= \langle \psi_0(x)\psi_0(y)\psi_1(z)|\lambda x^2yz|\psi_0(x)\psi_1(y)\psi_0(z)\rangle = \lambda\langle x^2\rangle_0\langle 0|y|1\rangle\langle 1|z|0\rangle\\
&= \lambda\frac{\hbar}{2m\omega}|\langle 0|x|1\rangle|^2 = \lambda\left(\frac{\hbar}{2m\omega}\right)^2 \quad \text{[using Problems 2.11 and 3.39]}.\\
\langle 1|H'|3\rangle &= \langle \psi_0(x)\psi_0(y)\psi_1(z)|\lambda x^2yz|\psi_1(x)\psi_0(y)\psi_0(z)\rangle = \lambda\langle 0|x^2|1\rangle\langle y\rangle_0\langle 1|z|0\rangle = 0,\\
\langle 2|H'|3\rangle &= \langle \psi_0(x)\psi_1(y)\psi_0(z)|\lambda x^2yz|\psi_1(x)\psi_0(y)\psi_0(z)\rangle = \lambda\langle 0|x^2|1\rangle\langle 1|y|0\rangle_0\langle z\rangle_0 = 0.
\end{aligned}$$

$$\mathsf{W} = \begin{pmatrix}0 & a & 0\\ a & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \quad \text{where} \quad a \equiv \lambda\left(\frac{\hbar}{2m\omega}\right)^2.$$

$$\text{Eigenvalues of } \mathsf{W}: \quad \begin{vmatrix}-E & a & 0\\ a & -E & 0\\ 0 & 0 & -E\end{vmatrix} = -E^3 + Ea^2 = 0 \Rightarrow E = \{0, \pm a\} = \boxed{0,\ \pm\lambda\left(\frac{\hbar}{2m\omega}\right)^2.}$$

Problem 7.37

(a) The first term is the nucleus/nucleus interaction, the second is the interaction between the nucleus of atom 2 and the electron in atom 1, the third is between nucleus 1 and electron 2, and the last term is the interaction between the electrons.

$$\frac{1}{R-x} = \frac{1}{R}\left(1-\frac{x}{R}\right)^{-1} = \frac{1}{R}\left[1+\left(\frac{x}{R}\right)+\left(\frac{x}{R}\right)^2+\dots\right],$$

so

$$\begin{aligned} H' &\cong \frac{1}{4\pi\epsilon_0}\frac{e^2}{R}\left\{1-\left[1+\left(\frac{x_1}{R}\right)+\left(\frac{x_1}{R}\right)^2\right]-\left[1-\left(\frac{x_2}{R}\right)+\left(\frac{x_2}{R}\right)^2\right]+\left[1+\left(\frac{x_1-x_2}{R}\right)+\left(\frac{x_1-x_2}{R}\right)^2\right]\right\} \\ &\approx \frac{1}{4\pi\epsilon_0}\frac{e^2}{R}\left(-\frac{2x_1x2}{R^2}\right) = -\frac{e^2x_1x_2}{2\pi\epsilon_0R^3}. \quad \checkmark \end{aligned}$$

(b) Expanding Eq. 7.106:

$$\begin{aligned} H &= \frac{1}{2m}\left(p_+^2+p_-^2\right)+\frac{1}{2}k\left(x_+^2+x_-^2\right)-\frac{e^2}{4\pi\epsilon_0R^3}\left(x_+^2-x_-^2\right) \\ &= \frac{1}{2m}\left(p_1^2+p_2^2\right)+\frac{1}{2}k\left(x_1^2+x_2^2\right)-\frac{e^2}{4\pi\epsilon_0R^3}(2x_1x_2) = H^0+H' \quad \text{(Eqs. 7.103 and 7.105).} \end{aligned}$$

(c)

$$\omega_\pm = \sqrt{\frac{k}{m}}\left(1\mp\frac{e^2}{2\pi\epsilon_0R^3k}\right)^{1/2} \cong \omega_0\left[1\mp\frac{1}{2}\left(\frac{e^2}{2\pi\epsilon_0R^3m\omega_0^2}\right)-\frac{1}{8}\left(\frac{e^2}{2\pi\epsilon_0R^3m\omega_0^2}\right)^2+\dots\right].$$

$$\begin{aligned} \Delta V &\cong \frac{1}{2}\hbar\omega_0\left[1-\frac{1}{2}\left(\frac{e^2}{2\pi\epsilon_0R^3m\omega_0^2}\right)-\frac{1}{8}\left(\frac{e^2}{2\pi\epsilon_0R^3m\omega_0^2}\right)^2+\right. \\ &\qquad\qquad \left.1+\frac{1}{2}\left(\frac{e^2}{2\pi\epsilon_0R^3m\omega_0^2}\right)-\frac{1}{8}\left(\frac{e^2}{2\pi\epsilon_0R^3m\omega_0^2}\right)^2\right]-\hbar\omega_0 \\ &= \frac{\hbar\omega_0}{2}\left(-\frac{1}{4}\right)\left(\frac{e^2}{2\pi\epsilon_0R^3m\omega_0^2}\right)^2 = -\frac{1}{8}\frac{\hbar}{m^2\omega_0^3}\left(\frac{e^2}{2\pi\epsilon_0}\right)^2\frac{1}{R^6}. \quad \checkmark \end{aligned}$$

(d) In first order:

$$E_0^1 = \langle 0|H'|0\rangle = -\frac{e^2}{2\pi\epsilon_0R^3}\langle\psi_0(x_1)\psi_0(x_2)|x_1x_2|\psi_0(x_1)\psi_0(x_2)\rangle = -\frac{e^2}{2\pi\epsilon_0R^3}\langle x\rangle_0\langle x\rangle_0 = 0.$$

In second order:

$$\begin{aligned} E_0^2 &= \sum_{n=1}^{\infty}\frac{|\langle\psi_n|H'|\psi_0\rangle|^2}{E_0-E_n}. \quad \text{Here} \quad |\psi_0\rangle = |0\rangle|0\rangle, \quad |\psi_n\rangle = |n_1\rangle|n_2\rangle, \quad \text{so} \\ &= \left(\frac{e^2}{2\pi\epsilon_0R^3}\right)^2\sum_{n_1=1}^{\infty}\sum_{n_2=1}^{\infty}\frac{|\langle n_1|x_1|0\rangle|^2\,|\langle n_2|x_2|0\rangle|^2}{E_{0,0}-E_{n_1,n_2}} \quad \text{[use Problem 3.39]} \\ &= \left(\frac{e^2}{2\pi\epsilon_0R^3}\right)^2\frac{|\langle 1|x|0\rangle|^2\,|\langle 1|x|0\rangle|^2}{(\frac{1}{2}\hbar\omega_0+\frac{1}{2}\hbar\omega_0)-(\frac{3}{2}\hbar\omega_0+\frac{3}{2}\hbar\omega_0)} \quad \text{[zero unless } n_1=n_2=1\text{]} \\ &= \left(\frac{e^2}{2\pi\epsilon_0R^3}\right)^2\left(-\frac{1}{2\hbar\omega_0}\right)\left(\frac{\hbar}{2m\omega_0}\right)^2 = -\frac{\hbar}{8m^2\omega_0^3}\left(\frac{e^2}{2\pi\epsilon_0}\right)^2\frac{1}{R^6}. \quad \checkmark \end{aligned}$$

[There is an interesting fraud in this well-known problem. If you expand H' to order $1/R^5$, the extra term has a nonzero expectation value in the ground state of H^0, so there is a non-zero first-order perturbation, and the dominant contribution goes like $1/R^5$, not $1/R^6$ (as desired). The model gets the power "right" in three dimensions (where the expectation value is zero), but not in one. See A. C. Ipsen and K. Splittorff, *Am. J. Phys.* **83**, 150 (2015).]

Problem 7.38

(a) Let the unperturbed Hamiltonian be $H(\lambda_0)$, for some fixed value λ_0. Now tweak λ to $\lambda_0 + d\lambda$. The perturbing Hamiltonian is $H' = H(\lambda_0 + d\lambda) - H(\lambda_0) = (\partial H/\partial\lambda)\, d\lambda$ (derivative evaluated at λ_0).

The change in energy is given by Eq. 7.9:

$$dE_n = E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle = \langle\psi_n|\frac{\partial H}{\partial\lambda}|\psi_n\rangle\, d\lambda \text{ (all evaluated at } \lambda_0); \quad \text{so} \quad \frac{\partial E_n}{\partial\lambda} = \langle\psi_n|\frac{\partial H}{\partial\lambda}|\psi_n\rangle.$$

[*Note:* Even though we used perturbation theory, the result is exact, since all we needed (to calculate the derivative) was the *infinitesimal* change in E_n.]

(b) $E_n = (n + \frac{1}{2})\hbar\omega; \quad H = -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2} + \dfrac{1}{2}m\omega^2x^2.$

(i)

$$\frac{\partial E_n}{\partial\omega} = (n + \frac{1}{2})\hbar; \quad \frac{\partial H}{\partial\omega} = m\omega x^2; \quad \text{so F-H} \Rightarrow (n + \frac{1}{2})\hbar = \langle n|m\omega x^2|n\rangle. \quad \text{But}$$

$$V = \frac{1}{2}m\omega^2x^2, \quad \text{so} \quad \langle V\rangle = \langle n|\frac{1}{2}m\omega^2x^2|n\rangle = \frac{1}{2}\omega(n + \frac{1}{2})\hbar; \quad \boxed{\langle V\rangle = \tfrac{1}{2}(n + \tfrac{1}{2})\hbar\omega.}$$

(ii)

$$\frac{\partial E_n}{\partial\hbar} = (n + \frac{1}{2})\omega; \quad \frac{\partial H}{\partial\hbar} = -\frac{\hbar}{m}\frac{d^2}{dx^2} = \frac{2}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) = \frac{2}{\hbar}T;$$

$$\text{so F-H} \Rightarrow (n + \frac{1}{2})\omega = \frac{2}{\hbar}\langle n|T|n\rangle, \quad \text{or} \quad \boxed{\langle T\rangle = \tfrac{1}{2}(n + \tfrac{1}{2})\hbar\omega.}$$

(iii)

$$\frac{\partial E_n}{\partial_m} = 0; \quad \frac{\partial H}{\partial m} = \frac{\hbar^2}{2m^2}\frac{d^2}{dx^2} + \frac{1}{2}\omega^2x^2 = -\frac{1}{m}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) + \frac{1}{m}\left(\frac{1}{2}m\omega^2x^2\right) = -\frac{1}{m}T + \frac{1}{m}V.$$

So F-H $\Rightarrow 0 = -\dfrac{1}{m}\langle T\rangle + \dfrac{1}{m}\langle V\rangle$, or $\boxed{\langle T\rangle = \langle V\rangle.}$ These results are consistent with what we found in Problems 2.12 and 3.37.

Problem 7.39

(a)

$$\begin{vmatrix} \epsilon_a - \lambda & 0 & V \\ 0 & \epsilon_a - \lambda & V \\ V^* & V^* & \epsilon_c - \lambda \end{vmatrix} = (\epsilon_a - \lambda)^2(\epsilon_c - \lambda) - 2VV^*(\epsilon_a - \lambda) = 0$$

$$\Rightarrow \boxed{\lambda_1 = \epsilon_a, \quad \lambda_\pm = \left(\frac{\epsilon_a + \epsilon_c}{2}\right) \pm \sqrt{\left(\frac{\epsilon_a - \epsilon_c}{2}\right)^2 + 2|V|^2}.}$$

(b)

$$\lambda_\pm = \left(\frac{\epsilon_a + \epsilon_c}{2}\right) \pm \left(\frac{\epsilon_a - \epsilon_c}{2}\right)\sqrt{1 + \frac{8|V|^2}{(\epsilon_a - \epsilon_c)^2}} \approx \left(\frac{\epsilon_a + \epsilon_c}{2}\right) \pm \left(\frac{\epsilon_a - \epsilon_c}{2}\right)\left[1 + \frac{4|V|^2}{(\epsilon_a - \epsilon_c)^2}\right]$$

$$= \left(\frac{\epsilon_a + \epsilon_c}{2}\right) \pm \left[\left(\frac{\epsilon_a - \epsilon_c}{2}\right) + \frac{2|V|^2}{(\epsilon_a - \epsilon_c)}\right].$$

$$\boxed{\lambda_1 = \epsilon_a, \quad \lambda_+ \approx \epsilon_a + \frac{2|V|^2}{\epsilon_a - \epsilon_c}, \quad \lambda_- \approx \epsilon_c - \frac{2|V|^2}{\epsilon_a - \epsilon_c}.}$$

(c) Naively applying nondegenerate perturbation theory to the states (1,0,0), (0,1,0), and (0,0,1):

$$E_1 = \epsilon_a + H'_{11} + \sum_{n \neq 1} \frac{|H'_{n1}|^2}{\epsilon_a - E_n^0} + \cdots = \epsilon_a + \frac{|H'_{21}|^2}{\epsilon_a - \epsilon_a} + \frac{|H'_{31}|^2}{\epsilon_a - \epsilon_c} = \epsilon_a + \frac{0}{0} + \frac{|V|^2}{\epsilon_a - \epsilon_c}.$$

$$E_2 = \epsilon_a + H'_{22} + \sum_{n \neq 2} \frac{|H'_{n2}|^2}{\epsilon_a - E_n^0} + \cdots = \epsilon_a + \frac{|H'_{12}|^2}{\epsilon_a - \epsilon_a} + \frac{|H'_{32}|^2}{\epsilon_a - \epsilon_c} = \epsilon_a + \frac{0}{0} + \frac{|V|^2}{\epsilon_a - \epsilon_c}.$$

$$E_3 = \epsilon_c + H'_{33} + \sum_{n \neq 3} \frac{|H'_{n3}|^2}{\epsilon_c - E_n^0} + \cdots = \epsilon_c + \frac{|H'_{13}|^2}{\epsilon_c - \epsilon_a} + \frac{|H'_{23}|^2}{\epsilon_c - \epsilon_a} = \epsilon_c - 2\frac{|V|^2}{\epsilon_a - \epsilon_c}.$$

The nondegenerate state comes out right ($E_3 = \lambda_-$), but the other two are at best ambiguous (the 0/0 terms warning us, perhaps, that something is amiss).

Problem 7.40

(a) In Equation 7.10, let $\psi_n \to \psi \equiv \alpha\psi_a + \beta\psi_b$:

$$(H^0 - E^0)\psi^1 = -(H' - E^1)\psi^0.$$

Now take the inner product with ψ_m^0, where $m \neq a, b$:

$$E_m^0\langle\psi_m^0|\psi^1\rangle - E^0\langle\psi_m^0|\psi^1\rangle = -\langle\psi_m^0|H'|\psi^0\rangle + E^1\cancel{\langle\psi_m^0|\psi^0\rangle},$$

so

$$\langle\psi_m^0|\psi^1\rangle = \frac{\langle\psi_m^0|H'|\psi^0\rangle}{E^0 - E_m^0} = \frac{\alpha H'_{ma} + \beta H'_{mb}}{E^0 - E_m^0}, \text{ and (Equation 7.13) } \boxed{\psi^1 = \sum_{m \neq a,b} \frac{\alpha H'_{ma} + \beta H'_{mb}}{E^0 - E_m^0}\psi_m^0.}$$

(b) Similarly, write Equation 7.8 for $\psi_n \to \psi$:

$$H^0\psi^2 + H'\psi^1 = E^0\psi^2 + E^1\psi^1 + E^2\psi^0$$

and take the inner product with ψ_a^0 and ψ_b^0:

$$\cancel{E^0\langle\psi_a^0|\psi^2\rangle} + \langle\psi_a^0|H'|\psi^1\rangle = \cancel{E^0\langle\psi_a^0|\psi^2\rangle} + E^1\langle\psi_a^0|\psi^1\rangle + E^2\langle\psi_a^0|\psi^0\rangle.$$

As before (Equation 7.11) we might as well choose $\langle\psi_a^0|\psi^1\rangle = 0$. And $\langle\psi_a^0|\psi^0\rangle = \alpha$. So

$$\langle\psi_a^0|H'|\psi^1\rangle = E^2\alpha, \text{ and similarly } \langle\psi_b^0|H'|\psi^1\rangle = E^2\beta.$$

Putting in the result of part (a):

$$\sum_{m\neq a,b} \frac{\alpha H'_{ma} + \beta H'_{mb}}{E^0 - E_m^0} H'_{am} = E^2\alpha, \qquad \sum_{m\neq a,b} \frac{\alpha H'_{ma} + \beta H'_{mb}}{E^0 - E_m^0} H'_{bm} = E^2\beta$$

This has the form of an eigenvalue equation:

$$\underbrace{\sum_{m\neq a,b} \frac{1}{E^0 - E_m^0} \begin{pmatrix} |H'_{ma}|^2 & H'_{am}H'_{mb} \\ H'_{bm}H'_{ma} & |H'_{mb}|^2 \end{pmatrix}}_{\mathsf{W}^2} \begin{pmatrix}\alpha \\ \beta\end{pmatrix} = E^2 \begin{pmatrix}\alpha \\ \beta\end{pmatrix}.$$

(c) In the case of Problem 7.39 the matrix is

$$\mathsf{W}^2 = \frac{1}{\epsilon_a - \epsilon_c}\begin{pmatrix} |V|^2 & |V|^2 \\ |V|^2 & |V|^2 \end{pmatrix}.$$

Its (normalized) eigenvectors are

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1\end{pmatrix}, \qquad \text{so the “good” states are} \quad \psi_\pm^0 = \frac{\psi_a^0 \pm \psi_b^0}{\sqrt{2}},$$

and the second-order correction to the energies are the eigenvalues

$$E_+^2 = 2\frac{|V|^2}{\epsilon_a - \epsilon_c}, \quad E_-^2 = 0.$$

This agrees precisely with the result in Problem 7.39(b), obtained by Taylor expansion of the exact energies.

Problem 7.41

(a)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \;\Rightarrow\; \frac{d^2\psi}{dx^2} = -k^2\psi \;\Rightarrow\; \psi = Ae^{ikx};\; \psi(x+L) = \psi(x) \;\Rightarrow\; e^{ikL} = 1$$

$$\Rightarrow kL = 2n\pi \;(n = 0, \pm1, \pm2, \ldots);\; \psi_n^0(x) = \frac{1}{\sqrt{L}}e^{i2\pi nx/L}. \quad \checkmark$$

(b)

$$H'_{mn} = \frac{V_0}{L}\int_0^L e^{-i2\pi mx/L}\cos\left(2\pi\frac{x}{L}\right)e^{i2\pi nx/L}\,dx = \frac{V_0}{2L}\int_0^L e^{i2\pi(n-m)x/L}\left(e^{i2\pi x/L}+e^{-i2\pi x/L}\right)dx$$
$$= \frac{V_0}{2L}\int_0^L \left[e^{i2\pi(n-m+1)x/L} + e^{i2\pi x(n-m-1)/L}\right]dx.$$

But, for any nonzero integer N,

$$\int_0^L e^{i2\pi Nx/L}\,dx = \left.\frac{e^{i2\pi Nx/L}}{i2\pi N/L}\right|_0^L = \frac{e^{i2\pi N}-1}{i2\pi N/L} = \frac{1-1}{i2\pi N/L} = 0,$$

while for $N=0$ the integral is (obviously) L, so

$$\boxed{H'_{mn} = \frac{V_0}{2}\left(\delta_{m,n+1}+\delta_{m,n-1}\right).}$$

(c)

$$[W]_{1,1} = H'_{11} = 0,\ [W]_{1,-1} = H'_{1\,-1} = 0,\ [W]_{-1,1} = H'_{-1\,1} = 0,\ [W]_{-1,-1} = H'_{-1\,-1} = 0,$$

so

$\boxed{\mathsf{W} = \begin{pmatrix}0&0\\0&0\end{pmatrix},}$ and (Equation 7.33) there are no first-order corrections to the energies.

(d)

$$[W^2]_{1,1} = \sum_{n\neq 1,-1}\frac{H'_{1n}H'_{n1}}{E_1^0-E_n^0} = \frac{|H'_{10}|^2}{E_1^0-E_0^0} + \frac{|H'_{21}|^2}{E_1^0-E_2^0} = \left(\frac{V_0}{2}\right)^2\left(\frac{1}{E_1^0-0}+\frac{1}{E_1^0-4E_1^0}\right) = \frac{V_0^2}{6E_1^0},$$
$$[W^2]_{1,-1} = \sum_{n\neq 1,-1}\frac{H'_{1n}H'_{n\,-1}}{E_1^0-E_n^0} = \frac{H'_{10}H'_{0\,-1}}{E_1^0-E_0^0} = \left(\frac{V_0}{2}\right)^2\left(\frac{1}{E_1^0-0}\right) = \frac{V_0^2}{4E_1^0},$$
$$[W^2]_{-1,1} = \sum_{n\neq 1,-1}\frac{H'_{-1\,n}H'_{n\,1}}{E_1^0-E_n^0} = \frac{H'_{-1\,0}H'_{0\,1}}{E_1^0-E_0^0} = \left(\frac{V_0}{2}\right)^2\left(\frac{1}{E_1^0-0}\right) = \frac{V_0^2}{4E_1^0},$$
$$[W^2]_{-1,-1} = \sum_{n\neq 1,-1}\frac{H'_{-1\,n}H'_{n\,-1}}{E_1^0-E_n^0} = \frac{|H'_{-1\,0}|^2}{E_1^0-E_0^0} + \frac{|H'_{-2\,-1}|^2}{E_1^0-E_2^0} = \left(\frac{V_0}{2}\right)^2\left(\frac{1}{E_1^0-0}+\frac{1}{E_1^0-4E_1^0}\right) = \frac{V_0^2}{6E_1^0}.$$

so

$$\boxed{\mathsf{W}^2 = \frac{V_0^2}{12E_1^0}\begin{pmatrix}2&3\\3&2\end{pmatrix}.}$$

The eigenvalues of $\begin{pmatrix}2&3\\3&2\end{pmatrix}$ are given by

$$\begin{vmatrix}(2-\lambda) & 3\\ 3 & (2-\lambda)\end{vmatrix} = (2-\lambda)^2 - 9 \Rightarrow \lambda_\pm = 2\pm 3;\ \lambda_+ = 5,\ \lambda_- = -1,$$

so the degeneracy lifts at second order. The eigenvectors are given by

$$\begin{pmatrix}2&3\\3&2\end{pmatrix}\begin{pmatrix}x\\y\end{pmatrix} = \lambda\begin{pmatrix}x\\y\end{pmatrix} \Rightarrow 2x+3y=\lambda x \Rightarrow 2x+3y=\lambda x.$$

$$\lambda_+ = 5 \;\Rightarrow\; 2x + 3y = 5x \;\Rightarrow\; y = x \Rightarrow\; v_+ = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix};$$

$$\lambda_- = -1 \;\Rightarrow\; 2x + 3y = -x \;\Rightarrow\; y = -x \Rightarrow\; v_- = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix},$$

so the "good" states are

$$\psi_+ = \frac{1}{\sqrt{2}}(\psi_1 + \psi_{-1}) = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{L}}\left(e^{i2\pi x/L} + e^{-i2\pi x/L}\right) = \boxed{\sqrt{\frac{2}{L}}\cos\left(\frac{2\pi x}{L}\right),}$$

$$\psi_- = \frac{1}{\sqrt{2}}(\psi_1 - \psi_{-1}) = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{L}}\left(e^{i2\pi x/L} - e^{-i2\pi x/L}\right) = \boxed{i\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right).}$$

(e) The energy, to second order, is

$$E = E^0 + E^1 + E^2 = E_1^0 + 0 + \left(\frac{V_0^2}{12E_1^0}\right)(2 \pm 3), \text{ where } E_1^0 = \frac{\hbar^2 k^2}{2m} = \frac{2\pi^2\hbar^2}{mL^2},$$

so the perturbed energies are

$$\boxed{E_+ = \frac{2\pi^2\hbar^2}{mL^2} + 5\frac{V_0^2 mL^2}{24\pi^2\hbar^2}, \quad E_- = \frac{2\pi^2\hbar^2}{mL^2} - \frac{V_0^2 mL^2}{24\pi^2\hbar^2}.}$$

Problem 7.42

(a)

$$\frac{\partial E_n}{\partial e} = -\frac{4me^3}{32\pi^2\epsilon_0^2\hbar^2(j_{\max} + \ell + 1)^2} = \frac{4}{e}E_n; \quad \frac{\partial H}{\partial e} = -\frac{2e}{4\pi\epsilon_0}\frac{1}{r}. \quad \text{So the F-H theorem says:}$$

$$\frac{4}{e}E_n = -\frac{e}{2\pi\epsilon_0}\left\langle\frac{1}{r}\right\rangle, \text{ or } \left\langle\frac{1}{r}\right\rangle = -\frac{8\pi\epsilon_0}{e^2}E_n = -\frac{8\pi\epsilon_0 E_1}{e^2 n^2} = -\frac{8\pi\epsilon_0}{e^2}\left[-\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{e^2 m}{4\pi\epsilon_0\hbar^2}\frac{1}{n^2}.$$

$$\text{But } \frac{4\pi\epsilon_0\hbar^2}{me^2} = a \text{ (by Eq. 4.72), so } \boxed{\left\langle\frac{1}{r}\right\rangle = \frac{1}{n^2 a}.} \quad \text{(Agrees with Eq. 7.56.)}$$

(b)

$$\frac{\partial E_n}{\partial \ell} = \frac{2me^4}{32\pi^2\epsilon_0^2\hbar^2(j_{\max} + \ell + 1)^3} = -\frac{2E_n}{n}; \quad \frac{\partial H}{\partial \ell} = \frac{\hbar^2}{2mr^2}(2\ell + 1); \quad \text{so F-H says}$$

$$-\frac{2E_n}{n} = \frac{\hbar^2(2\ell + 1)}{2m}\left\langle\frac{1}{r^2}\right\rangle, \quad \text{or } \left\langle\frac{1}{r^2}\right\rangle = -\frac{4mE_n}{n(2\ell + 1)\hbar^2} = -\frac{4mE_1}{n^3(2\ell + 1)\hbar^2}.$$

$$\text{But } -\frac{4mE_1}{\hbar^2} = \frac{2}{a^2}, \quad \text{so } \boxed{\left\langle\frac{1}{r^2}\right\rangle = \frac{1}{n^3(\ell + \frac{1}{2})a^2}.} \quad \text{(Agrees with Eq. 7.57.)}$$

Problem 7.43

Equation 4.53 $\Rightarrow u'' = \left[\frac{\ell(\ell+1)}{r^2} - \frac{2mE_n}{\hbar^2} - \frac{2m}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{r}\right]u.$

But $\frac{me^2}{4\pi\epsilon_0\hbar^2} = \frac{1}{a}$ (Eq. 4.72), and $-\frac{2mE_n}{\hbar^2} = \frac{2m}{\hbar^2}\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{1}{n^2} = \frac{1}{a^2n^2}$. So

$\bigstar \quad u'' = \left[\frac{\ell(\ell+1)}{r^2} - \frac{2}{ar} + \frac{1}{n^2a^2}\right]u.$

$\therefore \int (ur^s u'')\,dr = \int ur^s\left[\frac{\ell(\ell+1)}{r^2} - \frac{2}{ar} + \frac{1}{n^2a^2}\right]u\,dr = \ell(\ell+1)\langle r^{s-2}\rangle - \frac{2}{a}\langle r^{s-1}\rangle + \frac{1}{n^2a^2}\langle r^s\rangle$

$\blacklozenge \qquad = -\int \frac{d}{dr}(ur^s)u'\,dr = -\int (u'r^su')\,dr - s\int (ur^{s-1}u')\,dr.$

Lemma 1: $\int (ur^su')\,dr = -\int \frac{d}{dr}(ur^s)u\,dr = -\int (u'r^su)\,dr - s\int ur^{s-1}u\,dr \quad \Rightarrow$

$2\int (ur^su')\,dr = -s\langle r^{s-1}\rangle$, or $\int (ur^su')\,dr = -\frac{s}{2}\langle r^{s-1}\rangle.$

Lemma 2: $\int (u''r^{s+1}u')\,dr = -\int u'\frac{d}{dr}(r^{s+1}u')\,dr = -(s+1)\int (u'r^su')\,dr - \int (u'r^{s+1}u'')\,dr.$

$2\int (u''r^{s+1}u')\,dr = -(s+1)\int (u'r^su')\,dr$, or: $\int (u'r^su')\,dr = -\frac{2}{s+1}\int (u''r^{s+1}u')\,dr.$

Lemma 3: Use $\bigstar$ in Lemma 2, and exploit Lemma 1:

$$\begin{aligned}
\int (u'r^su')\,dr &= -\frac{2}{s+1}\int\left[\frac{\ell(\ell+1)}{r^2} - \frac{2}{ar} + \frac{1}{n^2a^2}\right](ur^{s+1}u')\,dr \\
&= -\frac{2}{s+1}\left[\ell(\ell+1)\int (ur^{s-1}u')\,dr - \frac{2}{a}\int (ur^su')\,dr + \frac{1}{n^2a^2}\int (ur^{s+1}u')\,dr\right] \\
&= -\frac{2}{s+1}\left[\ell(\ell+1)\left(-\frac{s-1}{2}\langle r^{s-2}\rangle\right) - \frac{2}{a}\left(-\frac{s}{2}\langle r^{s-1}\rangle\right) + \frac{1}{n^2a^2}\left(-\frac{s+1}{2}\langle r^s\rangle\right)\right] \\
&= \ell(\ell+1)\left(\frac{s-1}{s+1}\right)\langle r^{s-2}\rangle - \frac{2}{a}\left(\frac{s}{s+1}\right)\langle r^{s-1}\rangle + \frac{1}{n^2a^2}\langle r^s\rangle.
\end{aligned}$$

Plug Lemmas 1 and 3 into $\blacklozenge$:

$$\begin{aligned}
&\ell(\ell+1)\langle r^{s-2}\rangle - \frac{2}{a}\langle r^{s-1}\rangle + \frac{1}{n^2a^2}\langle r^s\rangle \\
&\qquad = -\ell(\ell+1)\left(\frac{s-1}{s+1}\right)\langle r^{s-2}\rangle + \frac{2}{a}\left(\frac{s}{s+1}\right)\langle r^{s-1}\rangle - \frac{1}{n^2a^2}\langle r^s\rangle + \frac{s(s-1)}{2}\langle r^{s-2}\rangle.
\end{aligned}$$

$$\frac{2}{n^2a^2}\langle r^s\rangle - \frac{2}{a}\underbrace{\left[1 + \frac{s}{s+1}\right]}_{\frac{2s+1}{s+1}}\langle r^{s-1}\rangle + \left\{\ell(\ell+1)\underbrace{\left[1 + \frac{s-1}{s+1}\right]}_{\frac{2s}{s+1}} - \frac{s(s-1)}{2}\right\}\langle r^{s-2}\rangle = 0.$$

$\frac{2(s+1)}{n^2a^2}\langle r^s\rangle - \frac{2}{a}(2s+1)\langle r^{s-1}\rangle + 2s\left[\ell^2 + \ell - \frac{(s^2-1)}{4}\right]\langle r^{s-2}\rangle = 0$, or, finally,

$\frac{(s+1)}{n^2}\langle r^s\rangle - a(2s+1)\langle r^{s-1}\rangle + \frac{sa^2}{4}(\underbrace{4\ell^2 + 4\ell + 1}_{(2\ell+1)^2} - s^2)\langle r^{s-2}\rangle = 0.$ QED

Problem 7.44

(a)

$$\frac{1}{n^2}\langle 1\rangle - a\left\langle\frac{1}{r}\right\rangle + 0 = 0 \Rightarrow \boxed{\left\langle\frac{1}{r}\right\rangle = \frac{1}{n^2 a}.}$$

$$\frac{2}{n^2}\langle r\rangle - 3a\langle 1\rangle + \frac{1}{4}\left[(2\ell+1)^2 - 1\right]a^2\left\langle\frac{1}{r}\right\rangle = 0 \Rightarrow \frac{2}{n^2}\langle r\rangle = 3a - \ell(\ell+1)a^2\frac{1}{n^2 a} = \frac{a}{n^2}\left[3n^2 - \ell(\ell+1)\right].$$

$$\boxed{\langle r\rangle = \frac{a}{2}\left[3n^2 - \ell(\ell+1)\right].}$$

$$\frac{3}{n^2}\langle r^2\rangle - 5a\langle r\rangle + \frac{1}{2}\left[(2\ell+1)^2 - 4\right]a^2 = 0 \Rightarrow \frac{3}{n^2}\langle r^2\rangle = 5a\frac{a}{2}\left[3n^2 - \ell(\ell+1)\right] - \frac{a^2}{2}\left[(2\ell+1)^2 - 4\right]$$

$$\begin{aligned}\frac{3}{n^2}\langle r^2\rangle &= \frac{a^2}{2}\left[15n^2 - 5\ell(\ell+1) - 4\ell(\ell+1) - 1 + 4\right] = \frac{a^2}{2}\left[15n^2 - 9\ell(\ell+1) + 3\right]\\ &= \frac{3a^2}{2}\left[5n^2 - 3\ell(\ell+1) + 1\right]; \quad \boxed{\langle r^2\rangle = \frac{n^2a^2}{2}\left[5n^2 - 3\ell(\ell+1) + 1\right].}\end{aligned}$$

$$\frac{4}{n^2}\langle r^3\rangle - 7a\langle r^2\rangle + \frac{3}{4}\left[(2\ell+1)^2 - 9\right]a^2\langle r\rangle = 0 \Longrightarrow$$

$$\begin{aligned}\frac{4}{n^2}\langle r^3\rangle &= 7a\frac{n^2a^2}{2}\left[5n^2 - 3\ell(\ell+1) + 1\right] - \frac{3}{4}\left[4\ell(\ell+1) - 8\right]a^2\frac{a}{2}\left[3n^2 - \ell(\ell+1)\right]\\ &= \frac{a^3}{2}\left\{35n^4 - 21\ell(\ell+1)n^2 + 7n^2 - \left[3\ell(\ell+1) - 6\right]\left[3n^2 - \ell(\ell+1)\right]\right\}\\ &= \frac{a^3}{2}\left[35n^4 - 21\ell(\ell+1)n^2 + 7n^2 - 9\ell(\ell+1)n^2 + 3\ell^2(\ell+1)^2 + 18n^2 - 6\ell(\ell+1)\right]\\ &= \frac{a^3}{2}\left[35n^4 + 25n^2 - 30\ell(\ell+1)n^2 + 3\ell^2(\ell+1)^2 - 6\ell(\ell+1)\right].\end{aligned}$$

$$\boxed{\langle r^3\rangle = \frac{n^2a^3}{8}\left[35n^4 + 25n^2 - 30\ell(\ell+1)n^2 + 3\ell^2(\ell+1)^2 - 6\ell(\ell+1)\right].}$$

(b)

$$0 + a\left\langle\frac{1}{r^2}\right\rangle - \frac{1}{4}\left[(2\ell+1)^2 - 1\right]a^2\left\langle\frac{1}{r^3}\right\rangle = 0 \Rightarrow \boxed{\left\langle\frac{1}{r^2}\right\rangle = a\ell(\ell+1)\left\langle\frac{1}{r^3}\right\rangle.}$$

(c)

$$a\ell(\ell+1)\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{(\ell+1/2)n^3a^2} \Rightarrow \boxed{\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{\ell(\ell+1/2)(\ell+1)n^3a^3}.} \quad \text{Agrees with Eq. 7.66.}$$

Notice a curious fact about these results: for a given n,
$\langle r\rangle$ *decreases* with increasing ℓ, whereas $\langle 1/r\rangle$ is *constant*;
$\langle r^2\rangle$ *decreases* with increasing ℓ, but so does $\langle 1/r^2\rangle$;
$\langle r^3\rangle$ *decreases* with increasing ℓ, and so does $\langle 1/r^3\rangle$.
Off hand, you might suppose that if $\langle r^s\rangle$ decreases, $\langle 1/r^s\rangle$ should *increase*, but this is not the case. What happens (as Paul Muzikar points out) is that the electron density is *more sharply peaked* as ℓ increases; for small ℓ it is both closer in *and* farther out than it is for large ℓ.

Problem 7.45

(a)

$$|1\,0\,0\rangle = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \text{ (Eq. 4.80)}, \; E_s^1 = \langle 1\,0\,0|H'|1\,0\,0\rangle = eE_{\text{ext}} \frac{1}{\pi a^3} \int e^{-2r/a} (r\cos\theta) r^2 \sin\theta \, dr\, d\theta\, d\phi.$$

But the θ integral is zero: $\displaystyle\int_0^\pi \cos\theta \sin\theta \, d\theta = \left.\frac{\sin^2\theta}{2}\right|_0^\pi = 0.$ So $E_s^1 = 0.$ QED

(b) From Problem 4.13:
$$\begin{cases} |1\rangle = \psi_{2\,0\,0} = & \dfrac{1}{\sqrt{2\pi a}} \dfrac{1}{2a} \left(1 - \dfrac{r}{2a}\right) e^{-r/2a} \\ |2\rangle = \psi_{2\,1\,1} = & -\dfrac{1}{\sqrt{\pi a}} \dfrac{1}{8a^2} r e^{-r/2a} \sin\theta e^{i\phi} \\ |3\rangle = \psi_{2\,1\,0} = & \dfrac{1}{\sqrt{2\pi a}} \dfrac{1}{4a^2} r e^{-r/2a} \cos\theta \\ |4\rangle = \psi_{2\,1\,-1} = & \dfrac{1}{\sqrt{\pi a}} \dfrac{1}{8a^2} r e^{-r/2a} \sin\theta e^{-i\phi} \end{cases}$$

$$\left.\begin{aligned} \langle 1|H_s'|1\rangle &= \{\ldots\} \int_0^\pi \cos\theta\sin\theta\, d\theta = 0 \\ \langle 2|H_s'|2\rangle &= \{\ldots\} \int_0^\pi \sin^2\theta\cos\theta\sin\theta\, d\theta = 0 \\ \langle 3|H_s'|3\rangle &= \{\ldots\} \int_0^\pi \cos^2\theta\cos\theta\sin\theta\, d\theta = 0 \\ \langle 4|H_s'|4\rangle &= \{\ldots\} \int_0^\pi \sin^2\theta\cos\theta\sin\theta\, d\theta = 0 \\ \langle 1|H_s'|2\rangle &= \{\ldots\} \int_0^{2\pi} e^{i\phi}\, d\phi = 0 \\ \langle 1|H_s'|4\rangle &= \{\ldots\} \int_0^{2\pi} e^{-i\phi}\, d\phi = 0 \\ \langle 2|H_s'|3\rangle &= \{\ldots\} \int_0^{2\pi} e^{-i\phi}\, d\phi = 0 \\ \langle 2|H_s'|4\rangle &= \{\ldots\} \int_0^{2\pi} e^{-2i\phi}\, d\phi = 0 \\ \langle 3|H_s'|4\rangle &= \{\ldots\} \int_0^{2\pi} e^{-i\phi}\, d\phi = 0 \end{aligned}\right\}$$

All matrix elements of H_s' are zero except $\langle 1|H_s'|3\rangle$ and $\langle 3|H_s'|1\rangle$ (which are complex conjugates, so only one needs to be evaluated).

$$\begin{aligned} \langle 1|H_s'|3\rangle &= eE_{\text{ext}} \frac{1}{\sqrt{2\pi a}} \frac{1}{2a} \frac{1}{\sqrt{2\pi a}} \frac{1}{4a^2} \int \left(1 - \frac{r}{2a}\right) e^{-r/2a} r e^{-r/2a} \cos\theta (r\cos\theta) r^2 \sin\theta \, dr\, d\theta\, d\phi \\ &= \frac{eE_{\text{ext}}}{2\pi a 8a^3} (2\pi) \left[\int_0^\pi \cos^2\theta \sin\theta\, d\theta\right] \int_0^\infty \left(1 - \frac{r}{2a}\right) e^{-r/a} r^4\, dr \\ &= \frac{eE_{\text{ext}}}{8a^4} \frac{2}{3} \left\{\int_0^\infty r^4 e^{-r/a}\, dr - \frac{1}{2a}\int_0^\infty r^5 e^{-r/a}\, dr\right\} = \frac{eE_{\text{ext}}}{12a^4}\left(4!a^5 - \frac{1}{2a}5!a^6\right) \\ &= \frac{eE_{\text{ext}}}{12a^4} 24a^5 \left(1 - \frac{5}{2}\right) = eaE_{\text{ext}}(-3) = -3aeE_{\text{ext}}. \end{aligned}$$

$$\mathsf{W} = -3aeE_{\text{ext}} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

We need the eigenvalues of this matrix. The characteristic equation is:

$$\begin{vmatrix} -\lambda & 0 & 1 & 0 \\ 0 & -\lambda & 0 & 0 \\ 1 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & -\lambda \end{vmatrix} = -\lambda \begin{vmatrix} -\lambda & 0 & 0 \\ 0 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{vmatrix} + \begin{vmatrix} 0 & -\lambda & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -\lambda \end{vmatrix} = -\lambda(-\lambda)^3 + (-\lambda^2) = \lambda^2(\lambda^2 - 1) = 0.$$

The eigenvalues are 0, 0, 1, and -1, so the perturbed energies are

$$\boxed{E_2,\ E_2,\ E_2 + 3aeE_{\text{ext}},\ E_2 - 3aeE_{\text{ext}}. \quad \text{Three levels.}}$$

(c) The eigenvectors with eigenvalue 0 are $|2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$ and $|4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$; the eigenvectors with eigenvalues ± 1 are $|\pm\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ \pm 1 \\ 0 \end{pmatrix}$. So the "good" states are $\boxed{\psi_{2\,1\,1},\ \psi_{2\,1\,-1},\ \frac{1}{\sqrt{2}}(\psi_{2\,0\,0} + \psi_{2\,1\,0}),\ \frac{1}{\sqrt{2}}(\psi_{2\,0\,0} - \psi_{2\,1\,0}).}$

$$\langle \mathbf{p}_e \rangle_4 = -e \frac{1}{\pi a} \frac{1}{64 a^4} \int r^2 e^{-r/a} \sin^2\theta \left[r \sin\theta \cos\phi \hat{\imath} + r \sin\theta \sin\phi \hat{\jmath} + r \cos\theta \hat{k} \right] r^2 \sin\theta \, dr \, d\theta \, d\phi.$$

But $\int_0^{2\pi} \cos\phi \, d\phi = \int_0^{2\pi} \sin\phi \, d\phi = 0, \quad \int_0^{\pi} \sin^3\theta \cos\theta \, d\theta = \left| \frac{\sin^4\theta}{4} \right|_0^{\pi} = 0,$ so

$$\boxed{\langle \mathbf{p}_e \rangle_4 = 0. \quad \text{Likewise} \quad \langle \mathbf{p}_e \rangle_2 = 0.}$$

$$\begin{aligned} \langle \mathbf{p}_e \rangle_\pm &= -\frac{1}{2} e \int (\psi_1 \pm \psi_3)^2 (\mathbf{r}) r^2 \sin\theta \, dr \, d\theta \, d\phi \\ &= -\frac{1}{2} e \frac{1}{2\pi a} \frac{1}{4a^2} \int \left[\left(1 - \frac{r}{2a}\right) \pm \frac{r}{2a} \cos\theta \right]^2 e^{-r/a} r (\sin\theta \cos\phi \, \hat{\imath} + \sin\theta \sin\phi \, \hat{\jmath} + \cos\theta \, \hat{k}) r^2 \sin\theta \, dr \, d\theta \, d\phi \\ &= -\frac{e}{2} \frac{\hat{k}}{2\pi a} \frac{1}{4a^2} 2\pi \int \left[\left(1 - \frac{r}{2a}\right) \pm \frac{r}{2a} \cos\theta \right]^2 r^3 e^{-r/a} \cos\theta \sin\theta \, dr \, d\theta. \end{aligned}$$

But $\int_0^{\pi} \cos\theta \sin\theta \, d\theta = \int_0^{\pi} \cos^3\theta \sin\theta \, d\theta = 0$, so only the cross-term survives:

$$\begin{aligned} \langle \mathbf{p}_e \rangle_\pm &= -\frac{e}{8a^3} \hat{k} \left(\pm \frac{1}{a} \right) \int \left(1 - \frac{r}{2a}\right) r \cos\theta \, r^3 e^{-r/a} \cos\theta \sin\theta \, dr \, d\theta \\ &= \mp \left(\frac{e}{8a^4} \hat{k} \right) \left[\int_0^{\pi} \cos^2\theta \sin\theta \, d\theta \right] \int_0^{\infty} \left(1 - \frac{r}{2a}\right) r^4 e^{-r/a} dr = \mp \left(\frac{e}{8a^4} \hat{k} \right) \frac{2}{3} \left[4! a^5 - \frac{1}{2a} 5! a^6 \right] \\ &= \mp e\hat{k} \left(\frac{1}{12a^4} \right) 24a^5 \left(1 - \frac{5}{2}\right) = \boxed{\pm 3ae\hat{k}.} \end{aligned}$$

Problem 7.46

(a) The nine states are:

$$\begin{cases} \underline{\ell=0}: |3\,0\,0\rangle & = R_{30}Y_0^0 \\ \underline{\ell=1}: |3\,1\,1\rangle & = R_{31}Y_1^1 \\ \qquad\quad |3\,1\,0\rangle & = R_{31}Y_1^0 \\ \qquad\quad |3\,1-1\rangle & = R_{31}Y_1^{-1} \\ \underline{\ell=2}: |3\,2\,2\rangle & = R_{32}Y_2^2 \\ \qquad\quad |3\,2\,1\rangle & = R_{32}Y_2^1 \\ \qquad\quad |3\,2\,0\rangle & = R_{32}Y_2^0 \\ \qquad\quad |3\,2-1\rangle & = R_{32}Y_2^{-1} \\ \qquad\quad |3\,2-2\rangle & = R_{32}Y_2^{-2} \end{cases}$$

H_s' contains no ϕ dependence, so the ϕ integral will be:

$$\langle n\,\ell\,m|H_s'|n'\,\ell'\,m'\rangle = \{\cdots\}\int_0^{2\pi} e^{-im\phi}e^{im'\phi}\,d\phi, \quad \text{which is zero unless} \quad m'=m.$$

For diagonal elements: $\langle n\,\ell\,m|H_s'|n\,\ell\,m\rangle = \{\cdots\}\int_0^\pi [P_\ell^m(\cos\theta)]^2\cos\theta\sin\theta\,d\theta$. But (p. 136 in the text) P_ℓ^m is a polynomial (even or odd) in $\cos\theta$, multiplied (if m is odd) by $\sin\theta$. Since $\sin^2\theta = 1-\cos^2\theta$, $[P_\ell^m(\cos\theta)]^2$ is a polynomial in even powers of $\cos\theta$. So the θ integral is of the form

$$\int_0^\pi (\cos\theta)^{2j+1}\sin\theta\,d\theta = -\left.\frac{(\cos\theta)^{2j+2}}{(2j+2)}\right|_0^\pi = 0. \quad \textit{All diagonal elements are zero.}$$

There remain just 4 elements to calculate:

$$m=m'=0:\ \langle 3\,0\,0|H_s'|3\,1\,0\rangle,\ \langle 3\,0\,0|H_s'|3\,2\,0\rangle,\ \langle 3\,1\,0|H_s'|3\,2\,0\rangle;\ m=m'=\pm1:\ \langle 3\,1\,\pm1|H_s'|3\,2\,\pm1\rangle.$$

$$\langle 3\,0\,0|H_s'|3\,1\,0\rangle = eE_{\text{ext}}\int R_{30}R_{31}r^3dr\int Y_0^0Y_1^0\cos\theta\sin\theta\,d\theta\,d\phi. \quad \text{From Table 4.7}:$$

$$\int R_{30}R_{31}r^3\,dr = \frac{2}{\sqrt{27}}\frac{1}{a^{3/2}}\frac{8}{27\sqrt{6}}\frac{1}{a^{3/2}}\frac{1}{a}\int\left(1-\frac{2r}{3a}+\frac{2r^2}{27a^2}\right)e^{-r/3a}\left(1-\frac{r}{6a}\right)re^{-r/3a}r^3\,dr.$$

Let $x \equiv 2r/3a$:

$$\begin{aligned}\int R_{30}R_{31}r^3\,dr &= \frac{2^4}{3^5\sqrt{2}a^4}\left(\frac{3a}{2}\right)^5\int_0^\infty\left(1-x+\frac{x^2}{6}\right)\left(1-\frac{x}{4}\right)x^4e^{-x}dx \\ &= \frac{a}{2\sqrt{2}}\int_0^\infty\left(1-\frac{5}{4}x+\frac{5}{12}x^2-\frac{1}{24}x^3\right)x^4e^{-x}dx = \frac{a}{2\sqrt{2}}\left(4!-\frac{5}{4}5!+\frac{5}{12}6!-\frac{1}{24}7!\right) \\ &= -9\sqrt{2}a.\end{aligned}$$

$$\int Y_0^0Y_1^0\cos\theta\sin\theta\,d\theta\,d\phi = \frac{1}{\sqrt{4\pi}}\sqrt{\frac{3}{4\pi}}\int\cos\theta\cos\theta\sin\theta\,d\theta\,d\phi = \frac{\sqrt{3}}{4\pi}2\pi\int_0^\pi\cos^2\theta\sin\theta\,d\theta = \frac{\sqrt{3}}{2}\frac{2}{3} = \frac{\sqrt{3}}{3}.$$

$$\langle 3\,0\,0|H_s'|3\,1\,0\rangle = eE_{\text{ext}}(-9\sqrt{2}a)\left(\frac{\sqrt{3}}{3}\right) = \boxed{-3\sqrt{6}aeE_{\text{ext}}.}$$

$$\langle 3\,0\,0|H_s'|3\,2\,0\rangle = eE_{\text{ext}}\int R_{30}R_{32}r^3dr\int Y_0^0Y_2^0\cos\theta\sin\theta\,d\theta\,d\phi.$$

$$\int Y_0^0Y_2^0\cos\theta\sin\theta\,d\theta\,d\phi = \frac{1}{\sqrt{4\pi}}\sqrt{\frac{5}{16\pi}}\int(3\cos^2\theta-1)\cos\theta\sin\theta\,d\theta\,d\phi = 0. \quad \boxed{\langle 3\,0\,0\,|H_s'|3\,2\,0\rangle = 0.}$$

$$\langle 3\,1\,0|H_s'|3\,2\,0\rangle = eE_{\text{ext}} \int R_{31}R_{32}r^3 dr \int Y_1^0 Y_2^0 \cos\theta \sin\theta \, d\theta \, d\phi.$$

$$\begin{aligned}\int R_{31}R_{32}r^3 dr &= \frac{8}{27\sqrt{6}}\frac{1}{a^{3/2}}\frac{1}{a}\frac{4}{81\sqrt{30}}\frac{1}{a^{3/2}}\frac{1}{a^2}\int\left(1-\frac{r}{6a}\right) re^{-r/3a}r^2e^{-r/3a}r^3 dr \\ &= \frac{2^4}{3^8\sqrt{5}a^6}\left(\frac{3a}{2}\right)^7\int_0^\infty\left(1-\frac{x}{4}\right)x^6e^{-x}dx = \frac{a}{24\sqrt{5}}\left(6!-\frac{1}{4}7!\right) = -\frac{9\sqrt{5}}{2}a.\end{aligned}$$

$$\begin{aligned}\int Y_1^0Y_2^0 \sin\theta\cos\theta\,d\theta\,d\phi &= \sqrt{\frac{3}{4\pi}}\sqrt{\frac{5}{16\pi}}\int\cos\theta(3\cos^2\theta-1)\cos\theta\sin\theta\,d\theta\,d\phi \\ &= \frac{\sqrt{15}}{8\pi}2\pi\int_0^\pi(3\cos^4\theta-\cos^2\theta)\sin\theta\,d\theta = \frac{\sqrt{15}}{4}\left[-\frac{3}{5}\cos^5\theta+\frac{1}{3}\cos^3\theta\right]\Bigg|_0^\pi = \frac{2}{\sqrt{15}}.\end{aligned}$$

$$\langle 3\,1\,0|H_s'|3\,2\,0\rangle = eE_{\text{ext}}\left(-\frac{9\sqrt{5}}{2}a\right)\left(\frac{2}{\sqrt{15}}\right) = \boxed{-3\sqrt{3}aeE_{\text{ext}}.}$$

$$\langle 3\,1\,\pm1|H_s'|3\,2\,\pm1\rangle = eE_{\text{ext}}\int R_{31}R_{32}r^3dr\int\left(Y_1^{\pm1}\right)^* Y_2^{\pm1}\cos\theta\sin\theta\,d\theta\,d\phi.$$

$$\begin{aligned}\int\left(Y_1^{\pm1}\right)^*Y_2^{\pm1}\cos\theta\sin\theta\,d\theta\,d\phi &= \left(\mp\sqrt{\frac{3}{8\pi}}\right)\left(\mp\sqrt{\frac{15}{8\pi}}\right)\int\sin\theta e^{\mp i\phi}\sin\theta\cos\theta e^{\pm i\phi}\cos\theta\sin\theta\,d\theta\,d\phi \\ &= \frac{3\sqrt{5}}{8\pi}2\pi\int_0^\pi\cos^2\theta(1-\cos^2\theta)\sin\theta\,d\theta = \frac{3}{4}\sqrt{5}\left(-\frac{\cos^3\theta}{3}+\frac{\cos^5\theta}{5}\right)\Bigg|_0^\pi \\ &= \frac{1}{\sqrt{5}}.\end{aligned}$$

$$\langle 3\,1\,\pm1|H_s'|3\,2\,\pm1\rangle = eE_{\text{ext}}\left(-9\frac{\sqrt{5}}{2}a\right)\left(\frac{1}{\sqrt{5}}\right) = \boxed{-\frac{9}{2}aeE_{\text{ext}}.}$$

Thus the matrix representing H_s' is (all empty boxes are zero; all numbers multiplied by $-aeE_{\text{ext}}$):

	300	310	320	311	321	31-1	32-1	322	32-2
300		$3\sqrt{6}$							
310	$3\sqrt{6}$		$3\sqrt{3}$						
320		$3\sqrt{3}$							
311					9/2				
321				9/2					
31-1							9/2		
32-1						9/2			
322									
32-2									

(b) The perturbing matrix (below) breaks into a 3×3 block, two 2×2 blocks, and two 1×1 blocks, so we can work out the eigenvalues in each block separately.

$$\underline{3\times 3}: \quad 3\sqrt{3}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \quad \begin{vmatrix} -\lambda & \sqrt{2} & 0 \\ \sqrt{2} & -\lambda & 1 \\ 0 & 1 & -\lambda \end{vmatrix} = -\lambda^3 + \lambda + 2\lambda = -\lambda(\lambda^2 - 3) = 0;$$

$$\lambda = 0, \pm\sqrt{3} \quad \Rightarrow \quad E_1^1 = 0,\ E_2^1 = 9aeE_{\text{ext}},\ E_3^1 = -9aeE_{\text{ext}}.$$

$$\underline{2\times 2}: \quad \frac{9}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = \lambda^2 - 1 = 0 \Rightarrow \lambda = \pm 1.$$

$E_4^1 = \dfrac{9}{2}aeE_{\text{ext}},\ E_5^1 = -\dfrac{9}{2}aeE_{\text{ext}}$. From the other 2×2 we get $E_6^1 = E_4^1,\ E_7^1 = E_5^1$, and from the 1×1's we get $E_8^1 = E_9^1 = 0$. Thus the perturbations to the energy (E_3) are:

$$\boxed{\begin{array}{ll} 0 & \text{(degeneracy 3)} \\ (9/2)aeE_{\text{ext}} & \text{(degeneracy 2)} \\ -(9/2)aeE_{\text{ext}} & \text{(degeneracy 2)} \\ 9aeE_{\text{ext}} & \text{(degeneracy 1)} \\ -9aeE_{\text{ext}} & \text{(degeneracy 1)} \end{array}}$$

Problem 7.47

$$\text{Equation 7.93} \Rightarrow E_{\text{hf}}^1 = \frac{\mu_0 g_d e^2}{3\pi m_d m_e a^3}\langle \mathbf{S}_d \cdot \mathbf{S}_e\rangle; \quad \text{Eq. 7.95} \Rightarrow \mathbf{S}_d \cdot \mathbf{S}_e = \frac{1}{2}(S^2 - S_e^2 - S_d^2).$$

Electron has spin $\frac{1}{2}$, so $S_e^2 = \frac{1}{2}\left(\frac{3}{2}\right)\hbar^2 = \frac{3}{4}\hbar^2$; deuteron has spin 1, so $S_d^2 = 1(2)\hbar^2 = 2\hbar^2$.
Total spin could be $\frac{3}{2}$ [in which case $S^2 = \frac{3}{2}\left(\frac{5}{2}\right)\hbar^2 = \frac{15}{4}\hbar^2$] or $\frac{1}{2}$ [in which case $S^2 = \frac{3}{4}\hbar^2$]. Thus

$$\langle \mathbf{S}_d \cdot \mathbf{S}_e\rangle = \left\{\begin{array}{ll} \frac{1}{2}\left(\frac{15}{4}\hbar^2 - \frac{3}{4}\hbar^2 - 2\hbar^2\right) & = \frac{1}{2}\hbar^2 \\ \frac{1}{2}\left(\frac{3}{4}\hbar^2 - \frac{3}{4}\hbar^2 - 2\hbar^2\right) & = -\hbar^2 \end{array}\right\}; \text{ the difference is } \frac{3}{2}\hbar^2, \text{ so} \quad \Delta E = \frac{\mu_0 g_d e^2\hbar^2}{2\pi m_d m_e a^3}.$$

But $\quad \mu_0\epsilon_0 = \dfrac{1}{c^2} \Rightarrow \mu_0 = \dfrac{1}{\epsilon_0 c^2}, \quad$ so $\quad \Delta E = \dfrac{2g_d e^2\hbar^2}{4\pi\epsilon_0 m_d m_e c^2 a^3} = \dfrac{2g_d\hbar^4}{m_d m_e^2 c^2 a^4} = \dfrac{3}{2}\dfrac{g_d}{g_p}\dfrac{m_p}{m_d}\Delta E_{\text{hydrogen}}$ (Eq. 7.97).

Now, $\lambda = \dfrac{c}{\nu} = \dfrac{ch}{\Delta E}, \quad$ so $\quad \lambda_d = \dfrac{2}{3}\dfrac{g_p}{g_d}\dfrac{m_d}{m_p}\lambda_h$, and since $m_d = 2m_p$, $\lambda_d = \dfrac{4}{3}\left(\dfrac{5.59}{1.71}\right)(21\text{ cm}) = \boxed{92\text{ cm.}}$

Problem 7.48

(a) The potential energy of the electron (charge $-e$) at (x, y, z) due to q's at $x = \pm d$ alone is:

$$V = -\frac{eq}{4\pi\epsilon_0}\left[\frac{1}{\sqrt{(x+d)^2 + y^2 + z^2}} + \frac{1}{\sqrt{(x-d)^2 + y^2 + z^2}}\right]. \quad \text{Expanding (with } d \gg x, y, z):$$

$$\frac{1}{\sqrt{(x\pm d)^2 + y^2 + z^2}} = (x^2 \pm 2dx + d^2 + y^2 + z^2)^{-1/2} = (d^2 \pm 2dx + r^2)^{-1/2} = \frac{1}{d}\left(1 \pm \frac{2x}{d} + \frac{r^2}{d^2}\right)^{-1/2}$$

$$\approx \frac{1}{d}\left(1 \mp \frac{x}{d} - \frac{r^2}{2d^2} + \frac{3}{8}\frac{4x^2}{d^2}\right) = \frac{1}{d}\left[1 \mp \frac{x}{d} + \frac{1}{2d^2}(3x^2 - r^2)\right].$$

$$V = -\frac{eq}{4\pi\epsilon_0 d}\left[1 - \frac{x}{d} + \frac{1}{2d^2}(3x^2 - r^2) + 1 + \frac{x}{d} + \frac{1}{2d^2}(3x^2 - r^2)\right] = -\frac{2eq}{4\pi\epsilon_0 d} - \frac{eq}{4\pi\epsilon_0 d^3}(3x^2 - r^2)$$
$$= 2\beta d^2 + 3\beta x^2 - \beta r^2, \quad \text{where} \quad \beta \equiv -\frac{e}{4\pi\epsilon_0}\frac{q}{d^3}.$$

Thus with all six charges in place

$$H' = 2(\beta_1 d_1^2 + \beta_2 d_2^2 + \beta_3 d_3^2) + 3(\beta_1 x^2 + \beta_2 y^2 + \beta_3 z^2) - r^2(\beta_1 + \beta_2 + \beta_3). \quad \text{QED}$$

(b) $\langle 1\,0\,0|H'|1\,0\,0\rangle = \dfrac{1}{\pi a^3}\displaystyle\int e^{-2r/a} H' r^2 \sin\theta\, dr\, d\theta\, d\phi$

$$= V_0 + \frac{3}{\pi a^3}\int e^{-2r/a}(\beta_1 x^2 + \beta_2 y^2 + \beta_3 z^2) r^2 \sin\theta dr\, d\theta\, d\phi - \frac{(\beta_1 + \beta_2 + \beta_3)}{\pi a^3}\int r^2 e^{-2r/a} r^2 \sin\theta\, dr\, d\theta\, d\phi.$$

$$I_1 \equiv \int r^2 e^{-2r/a} r^2 \sin\theta\, dr\, d\theta\, d\phi = 4\pi\int_0^\infty r^4 e^{-2r/a} dr = 4\pi 4!(\frac{a}{2})^5 = 3\pi a^5.$$
$$I_2 \equiv \int e^{-2r/a}(\beta_1 x^2 + \beta_2 y^2 + \beta_3 z^2) r^2 \sin\theta\, dr\, d\theta\, d\phi$$
$$= \int r^4 e^{-2r/a}(\beta_1 \sin^2\theta\cos^2\phi + \beta_2 \sin^2\theta\sin^2\phi + \beta_3\cos^2\theta)\sin\theta\, dr\, d\theta\, d\phi.$$

But $\displaystyle\int_0^{2\pi}\cos^2\phi\, d\phi = \int_0^{2\pi}\sin^2\phi\, d\phi = \pi, \quad \int_0^{2\pi} d\phi = 2\pi.$ So

$$= \int_0^\infty r^4 e^{-2r/a} dr \int_0^\pi \left[\pi(\beta_1 + \beta_2)\sin^2\theta + 2\pi\beta_3\cos^2\theta\right]\sin\theta\, d\theta.$$

But $\displaystyle\int_0^\pi \sin^3\theta\, d\theta = \frac{4}{3}, \quad \int_0^\pi \cos^2\theta\sin\theta\, d\theta = \frac{2}{3}.$ So

$$= 4!\left(\frac{a}{2}\right)^5\left[\frac{4\pi}{3}(\beta_1 + \beta_2) + \frac{4\pi}{3}\beta_3\right] = \pi a^5(\beta_1 + \beta_2 + \beta_3).$$

$$\langle 1\,0\,0|H'|1\,0\,0\rangle = V_0 + \frac{3}{\pi a^3}\pi a^5(\beta_1 + \beta_2 + \beta_3) - \frac{(\beta_1 + \beta_2 + \beta_3)}{\pi a^3}3\pi a^5 = \boxed{V_0.}$$

(c) The four states are $\left\{\begin{array}{ll} |2\,0\,0\rangle & = R_{20}Y_0^0 \\ |2\,1\,1\rangle & = R_{21}Y_1^1 \\ |2\,1\,-1\rangle & = R_{21}Y_1^{-1} \\ |2\,1\,0\rangle & = R_{21}Y_1^0 \end{array}\right\}$ (functional forms in Problem 4.13).

Diagonal elements: $\langle n\,\ell\,m|H'|n\,\ell\,m\rangle = V_0 + 3\left(\beta_1\langle x^2\rangle + \beta_2\langle y^2\rangle + \beta_3\langle z^2\rangle\right) - (\beta_1 + \beta_2 + \beta_3)\langle r^2\rangle$.

For $|2\,0\,0\rangle, \langle x^2\rangle = \langle y^2\rangle = \langle z^2\rangle = \frac{1}{3}\langle r^2\rangle$ (Y_0^0 does not depend on ϕ, θ; this state has spherical symmetry), so $\boxed{\langle 2\,0\,0|H'|2\,0\,0\rangle = V_0.}$ (I could have used the same argument in (b).)

From Problem 7.44(a), $\langle r^2\rangle = \dfrac{n^2a^2}{2}\left[5n^2 - 3\ell(\ell+1) + 1\right]$, so for $n = 2, \ell = 1:$ $\langle r^2\rangle = 30a^2$. Moreover, since $\langle x^2\rangle = \{\ldots\}\displaystyle\int_0^{2\pi}\cos^2\phi\, d\phi = \{\ldots\}\int_0^{2\pi}\sin^2\phi\, d\phi = \langle y^2\rangle$, and $\langle x^2\rangle + \langle y^2\rangle + \langle z^2\rangle = \langle r^2\rangle$, it follows that $\langle x^2\rangle = \langle y^2\rangle = \dfrac{1}{2}(\langle r^2\rangle - \langle z^2\rangle) = 15a^2 - \dfrac{1}{2}\langle z^2\rangle$. So all we need to calculate is $\langle z^2\rangle$.

$$\langle 2\,1\,0|z^2|2\,1\,0\rangle = \frac{1}{2\pi a}\frac{1}{16a^4}\int r^2 e^{-r/a}\cos^2\theta(r^2\cos^2\theta) r^2 \sin\theta\, dr\, d\theta\, d\phi$$

$$= \frac{1}{16a^5}\int_0^\infty r^6 e^{-r/a}dr \int_0^\pi \cos^4\theta \sin\theta\, d\theta = \frac{1}{16a^5}6!a^7\frac{2}{5} = 18a^2; \quad \langle x^2\rangle = \langle y^2\rangle = 15a^2 - 9a^2 = 6a^2.$$

$$\begin{aligned}\langle 2\,1\,0|H'|2\,1\,0\rangle &= V_0 + 3(6a^2\beta_1 + 6a^2\beta_2 + 18a^2\beta_3) - 30a^2(\beta_1+\beta_2+\beta_3)\\ &= \boxed{V_0 - 12a^2(\beta_1+\beta_2+\beta_3) + 36a^2\beta_3.}\end{aligned}$$

$$\langle 2\,1\,\pm1|z^2|2\,1\,\pm1\rangle = \frac{1}{\pi a}\frac{1}{64a^4}\int r^2 e^{-r/a}\sin^2\theta(r^2\cos^2\theta)r^2\sin\theta\,dr\,d\theta\,d\phi$$

$$= \frac{1}{32a^5}\int_0^\infty r^6 e^{-r/a}dr\int_0^\pi (1-\cos^2\theta)\cos^2\theta\sin\theta\,d\theta = \frac{1}{32a^5}6!a^7\left(\frac{2}{3}-\frac{2}{5}\right) = 6a^2;$$

$\langle x^2\rangle = \langle y^2\rangle = 15a^2 - 3a^2 = 12a^2.$

$$\begin{aligned}\langle 2\,1\,\pm1|H'|2\,1\,\pm1\rangle &= V_0 + 3(12a^2\beta_1 + 12a^2\beta_2 + 6a^2\beta_3) - 30a^2(\beta_1+\beta_2+\beta_3)\\ &= \boxed{V_0 + 6a^2(\beta_1+\beta_2+\beta_3) - 18a^2\beta_3.}\end{aligned}$$

Off-diagonal elements: We need $\langle 2\,0\,0|H'|2\,1\,0\rangle, \langle 2\,0\,0|H'|2\,1\pm1\rangle, \langle 2\,1\,0|H'|2\,1\pm1\rangle$, and $\langle 2\,1-1|H'|2\,1\,1\rangle$. Now $\langle n\,\ell\,m|V_0|n'\,\ell'\,m'\rangle = 0$, by orthogonality, and $\langle n\,\ell\,m|r^2|n'\,\ell'\,m'\rangle = 0$, by orthogonality of Y_ℓ^m, so all we need are the matrix elements of x^2 and y^2 ($\langle|z^2|\rangle = -\langle|x^2|\rangle - \langle|y^2|\rangle$). For $\langle 2\,0\,0|x^2|2\,1\pm1\rangle$ and $\langle 2\,1\,0|x^2|2\,1\pm1\rangle$ the ϕ integral is $\int_0^{2\pi}\cos^2\phi e^{\pm i\phi}\,d\phi = \int_0^{2\pi}\cos^3\phi\,d\phi \pm i\int_0^{2\pi}\cos^2\phi\sin\phi\,d\phi = 0$, and the same goes for y^2. So $\boxed{\langle 2\,0\,0|H'|2\,1\pm1\rangle = \langle 2\,1\,0|H'|2\,1\pm1\rangle = 0.}$

For $\langle 2\,0\,0|x^2|2\,1\,0\rangle$ and $\langle 2\,0\,0|y^2|2\,1\,0\rangle$ the θ integral is $\int_0^\pi \cos\theta(\sin^2\theta)\sin\theta\,d\theta = \sin^4\theta/4\big|_0^\pi = 0$, so $\boxed{\langle 2\,0\,0|H'|2\,1\,0\rangle = 0.}$ Finally:

$$\begin{aligned}\langle 2\,1-1|x^2|2\,1\,1\rangle &= -\frac{1}{\pi a}\frac{1}{64a^4}\int r^2 e^{-r/a}\sin^2\theta e^{2i\phi}(r^2\sin^2\theta\cos^2\phi)r^2\sin\theta\,dr\,d\theta\,d\phi\\ &= -\frac{1}{64\pi a^5}\underbrace{\int_0^\infty r^6 e^{-r/a}dr}_{6!a^7}\underbrace{\int_0^\pi \sin^5\theta d\theta}_{16/15}\underbrace{\int_0^{2\pi} e^{2i\phi}\cos^2\phi\,d\phi}_{\pi/2}\\ &= -\frac{1}{64\pi a^5}6!a^7\frac{16}{15}\frac{\pi}{2} = -6a^2.\end{aligned}$$

For y^2, the ϕ integral is $\int_0^{2\pi} e^{2i\phi}\sin^2\phi\,d\phi = -\pi/2$, so $\langle 2\;1\;-1|y^2|2\;1\;1\rangle = 6a^2$, and $\langle 2\,1-1|z^2|2\,1\,1\rangle = 0$.

$$\langle 2\,1-1|H'|2\,1\,1\rangle = 3\left[\beta_1(-6a^2) + \beta_2(6a^2)\right] = \boxed{-18a^2(\beta_1-\beta_2).}$$

The perturbation matrix is:

	2 0 0	2 1 0	2 1 1	2 1 -1
2 0 0	V_0	0	0	0
2 1 0	0	$V_0 - 12a^2(\beta_1+\beta_2) + 24a^2\beta_3$	0	0
2 1 1	0	0	$V_0 + 6a^2(\beta_1+\beta_2) - 12a^2\beta_3$	$-18a^2(\beta_1-\beta_2)$
2 1 -1	0	0	$-18a^2(\beta_1-\beta_2)$	$V_0 + 6a^2(\beta_1+\beta_2) - 12a^2\beta_3$

The 2×2 block has the form $\begin{pmatrix} A & B \\ B & A \end{pmatrix}$; its characteristic equation is $(A-\lambda)^2 - B^2 = 0$, so $A-\lambda = \pm B$, or

$$\lambda = A \mp B = V_0 + 6a^2(\beta_1+\beta_2) - 12a^2\beta_3 \pm 18a^2(\beta_1-\beta_2) = \begin{cases} V_0 + 24a^2\beta_1 - 12a^2\beta_2 - 12a^2\beta_3, \\ V_0 - 12a^2\beta_1 + 24a^2\beta_2 - 12a^2\beta_3. \end{cases}$$

The first-order corrections to the energy (E_2) are therefore: $\boxed{\begin{aligned} \epsilon_1 &= V_0 \\ \epsilon_2 &= V_0 - 12a^2(\beta_1+\beta_2-2\beta_3) \\ \epsilon_3 &= V_0 - 12a^2(-2\beta_1+\beta_2+\beta_3) \\ \epsilon_4 &= V_0 - 12a^2(\beta_1 - 2\beta_2 + \beta_3) \end{aligned}}$

(i) If $\beta_1 = \beta_2 = \beta_3$, then $\epsilon_1 = \epsilon_2 = \epsilon_3 = \epsilon_4 = V_0$: $\boxed{\text{one level}}$ (still 4-fold degenerate).

(ii) If $\beta_1 = \beta_2 \neq \beta_3$, then $\epsilon_1 = V_0,\ \epsilon_2 = V_0 - 24a^2(\beta_1-\beta_3),\ \epsilon_3 = \epsilon_4 = V_0 + 12a^2(\beta_1-\beta_3)$: $\boxed{\text{three levels}}$ (one remains doubly degenerate).

(iii) If all three β's are different, there are $\boxed{\text{four levels}}$ (no remaining degeneracy).

Problem 7.49

We first calculate the mechanical angular momentum:

$$\mathbf{L}_{\text{mechanical}} = \mathbf{L} - q(\mathbf{r}\times\mathbf{A}) = \mathbf{L} - q\left[\mathbf{r}\times\left(-\frac{1}{2}\mathbf{r}\times\mathbf{B}_0\right)\right] = \mathbf{L} - \frac{q}{2}\left[r^2\mathbf{B}_0 - \mathbf{r}(\mathbf{r}\cdot\mathbf{B}_0)\right].$$

The Hamiltonian (Problem 4.72) is

$$H = \frac{p^2}{2m} + q\varphi - \mathbf{B}\cdot(\gamma_o\mathbf{L} + \gamma\mathbf{S}) + \frac{q^2}{8m}\left[r^2B_0^2 - (\mathbf{r}\cdot\mathbf{B}_0)^2\right],$$

so

$$\frac{\partial H}{\partial B_0} = -(\gamma_o L_z + \gamma S_z) + \frac{q^2}{4m}\left[r^2 B_0 - (\mathbf{r}\cdot\mathbf{B}_0)z\right],$$

and since $\gamma_o = q^2/2m$,

$$\frac{\partial H}{\partial B_0} = -\gamma_o\left[L_z - \frac{q}{2}\left(r^2B_0 - (\mathbf{r}\cdot\mathbf{B}_0)z\right)\right] - \gamma S_z = -\gamma_o\mathbf{L}_{\text{mechanical}_\mathbf{z}} - \gamma\mathbf{S_z} = -\mu_\mathbf{z}.$$

Therefore, from the Feynman-Hellman theorem,

$$\frac{\partial E_n}{\partial B_0} = -\langle\psi_n|\mu_z|\psi_n\rangle. \quad \checkmark$$

Problem 7.50

(a) At first order in perturbation theory

$$E^1 = -B_0(\gamma_o\langle L_z\rangle + \gamma\langle S_z\rangle) + \frac{e^2}{8m}B_0^2\sum_{i=1}^{Z}\langle x_i^2 + y_i^2\rangle$$

and at second order

$$E^2 = B_0^2 \sum_{n\neq 0} \frac{|\langle\psi_n|(\gamma_o L_z + \gamma S_z)|\psi_0\rangle|^2}{E_0 - E_n}.$$

(I've ignored the second term in H', when computing E^2, because it will add higher powers of B_0.) Now, since ψ_0 is an eigenstate of L_z and S_z with eigenvalue 0, we are left with only one contribution:

$$\Delta E = \frac{e^2}{8m} B_0^2 \sum_{i=2}^{2} \langle x_i^2 + y_i^2\rangle.$$

The ground state is spherically symmetric, so $\langle x_i^2\rangle = \langle y_i^2\rangle = \langle r^2\rangle/3$, where $\langle r^2\rangle$ is the expectation value of r^2 in the ground state of hydrogen (Problem 4.15, only with $Z = 2$): $\langle r^2\rangle = 3a^2/Z^2$:

$$\Delta E = \frac{e^2}{6m} B_0^2 \langle r^2\rangle = \boxed{\frac{e^2}{2m} B_0^2 \left(\frac{a}{Z}\right)^2.}$$

(b) Combining these results, we get

$$\chi = -\frac{N}{V}\mu_0 \frac{\partial^2 E}{\partial B_0^2} = -\frac{N}{V}\mu_0 \frac{e^2}{m}\left(\frac{a}{Z}\right)^2.$$

Now $\frac{N}{V} = \left(\frac{\text{atoms}}{\text{volume}}\right) = \left(\frac{1}{\text{mass/atom}}\right)\left(\frac{\text{mass}}{\text{volume}}\right) = \frac{\rho}{m_{\text{He}}}$, so

$$\boxed{\chi = -\frac{\rho}{m_{\text{He}}} \frac{\mu_0 e^2}{m}\left(\frac{a}{Z}\right)^2.}$$

With $Z = 2$ this yields a numerical value of $\boxed{-6.2\times 10^{-10},}$ but if you use the screened value for Z of 1.69 (see Equation 8.34) it rises to -8.7×10^{-10}.

Problem 7.51

(a) (i) Equation 7.10: $(H^0 - E_0^0)\psi_0^1 = -(H' - E_0^1)\psi_0^0.$

$$\begin{aligned}
H^0 &= -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} = -\frac{\hbar^2}{2m}\left(\nabla^2 + \frac{2}{ar}\right), \quad \text{since} \quad a = \frac{4\pi\epsilon_0\hbar^2}{me^2}.\\
E_0^0 &= -\frac{\hbar^2}{2ma^2}.\\
H' &= eE_{\text{ext}} r\cos\theta; \quad E_0^1 = 0 \quad \text{(Problem 7.45(a))}.\\
\psi_0^0 &= \frac{1}{\sqrt{\pi a^3}} e^{-r/a}; \quad \psi_0^1 = f(r)e^{-r/a}\cos\theta.
\end{aligned}$$

Equation 4.13 $\Rightarrow$

$$\begin{aligned}
\nabla^2\psi_0^1 &= \frac{\cos\theta}{r^2}\frac{d}{dr}\left[r^2\frac{d}{dr}\left(fe^{-r/a}\right)\right] + \frac{fe^{-r/a}}{r^2\sin\theta}\frac{d}{d\theta}\left[\sin\theta\frac{d}{d\theta}(\cos\theta)\right] \\
&= \frac{\cos\theta}{r^2}\frac{d}{dr}\left[r^2\left(f'-\frac{1}{a}f\right)e^{-r/a}\right] + \frac{fe^{-r/a}}{r^2\sin\theta}\frac{d}{d\theta}\left[-\sin^2\theta\right] \\
&= \frac{\cos\theta}{r^2}\left[2r\left(f'-\frac{1}{a}f\right)e^{-r/a} + r^2\left(f''-\frac{2}{a}f'+\frac{1}{a^2}f\right)e^{-r/a}\right] - \frac{2\cos\theta}{r^2}fe^{-r/a} \\
&= \cos\theta e^{-r/a}\left[\left(f''-\frac{2}{a}f'+\frac{1}{a^2}f\right) + 2\left(f'-\frac{1}{a}f\right)\frac{1}{r} - 2f\frac{1}{r^2}\right].
\end{aligned}$$

Plug this into Eq. 7.10:

$$-\frac{\hbar^2}{2m}\cos\theta e^{-r/a}\left[\left(f''-\frac{2}{a}f'+\frac{1}{a^2}f\right)+2\left(f'-\frac{1}{a}f\right)\frac{1}{r}-2f\frac{1}{r^2}+2f\frac{1}{a}\frac{1}{r}-f\frac{1}{a^2}\right] = -eE_{\text{ext}}r\cos\theta\frac{1}{\sqrt{\pi a^3}}e^{-r/a},$$

$$\blacklozenge \quad \left(f''-\frac{2}{a}f'\right)+2f'\frac{1}{r}-2f\frac{1}{r^2} = \left(\frac{2meE_{\text{ext}}}{\hbar^2\sqrt{\pi a^3}}\right)r = \frac{4\gamma}{a}r, \quad \text{where} \quad \boxed{\gamma \equiv \frac{meE_{\text{ext}}}{2\hbar^2\sqrt{\pi a}}.}$$

Now let $f(r) = A + Br + Cr^2$, so $f' = B + 2Cr$ and $f'' = 2C$. Then

$$2C - \frac{2}{a}(B+2Cr) + \frac{2}{r}(B+2Cr) - \frac{2}{r^2}(A+Br+Cr^2) = \frac{4\gamma}{a}r.$$

Collecting like powers of r:

$$\begin{aligned}
r^{-2}: &\quad A = 0. \\
r^{-1}: &\quad 2B - 2B = 0 \quad \text{(automatic)}. \\
r^{0}: &\quad 2C - 2B/a + 4C - 2C = 0 \Rightarrow B = 2aC. \\
r^{1}: &\quad -4C/a = 4\gamma/a \Rightarrow C = -\gamma.
\end{aligned}$$

Evidently the function suggested *does* satisfy Eq. 7.10, with the coefficients $\boxed{A = 0,\ B = -2a\gamma,\ C = -\gamma;}$ the first-order correction to the wave function is

$$\psi_0^1 = -\gamma r(r+2a)e^{-r/a}\cos\theta.$$

(ii) Equation 7.14 says, in this case:

$$\begin{aligned}
E_0^2 &= \langle\psi_0^0|H'|\psi_0^1\rangle = -\frac{1}{\sqrt{\pi a^3}}\frac{meE_{\text{ext}}}{2\hbar^2\sqrt{\pi a}}eE_{\text{ext}}\int e^{-r/a}(r\cos\theta)r(r+2a)e^{-r/a}\cos\theta\, r^2\sin\theta\, dr\, d\theta\, d\phi \\
&= -\frac{m(eE_{\text{ext}})^2}{2\pi a^2\hbar^2}2\pi\int_0^\infty r^4(r+2a)e^{-2r/a}dr\int_0^\pi\cos^2\theta\sin\theta\, d\theta \\
&= -m\left(\frac{eE_{\text{ext}}}{a\hbar}\right)^2\left[5!\left(\frac{a}{2}\right)^6 + 2a\,4!\left(\frac{a}{2}\right)^5\right]\left(-\frac{\cos^3\theta}{3}\right)\Bigg|_0^\pi \\
&= -m\left(\frac{eE_{\text{ext}}}{a\hbar}\right)^2\left(\frac{27}{8}a^6\right)\frac{2}{3} = \boxed{-m\left(\frac{3eE_{\text{ext}}a^2}{2\hbar}\right)^2.}
\end{aligned}$$

(b) (i) This is the same as (a) [note that $E_0^1 = 0$, as before, since ψ_0^0 is spherically symmetric, so $\langle\cos\theta\rangle = 0$] except for the r-dependence of H'. So Eq. ♦ ⇒

$$f'' + 2f'\left(\frac{1}{r} - \frac{1}{a}\right) - 2f\frac{1}{r^2} = -\left(\frac{2mep}{4\pi\epsilon_0\hbar^2\sqrt{\pi a^3}}\right)\frac{1}{r^2} = -\frac{2\beta}{r^2}, \quad \text{where} \quad \boxed{\beta \equiv \frac{mep}{4\pi\epsilon_0\hbar^2\sqrt{\pi a^3}}.}$$

The solution this time it obvious: $f(r) = \beta$ (constant). [For the *general* solution we would add the general solution to the homogeneous equation (right side set equal to zero), but this would simply reproduce the unperturbed ground state, ψ_0^0, which we exclude—see p. 282.] So

$$\boxed{\psi_0^1 = \beta e^{-r/a}\cos\theta.}$$

(ii) The electric dipole moment of the electron is

$$\langle p_e\rangle = \langle -er\cos\theta\rangle = -e\langle\psi_0^0+\psi_0^1|r\cos\theta|\psi_0^0+\psi_0^1\rangle = -e\left(\langle\psi_0^0|r\cos\theta|\psi_0^0\rangle + 2\langle\psi_0^0|r\cos\theta|\psi_0^1\rangle + \langle\psi_0^1|r\cos\theta|\psi_0^1\rangle\right).$$

But the first term is zero, and the third is higher order, so

$$\begin{aligned}
\langle p_e\rangle &= -2e\frac{1}{\sqrt{\pi a^3}}\beta\int e^{-r/a}(r\cos\theta)e^{-r/a}\cos\theta\, r^2\sin\theta\, dr\, d\theta\, d\phi \\
&= -2e\left(\frac{mep}{4\pi\epsilon_0\hbar^2\pi a^3}\right)2\pi\int_0^\infty r^3e^{-2r/a}dr\int_0^\pi\cos^2\theta\sin\theta\, d\theta = -\left(\frac{me^2p}{\epsilon_0\hbar^2\pi a^3}\right)\left[3!\left(\frac{a}{2}\right)^4\right]\left(\frac{2}{3}\right) \\
&= -\left(\frac{me^2p}{\epsilon_0\hbar^2\pi a^3}\right)\left(\frac{3a^4}{8}\right)\left(\frac{2}{3}\right) = -\left(\frac{me^2pa}{4\pi\epsilon_0\hbar^2}\right) = \boxed{-p.}
\end{aligned}$$

Evidently the dipole moment associated with the perturbation of the electron cloud cancels the dipole moment of the nucleus, and the total dipole moment of the atom is zero.

(iii) The first-order correction is zero (as noted in (i)). The second-order correction is

$$\begin{aligned}
E_0^2 &= \langle\psi_0^0|H'|\psi_0^1\rangle = \frac{1}{\sqrt{\pi a^3}}\left(-\frac{ep}{4\pi\epsilon_0}\right)\left(\frac{mep}{4\pi\epsilon_0\hbar^2\sqrt{\pi a^3}}\right)\int e^{-r/a}\left(\frac{\cos\theta}{r^2}\right)e^{-r/a}\cos\theta\, r^2\sin\theta\, dr\, d\theta\, d\phi \\
&= -m\frac{(ep)^2}{(4\pi\epsilon_0)^2\hbar^2\pi a^3}2\pi\int_0^\infty e^{-2r/a}dr\int_0^\pi\cos^2\theta\sin\theta\, d\theta = -2m\frac{(ep)^2}{(4\pi\epsilon_0)^2\hbar^2a^3}\left(\frac{a}{2}\right)\left(\frac{2}{3}\right) \\
&= \frac{4}{3}\left(-\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2}\right)\frac{p^2}{e^2a^2} = \boxed{\frac{4}{3}\left(\frac{p}{ea}\right)^2E_1.}
\end{aligned}$$

Problem 7.52

(a) The Schrödinger equation separates into two one-dimensional harmonic oscillators, and the solutions can be written as products, $\psi(x,y) = \psi_m(x)\psi_n(y)$, with energies $E_{mn} = (m+n+1)\hbar\omega$. The ground state is $m = n = 0$, and (Equation 2.60)

$$\boxed{\psi_0(x,y) = \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}, \quad E_0 = \hbar\omega.}$$

The first excited states are $m = 0, n = 1$ and $m = 1, n = 0$; using Equation 2.63:

$$\psi_1^a(x,y) = \psi_0(x)\psi_1(y) = \boxed{\sqrt{\frac{2}{\pi}}\left(\frac{m\omega}{\hbar}\right) y\, e^{-\frac{m\omega}{2\hbar}(x^2+y^2)},}$$

$$\psi_1^b(x,y) = \psi_1(x)\psi_0(y) = \boxed{\sqrt{\frac{2}{\pi}}\left(\frac{m\omega}{\hbar}\right) x\, e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}.}$$

Any orthonormal linear combination of these would also do; the energy is $\boxed{E_1 = 2\hbar\omega.}$

(b) For the ground state we use nondegenerate perturbation theory (Equation 7.9):

$$E_0^1 = \langle\psi_0|H'|\psi_0\rangle = \frac{m\omega}{\pi\hbar}\left(-\frac{qB_0}{2m}\right)\int e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}(xp_y - yp_x)e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}\,dx\,dy.$$

But

$$\begin{aligned}(xp_y - yp_x)e^{-\frac{m\omega}{2\hbar}(x^2+y^2)} &= -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]e^{-\frac{m\omega}{2\hbar}(x^2+y^2)} \\ &= -i\hbar\left[x\left(-\frac{m\omega}{\hbar}y\right)e^{-\frac{m\omega}{2\hbar}(x^2+y^2)} - y\left(-\frac{m\omega}{\hbar}x\right)e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}\right] = 0,\end{aligned}$$

so $\boxed{E_0^1 = 0.}$ For the first excited state(s) we need degenerate perturbation theory (Equation 7.33):

$$W_{aa} = \langle\psi_1^a|H'|\psi_1^a\rangle = \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2\left(-\frac{qB_0}{2m}\right)\int ye^{-\frac{m\omega}{2\hbar}(x^2+y^2)}(xp_y - yp_x)ye^{-\frac{m\omega}{2\hbar}(x^2+y^2)}\,dx\,dy.$$

But

$$\begin{aligned}(xp_y - yp_x)y\,e^{-\frac{m\omega}{2\hbar}(x^2+y^2)} &= -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]y\,e^{-\frac{m\omega}{2\hbar}(x^2+y^2)} \\ = -i\hbar\left[x\left(1 - \frac{m\omega}{\hbar}y^2\right)e^{-\frac{m\omega}{2\hbar}(x^2+y^2)} - y^2\left(-\frac{m\omega}{\hbar}x\right)e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}\right] &= -i\hbar\,xe^{-\frac{m\omega}{2\hbar}(x^2+y^2)},\end{aligned}$$

so

$$\begin{aligned}W_{aa} &= \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2\left(-\frac{qB_0}{2m}\right)(-i\hbar)\int x\,y\,e^{-\frac{m\omega}{\hbar}(x^2+y^2)}\,dx\,dy = 0, \\ W_{ba} &= \langle\psi_1^b|H'|\psi_1^a\rangle = \frac{2}{\pi}\left(\frac{m\omega}{\hbar}\right)^2\left(-\frac{qB_0}{2m}\right)(-i\hbar)\int x^2\,e^{-\frac{m\omega}{\hbar}(x^2+y^2)}\,dx\,dy \\ &= i\left(\frac{m\omega^2 qB_0}{\pi\hbar}\right)\left(\frac{\hbar}{2m\omega}\sqrt{\frac{\pi\hbar}{m\omega}}\right)\left(\sqrt{\frac{\pi\hbar}{m\omega}}\right) = i\left(\frac{qB_0\hbar}{2m}\right).\end{aligned}$$

(W_{ab} is the complex conjugate of W_{ba}; W_{bb} the same as W_{aa} with $x \leftrightarrow y$, so it too is zero.) From Equation 7.33:

$$\boxed{E_\pm^1 = \pm|W_{ab}| = \pm\left(\frac{qB_0\hbar}{2m}\right).}$$

Problem 7.53

(a) The first-order correction to the nth energy is

$$\begin{aligned} E_n^1 &= \langle \psi_n^0 \,|\, H' \,|\, \psi_n^0 \rangle \\ &= \lambda \int_0^a \left|\psi_n^0(x)\right|^2 \delta(x - x_0) \\ &= \lambda \left|\psi_n^0(x_0)\right|^2 \\ &= \frac{2\,\lambda}{a} \sin^2\!\Big(\frac{n\,\pi\,x_0}{L}\Big) . \end{aligned}$$

Here small means that

$$\left|\frac{V_{mn}}{E_m^0 - E_n^0}\right| \ll 1 .$$

The matrix element $|V_{mn}| = (2\,\lambda/a)\ |\sin(m\,\pi\,x_0/a)\ \sin(n\,\pi\,x_0/a)|$ is of order $2\,\lambda/a$ and the spacing between energy levels is of order $\pi^2\,\hbar^2/2\,m\,a^2$ so that we need to have

$$\lambda \ll \frac{a}{2}\,\frac{\pi^2\,\hbar^2}{2\,m\,a^2} .$$

(b) To compute the second-order correction we first need

$$\begin{aligned} V_{mn} &= \langle \psi_m^0 \,|\, H' \,|\, \psi_n^0 \rangle \\ &= \lambda \int \left[\psi_m^0(x)\right]^* \delta(x - x_0)\ \psi_n^0(x)\ dx \\ &= \frac{2\,\lambda}{a} \sin\!\Big(\frac{m\,\pi\,x_0}{a}\Big) \sin\!\Big(\frac{n\,\pi\,x_0}{a}\Big) . \end{aligned}$$

Then the second-order correction to the allowed energies is then

$$\begin{aligned} E_n^2 &= \sum_{m\neq n} \frac{|V_{mn}|^2}{E_n^0 - E_m^0} \\ &= \frac{(2\,\lambda/a)^2}{\pi^2\,\hbar^2/(2\,m\,a^2)} \sum_{m\neq n} \frac{\sin^2\big(\frac{m\,\pi\,x_0}{a}\big)\ \sin^2\big(\frac{n\,\pi\,x_0}{a}\big)}{n^2 - m^2} \\ &= \frac{8\,m\,\lambda^2}{\pi^2\,\hbar^2} \sin^2\!\Big(\frac{n\,\pi\,x_0}{a}\Big) \sum_{m\neq n} \frac{\sin^2\big(\frac{m\,\pi\,x_0}{a}\big)}{n^2 - m^2} . \end{aligned}$$

(c) We construct a piecewise solution. The time-independent Schrödinger equation for $0 < x < x_0$ or for $x_0 < x < a$ reads

$$-\frac{\hbar^2}{2\,m}\,\psi'' = E\,\psi$$

for which the general solution is $\psi(x) = A\,\sin(k\,x) + B\,\cos(k\,x)$ where $k = \sqrt{2\,m\,E/\hbar^2}$ so that our piecewise solution is

$$\psi(x) = \begin{cases} A\,\sin(k\,x) + B\,\cos(k\,x) & 0 < x < x_0 \\ C\,\sin(k\,x) + D\,\cos(k\,x) & x_0 < x < a \end{cases} .$$

The boundary condition at $x = 0$ gives $B = 0$ and the boundary condition at $x = a$ gives $D = -C \tan(k\,a)$ so with these two boundary conditions satisfied

$$\psi(x) = \begin{cases} A \sin(k\,x) & 0 < x < x_0 \\ C' \sin[k\,(a - x)] & x_0 < x < a \end{cases} .$$

where (unimportantly) we've defined a new constant $C' = -C/\cos(k\,a)$. Now we look at the boundary conditions at $x = x_0$. Continuity of the wave function requires

$$A \sin(k\,x_0) = C' \sin[k\,(a - x_0)] \qquad \bigstar$$

and the condition on the derivative (Equation 2.128) is

$$\begin{aligned} \Delta\psi' &= \frac{2\,m\,\lambda}{\hbar^2}\,\psi(x_0) \\ -C'\,k\,\cos[k\,(a - x_0)] - A\,k\,\cos(k\,x_0) &= \frac{2\,m\,\lambda}{\hbar^2}\,A\,\sin(k\,x_0) \\ A\,k\,\cos(k\,x_0) + \frac{2\,m\,\lambda}{\hbar^2}\,A\,\sin(k\,x_0) &= -C'\,k\,\cos[k\,(a - x_0)] \qquad \blacklozenge \end{aligned}$$

Dividing Equation $\blacklozenge$ by Equation $\bigstar$ gives

$$\begin{aligned} k\,\cot(k\,x_0) + \frac{2\,m\,\lambda}{\hbar^2} &= -k\,\cot[k\,(a - x_0)] \\ u\,\cot(p\,u) + \Lambda &= -u\,\cot[u\,(1 - p)] \\ u\,\cos(p\,u)\,\sin[u\,(1 - p)] + \Lambda\,\sin(p\,u)\,\sin[u\,(1 - p)] &= -u\,\cos[u\,(1 - p)]\,\sin(p\,u) \end{aligned}$$

which simplifies to

$$\boxed{u\,\sin(u) + \Lambda\,\sin(p\,u)\,\sin[u\,(1 - p)] = 0\,.} \qquad \bigstar\bigstar$$

Now, to calculate the corrections to the energy from this expression note that

$$\begin{aligned} u &= \sqrt{\frac{2\,m\,a^2\,E}{\hbar^2}} = \sqrt{\frac{2\,m\,a^2\,(E_n^0 + E_n^1 + \ldots)}{\hbar^2}} \\ &= \sqrt{\frac{2\,m\,a^2\,E_n^0}{\hbar^2}} + \sqrt{\frac{m\,a^2}{2\,E_n^0\,\hbar^2}}\,E_n^1 + \ldots \\ &= n\,\pi + \frac{m\,a^2}{n\,\pi\,\hbar^2}\,E_n^1 + \ldots \\ &= u_0 + \delta u + \ldots \end{aligned}$$

Plugging into Equation $\bigstar\bigstar$ and keeping terms of order δu gives

$$(u_0 + \delta u)\,\sin(u_0 + \delta u) + \Lambda\,\sin(p\,u_0)\,\sin[u_0\,(1 - p)] \approx 0$$

where we can ignore the δu in the second term because the Λ ensures that the whole term is already order δ. Expanding this

$$u_0\,\underbrace{\sin(u_0)}_{0} + \left[u_0\,\underbrace{\cos(u_0)}_{(-1)^n} + \sin(u_0)\right]\delta u + \Lambda\,\sin(p\,u_0) \approx 0 \qquad \blacklozenge\blacklozenge$$

and

$$\delta u = \frac{m\,a^2}{n\,\pi\,\hbar^2}\,E_n^1 = -(-1)^n\;\frac{\Lambda}{u_0}\;\sin(p\,u_0)\;\sin\left[u_0\,(1-p)\right]$$

$$\begin{aligned} E_n^1 &= -\,(-1)^n\;\frac{n\,\pi\,\hbar^2}{m\,a^2}\,\frac{2\,m\,a\,\lambda}{n\,\pi\,\hbar^2}\;\sin(p\,u_0)\;[\sin u_0\;\cos(p\,u_0) \\ &\quad -\sin(p\,u_0)\;\cos u_0] \\ &= \frac{2\,\lambda}{a}\;\left|\sin(p\,u_0)\right|^2 \end{aligned}$$

which is *precisely* the result obtained above in part (a) since $p\,u_0 = n\,\pi\,x_0/a$.

(d) In this case we want negative-energy solutions and we write

$$u = \sqrt{\frac{2\,m\,E\,a^2}{\hbar^2}} = i\,\sqrt{\frac{2\,m\;|E|\;a^2}{\hbar^2}} \equiv i\,v\,.$$

Plugging this into Equation ★★ and noting that $\sin(i\,z) = i\,\sinh z$ we have

$$\boxed{v\;\sinh v + \Lambda\sinh(p\,v)\sinh\left[(1-p)\;v\right] = 0\,.}$$

For the case $p = 1/2$,

$$\begin{aligned} v\;\sinh v + \Lambda\;\sinh^2\!\left(\frac{v}{2}\right) &= 0 \\ v &= -\frac{1}{2}\,\Lambda\;\tanh\!\left(\frac{v}{2}\right)\;. \end{aligned}$$

If a is huge so that the boundaries don't matter, then $\tanh(v/2) = \tanh(\kappa\,a/2) \approx 1$ and

$$v \approx -\frac{\Lambda}{2}$$

and then

$$E = -\frac{\hbar^2\,v^2}{2\,m\,a^2} \approx -\frac{\hbar^2\,\Lambda^2}{8\,m\,a^2} = -\frac{m\,\lambda^2}{2\,\hbar^2}\,,$$

which is precisely the energy of the delta-function well.

(e) For the case of $p = 1/2$,

$$v = \frac{1}{2}\;|\Lambda|\;\tanh\!\left(\frac{v}{2}\right)$$

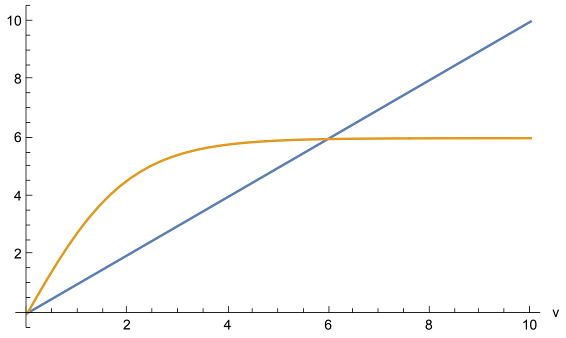
as shown above. From the graph (below) it's clear that the functions on the right- and left-hand sides of this equation intersect at most once. In order to intersect at all the slope of the function on the right-hand side must be greater than 1 at the origin.

$$\begin{aligned} \frac{d}{dv}\frac{1}{2}\;|\Lambda|\;\tanh\!\left(\frac{v}{2}\right)\bigg|_0 &> 1 \\ \frac{|\Lambda|}{4} &> 1 \end{aligned}$$

as claimed for $p = 1/2$.

```
In[∘]:= Λ = -12; Plot[{v, Abs[Λ]/2 Tanh[v/2]}, {v, 0, 10}, AxesLabel → {"v", None}]
```

Out[∘]=



As a function of p, solutions for v exist between

$$\frac{1}{2}\left(1-\sqrt{\frac{|\Lambda|-4}{|\Lambda|}}\right) < p < \frac{1}{2}\left(1+\sqrt{\frac{|\Lambda|-4}{|\Lambda|}}\right) .$$

These values are shown with gridlines in the following plot.

Transcendental equation (LHS) for negative-energy solutions:

```
In[◦]:= f[Λ_, p_, v_] := v Sinh[v] + Λ Sinh[p v] Sinh[(1 - p) v]
```

This will solve the transcendental equation. A starting guess of 4 works for this range of Λ values

```
In[◦]:= solution[λ_, P_] := v /. FindRoot[f[λ, P, v], {v, 4}]
```

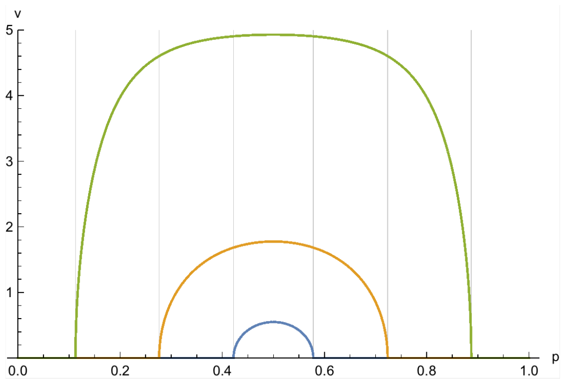
These are the minimum and maximum values of p for which there should be solutions for a given Λ

```
In[◦]:= p1[λ_] := 1/2 (1 - Sqrt[(-4 + Abs[λ])/Abs[λ]]); p2[λ_] := 1/2 (1 + Sqrt[(-4 + Abs[λ])/Abs[λ]]);
```

Here is a plot of the solutions. Vertical grid lines mark the boundaries of the regions for which we expect solutions and match up perfectly

```
In[◦]:= Plot[
 {solution[-4.1, P], solution[-5, P], solution[-10, P]}, {P, 0, 1},
 PlotRange → {0, 5},
 GridLines →
  {{p1[-41 / 10], p2[-41 / 10], p1[-5], p2[-5], p1[-10], p2[-10]}, None},
 AxesLabel → {"p", "v"}]
```

Out[◦]=



(f) Note that (for p = 1/2), for negative energy solutions to exist we must have

$$|\Lambda| > \frac{1}{1/2\,(1 - 1/2)} = 4\,.$$

So we need to switch between solving the two transcendental equations at this point.

Transcendental equation (LHS) for positive-energy solutions:

```
In[∘]:= g[Λ_, p_, u_] := u Sin[u] + Λ Sin[p u] Sin[(1 - p) u]
```

This solves the appropriate transcendental equation and returns u (or i v) depending on whether it is a positive- (or negative-) energy solution

```
In[∘]:= solutionF[λ_] := If[Abs[λ] > 4, I solution[λ, 1 / 2],
          u /. FindRoot[g[λ, 1 / 2, u], {u, 4}]]
```

This is the wave function for a given value of u = k (for p = 1/2)

```
In[∘]:= ψ[k_, x_] := If[x < 1 / 2, Sin[k x], Sin[k (1 - x)]]
```

This is a table with the wave function for each value of Λ we want to plot

```
In[∘]:= ψ[x_] = Table[ψ[solutionF[λ], x], {λ, {0, -2, -3, -3.5, -4.5, -5, -10}}];
```

This computes the norm for each ψ

```
In[∘]:= norm = Sqrt[Integrate[Abs[ψ[x]]^2, {x, 0, 1}]];
```

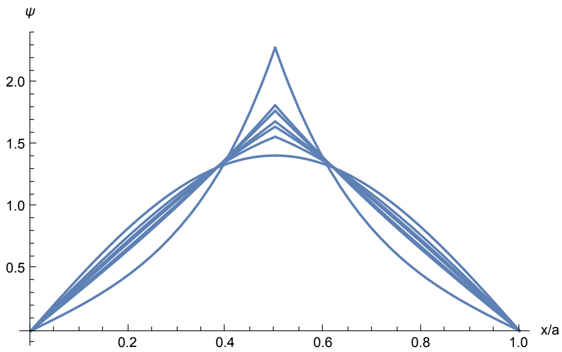
And the normalized wave function

```
In[∘]:= ψ[x_] = ψ[x] / norm;
```

Here it is...

```
In[∘]:= Plot[Abs[ψ[x]], {x, 0, 1}, AxesLabel → {"x/a", "ψ"}]
```

Out[∘]=



Problem 7.54

(a) $\langle H'\rangle = 2\,\mathrm{Re}\sum_{m\neq n}\frac{|\langle\psi_m^0|H'|\psi_n^0\rangle|^2}{E_n^0 - E_m^0}$. The sum is manifestly real (so we can drop the "Re"), and in fact it is precisely E_n^2 (Equation 7.15): $\boxed{\langle H'\rangle = 2E_n^2.}$

Explanation: The second-order correction to the energy is the term of order λ^2 in

$$\frac{\langle\psi_n|H_0+\lambda H'|\psi_n\rangle}{\langle\psi_n|\psi_n\rangle} = \frac{\langle\psi_n|H_0|\psi_n\rangle}{\langle\psi_n|\psi_n\rangle} + \lambda\frac{\langle\psi_n|H'|\psi_n\rangle}{\langle\psi_n|\psi_n\rangle},$$

where ψ_n is the exact nth eigenstate. We just calculated the second term; we need to evaluate the first term, to order λ^2.

$$\begin{aligned}
\langle\psi_n|H_0|\psi_n\rangle &= \langle(\psi_n^0+\lambda\psi_0^1+\lambda^2\psi_n^2+\cdots)|H_0|(\psi_n^0+\lambda\psi_0^1+\lambda^2\psi_n^2+\cdots)\rangle \\
&= \langle\psi_n^0|H_0|\psi_n^0\rangle + \lambda\left[\langle\psi_n^0|H_0|\psi_n^1\rangle + \langle\psi_n^1|H_0|\psi_n^0\rangle\right] \\
&\quad + \lambda^2\left[\langle\psi_n^0|H_0|\psi_n^2\rangle + \langle\psi_n^1|H_0|\psi_n^1\rangle + \langle\psi_n^2|H_0|\psi_n^0\rangle\right] + \cdots \\
&\approx E_n^0 + \lambda\left[E_n^0\left(\langle\psi_n^0|\psi_n^1\rangle + \langle\psi_n^1|\psi_n^0\rangle\right)\right] + \lambda^2\left[E_n^0\left(\langle\psi_n^0|\psi_n^2\rangle + \langle\psi_n^2|\psi_n^0\rangle\right) + \langle\psi_n^1|H_0|\psi_n^1\rangle\right] \\
&= E_n^0 + \lambda^2\langle\psi_n^1|H_0|\psi_n^1\rangle.
\end{aligned}$$

(As always, we choose $\langle\psi_n^i|\psi_n^0\rangle = 0$—see comments after Equation 7.11.) Similarly,

$$\begin{aligned}
\langle\psi_n|\psi_n\rangle &= \langle\psi_n^0|\psi_n^0\rangle + \lambda\left[\langle\psi_n^0|\psi_n^1\rangle + \langle\psi_n^1|\psi_n^0\rangle\right] + \lambda^2\left[\langle\psi_n^0|\psi_n^2\rangle + \langle\psi_n^1|\psi_n^1\rangle + \langle\psi_n^2|\psi_n^0\rangle\right] + \cdots \\
&\approx 1 + \lambda^2\langle\psi_n^1|\psi_n^1\rangle.
\end{aligned}$$

So

$$\begin{aligned}
\frac{\langle\psi_n|H_0|\psi_n\rangle}{\langle\psi_n|\psi_n\rangle} &= \left[E_n^0 + \lambda^2\langle\psi_n^1|H_0|\psi_n^1\rangle\right]\left(1+\lambda^2\langle\psi_n^1|\psi_n^1\rangle\right)^{-1} \approx \left[E_n^0 + \lambda^2\langle\psi_n^1|H_0|\psi_n^1\rangle\right]\left(1-\lambda^2\langle\psi_n^1|\psi_n^1\rangle\right) \\
&= E_n^0 + \lambda^2\left[\langle\psi_n^1|H_0|\psi_n^1\rangle - E_n^0\langle\psi_n^1|\psi_n^1\rangle\right] = E_n^0 + \lambda^2\langle\psi_n^1|(H_0-E_n^0)|\psi_n^1\rangle.
\end{aligned}$$

Finally, using Equation 7.13:

$$\begin{aligned}
\langle\psi_n^1|(H_0-E_n^0)|\psi_n^1\rangle &= \langle\psi_n^1|(H_0-E_n^0)\sum_{m\neq n}\frac{H'_{mn}}{(E_n^0-E_m^0)}|\psi_m^0\rangle = -\langle\psi_n^1|\sum_{m\neq n}H'_{mn}|\psi_m^0\rangle \\
&= -\sum_{p\neq n}\sum_{m\neq n}\frac{{H'_{pn}}^*}{E_n^0-E_p^0}H'_{mn}\langle\psi_p^0|\psi_m^0\rangle = -\sum_{m\neq n}\frac{|H'_{mn}|^2}{E_n^0-E_m^0} = -E_n^2
\end{aligned}$$

(Equation 7.15). So the second-order correction the nth energy is $-E_n^2 + 2E_n^2 = E_n^2$, as it should be.

(b) To first order, the expectation value of p_e in the nth state is

$$\langle p_e\rangle = 2\mathrm{Re}\sum_{m\neq n}\frac{\langle\psi_n^0|qx|\psi_m^0\rangle\langle\psi_m^0|(-qE_{\text{ext}}x)|\psi_n^0\rangle}{E_n^0-E_m^0} = -2q^2E_{\text{ext}}\sum_{m\neq n}\frac{|\langle\psi_n^0|x|\psi_m^0\rangle|^2}{E_n^0-E_m^0},$$

so

$$\alpha = -2q^2\sum_{m\neq n}\frac{|\langle\psi_n^0|x|\psi_m^0\rangle|^2}{E_n^0-E_m^0}. \quad \checkmark$$

For the one-dimensional oscillator (Equation 3.114)

$$\langle\psi_n^0|x|\psi_m^0\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{m}\,\delta_{n,m-1} + \sqrt{n}\,\delta_{m,n-1}\right) \Rightarrow \langle\psi_0^0|x|\psi_m^0\rangle = \sqrt{\frac{\hbar}{2m\omega}}\sqrt{m}\,\delta_{0,m-1} = \sqrt{\frac{\hbar}{2m\omega}}\,\delta_{m,1}.$$

(don't confuse the *mass* m, in the factor out front, with the *index* m), so

$$\alpha = -2q^2\frac{\hbar/2m\omega}{(\hbar\omega/2)-(3\hbar\omega/2)} = \boxed{\frac{q^2}{m\omega^2}.}$$

Classically, the electric force qE_{ext} balances the spring force kd, so $p_e = qd = q^2E_{\text{ext}}/k$, and hence $\alpha = q^2/k = q^2/(m\omega^2)$, in agreement with the quantum result.

(c)

$$\begin{aligned}
\langle x\rangle^1 &= 2\mathrm{Re}\left(\sum_{m\neq n}\frac{\langle\psi_n^0|x|\psi_m^0\rangle\langle\psi_m^0|\left(-\frac{1}{6}\kappa x^3\right)|\psi_n^0\rangle}{(n+\frac{1}{2})\hbar\omega-(m+\frac{1}{2})\hbar\omega}\right) = -\frac{\kappa}{3\hbar\omega}\mathrm{Re}\left(\sum_{m\neq n}\frac{\langle\psi_n^0|x|\psi_m^0\rangle\langle\psi_m^0|x^3|\psi_n^0\rangle}{(n-m)}\right)\\
&= -\frac{\kappa}{3\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}}\mathrm{Re}\left(\sum_{m\neq n}\frac{(\sqrt{m}\,\delta_{n,m-1}+\sqrt{n}\,\delta_{m,n-1})}{(n-m)}\langle\psi_m^0|x^3|\psi_n^0\rangle\right)\\
&= -\frac{\kappa}{3\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}}\mathrm{Re}\left[-\sqrt{n+1}\langle\psi_{n+1}^0|x^3|\psi_n^0\rangle+\sqrt{n}\langle\psi_{n-1}^0|x^3|\psi_n^0\rangle\right].
\end{aligned}$$

Now, from (Equation 2.70),

$$\begin{aligned}
x^3 &= \left(\frac{\hbar}{2m\omega}\right)^{3/2}(a_+ + a_-)^3\\
&= \left(\frac{\hbar}{2m\omega}\right)^{3/2}(a_+^3 + a_+^2 a_- + a_+a_-a_+ + a_+a_-^2 + a_-a_+^2 + a_-a_+a_- + a_-^2a_+ + a_-^3).
\end{aligned}$$

We need

$$\begin{aligned}
\langle n+1|x^3|n\rangle &= \left(\frac{\hbar}{2m\omega}\right)^{3/2}\langle n+1|\left(a_+^2a_- + a_+a_-a_+ + a_-a_+^2\right)|n\rangle,\\
\langle n-1|x^3|n\rangle &= \left(\frac{\hbar}{2m\omega}\right)^{3/2}\langle n-1|\left(a_+a_-^2 + a_-a_+a_- + a_-^2a_+\right)|n\rangle.
\end{aligned}$$

(In the first line we need two a_+'s and one a_-, to raise $|n\rangle$ up to $|n+1\rangle$; in the second line we need two a_-'s and one a_+, to lower $|n\rangle$ to $|n-1\rangle$.) Using Equation 2.67 repeatedly:

$$\begin{aligned}
a_+^2a_-|n\rangle &= \sqrt{n}\,a_+^2|n-1\rangle = \sqrt{n}\sqrt{n}\,a_+|n\rangle = n\sqrt{n+1}\,|n+1\rangle,\\
a_+a_-a_+|n\rangle &= \sqrt{n+1}\,a_+a_-|n+1\rangle = \sqrt{n+1}\sqrt{n+1}\,a_+|n\rangle = (n+1)\sqrt{n+1}\,|n+1\rangle,\\
a_-a_+^2|n\rangle &= \sqrt{n+1}\,a_-a_+|n+1\rangle = \sqrt{n+1}\sqrt{n+2}\,a_-|n+2\rangle = (n+2)\sqrt{n+1}\,|n+1\rangle,
\end{aligned}$$

so

$$\begin{aligned}
\langle n+1|\left(a_+^2a_- + a_+a_-a_+ + a_-a_+^2\right)|n\rangle &= \langle n+1|\left(n\sqrt{n+1}+(n+1)\sqrt{n+1}+(n+2)\sqrt{n+1}\right)|n+1\rangle\\
&= 3(n+1)\sqrt{n+1}.
\end{aligned}$$

In the same way,

$$\begin{aligned}
a_+a_-^2|n\rangle &= \sqrt{n}\,a_+a_-|n-1\rangle = \sqrt{n}\sqrt{n-1}\,a_+|n-2\rangle = (n-1)\sqrt{n}\,|n-1\rangle,\\
a_-a_+a_-|n\rangle &= \sqrt{n}\,a_-a_+|n-1\rangle = \sqrt{n}\sqrt{n}\,a_-|n\rangle = n\sqrt{n}\,|n-1\rangle,\\
a_-^2a_+|n\rangle &= \sqrt{n+1}\,a_-^2|n+1\rangle = \sqrt{n+1}\sqrt{n+1}\,a_-|n\rangle = (n+1)\sqrt{n}\,|n-1\rangle,
\end{aligned}$$

so

$$\begin{aligned}
\langle n-1|\left(a_+a_-^2 + a_-a_+a_- + a_-^2a_+\right)|n\rangle &= \langle n-1|\left((n-1)\sqrt{n}+n\sqrt{n}+(n+1)\sqrt{n}\right)|n-1\rangle\\
&= 3n\sqrt{n}.
\end{aligned}$$

Thus

$$\langle n+1|x^3|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{3/2} 3(n+1)\sqrt{n+1}, \quad \langle n-1|x^3|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{3/2} 3n\sqrt{n}.$$

Finally,

$$\begin{aligned}\langle x\rangle^1 &= -\frac{\kappa}{3\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}}\left(\frac{\hbar}{2m\omega}\right)^{3/2}\left[-\sqrt{n+1}\,3(n+1)\sqrt{n+1}+\sqrt{n}\,3n\sqrt{n}\right]\\ &= -\frac{\kappa}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^2\left[-(n+1)^2+n^2\right] = \boxed{(2n+1)\frac{\hbar\kappa}{4m^2\omega^3}.}\end{aligned}$$

Problem 7.55

In the absence of the perturbation, the ground state is

$$\psi_0(x) = \frac{1}{\sqrt{L}}$$

and the remaining stationary states come in degenerate pairs,

$$\begin{aligned}\psi_{n,e}(x) &= \sqrt{\frac{2}{L}}\cos\!\left(\frac{2\,n\,\pi\,x}{L}\right)\\ \psi_{n,o}(x) &= \sqrt{\frac{2}{L}}\cos\!\left(\frac{2\,n\,\pi\,x}{L}\right).\end{aligned}$$

The unperturbed energies are

$$E_n^0 = \frac{2\,n^2\,\pi^2\,\hbar^2}{m\,L^2}.$$

We now calculate the first-order energy corrections due to the perturbation. The correction to the ground state is

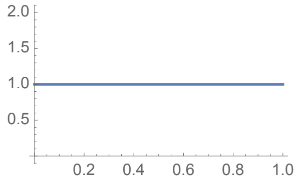
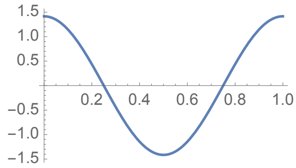
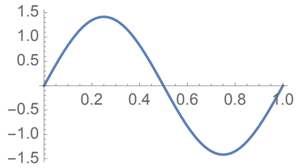
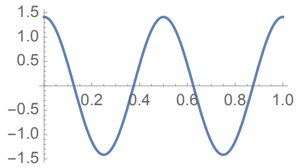
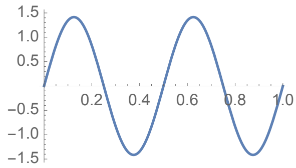
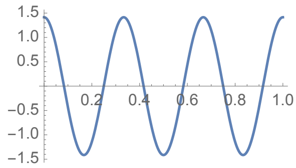
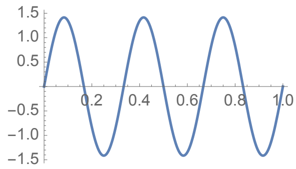
$$E_0^1 = \int_0^L [\psi_0(x)]^2\,[-\alpha\,\delta(x)]\,\psi_0(x)\,dx = -\frac{\alpha}{L}.$$

The degenerate states are already the good states (calculate the matrix W if you wish) since they are eigenstates of a reflection about $x=0$ with distinct eigenvalues (± 1), a symmetry of the Hamiltonian. The corrections to their energies are then

$$\begin{aligned}E_{n,e}^1 &= \int_0^L [\psi_n(x)]^2\,[-\alpha\,\delta(x)]\,\psi_n(x)\,dx = -\frac{2\,\alpha}{L}\\ E_{n,o}^1 &= \int_0^L [\psi_n(x)]^2\,[-\alpha\,\delta(x)]\,\psi_n(x)\,dx = 0.\end{aligned}$$

These results are shown on the next page fro the first seven states. The sequence of node numbers is $0, 2, 2, 4, 4, 6, 6, \ldots$.

Out[ ]//TableForm=

n	E	Nodes	Parity	
0	$-\frac{\alpha}{L}$	0	Even	
1	$-\frac{2\alpha}{L}+\frac{2\pi^2\hbar^2}{L^2 m}$	2	Even	
1	$\frac{2\pi^2\hbar^2}{L^2 m}$	2	Odd	
2	$-\frac{2\alpha}{L}+\frac{8\pi^2\hbar^2}{L^2 m}$	4	Even	
2	$\frac{8\pi^2\hbar^2}{L^2 m}$	4	Odd	
3	$-\frac{2\alpha}{L}+\frac{18\pi^2\hbar^2}{L^2 m}$	6	Even	
3	$\frac{18\pi^2\hbar^2}{L^2 m}$	6	Odd	

Problem 7.56

(a) The first order correction to the ground state is

$$E_0^1 = \left\langle \psi_0 \left| \frac{e^2}{4\pi\epsilon_0 r} \right| \psi_0 \right\rangle = \frac{e^2}{4\pi\epsilon_0 a} \left\langle \psi_0 \left| \frac{a}{r} \right| \psi_0 \right\rangle$$

where $r = |\mathbf{r}_1 - \mathbf{r}_2|$. The matrix element evaluates to 5/4; see the solution for Problem 5.15 for the details. Therefore

$$E_0^1 = \frac{5}{2}\,\frac{e^2}{8\,\pi\epsilon_0\,a} = \frac{5}{2}\,|E_1|$$

where $|E_1| = 13.6\,\mathrm{eV}$.

(b) Now we turn to the *degenerate* first-excited states. The states are

$$\psi_\pm(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\,\left[\psi_{100}(\mathbf{r}_1)\;\psi_{200}(\mathbf{r}_2) \pm \psi_{200}(\mathbf{r}_1)\;\psi_{100}(\mathbf{r}_2)\right]\,.$$

Of course we need to worry about whether to use *degenerate* perturbation theory. It turns out its unnecessary. The Hamiltonian is invariant under the interchange of $\mathbf{r}_1$ and $\mathbf{r}_2$ and these two states are even and odd under that interchange so they won't be mixed by the perturbation. We may therefore compute

$$\begin{aligned}
E_\pm^1 &= \left\langle \psi_\pm \,\middle|\, \frac{e^2}{4\,\pi\,\epsilon_0\,r} \,\middle|\, \psi_\pm \right\rangle \\
&= \frac{1}{2}\int\!\!\int \Bigg[\psi_{100}^*(\mathbf{r}_1)\;\psi_{200}^*(\mathbf{r}_2)\;\frac{e^2}{4\,\pi\,\epsilon_0\,r}\;\psi_{100}(\mathbf{r}_1)\;\psi_{200}(\mathbf{r}_2) \\
&\quad \pm \psi_{100}^*(\mathbf{r}_1)\;\psi_{200}^*(\mathbf{r}_2)\;\frac{e^2}{4\,\pi\,\epsilon_0\,r}\;\psi_{200}(\mathbf{r}_1)\;\psi_{100}(\mathbf{r}_2) \\
&\quad \pm \psi_{200}^*(\mathbf{r}_1)\;\psi_{100}^*(\mathbf{r}_2)\;\frac{e^2}{4\,\pi\,\epsilon_0\,r}\;\psi_{100}(\mathbf{r}_1)\;\psi_{200}(\mathbf{r}_2) \\
&\quad + \psi_{200}^*(\mathbf{r}_1)\;\psi_{100}^*(\mathbf{r}_2)\;\frac{e^2}{4\,\pi\,\epsilon_0\,r}\;\psi_{200}(\mathbf{r}_1)\;\psi_{100}(\mathbf{r}_2)\Bigg]\;d^3\mathbf{r}_1\,d^3\mathbf{r}_2\,.
\end{aligned}$$

The orbitals are real so we can drop the complex conjugation. Additionally, we can interchange $\mathbf{r}_1$ and $\mathbf{r}_2$ in the third and fourth terms to see that they are equal to the first two integrals and therefore

$$\boxed{E_\pm^1 = \frac{1}{2}(K \pm J)\,,}$$

with the integrals as given in the problem statement.

Now we turn to the business of actually evaluating these two integrals.

$$K = 2\int |\psi_{200}(\mathbf{r}_2)|^2 \underbrace{\int |\psi_{100}(\mathbf{r}_1)|^2\;\frac{e^2}{4\,\pi\,\epsilon_0\,r}\,d\mathbf{r}_1}_{\equiv V_1}\;d\mathbf{r}_2$$

where

$$\begin{aligned}
V_1 &= \frac{e^2}{4\,\pi\,\epsilon_0\,a}\int \frac{8}{\pi\,a^3}\,e^{-4\,r_1/a}\;\frac{a}{|\mathbf{r}_1 - \mathbf{r}_2|}\;d\mathbf{r}_1 \\
&= 2\;|E_1|\;\frac{16}{a^3}\int_0^\infty e^{-4\,r_1/a}\;\underbrace{\int_0^\pi \frac{a\,\sin\theta_1}{\sqrt{r_1^2 + r_2^2 - 2\,r_1\,r_2\,\cos\theta_1}}\,d\theta_1}_{Z_1}\;r_1^2\,dr_1\,,
\end{aligned}$$

having already done the trivial 2π integral. Next we compute (setting $u = \cos\theta$)

$$\begin{aligned}
Z_1 &= \int_{-1}^{1} \frac{a}{\sqrt{r_1^2 + r_2^2 - 2\, r_1\, r_2\, u}}\, du \\
&= -\frac{a}{r_1\, r_2}\, \sqrt{r_1^2 + r_2^2 - 2\, r_1, r_2\, u}\,\Big|_{-1}^{1} \\
&= \frac{a}{r_1\, r_2}\, (r_1 + r_2 - |r_1 - r_2|) \\
&= \begin{cases} 2\, a/r_1 & r_1 > r_2 \\ 2\, a/r_2 & r_1 < r_2 \end{cases} .
\end{aligned}$$

Returning with this result to the expression for V_1 we have

$$\begin{aligned}
V_1 &= 2\, |E_1|\, \frac{32}{a^3} \left[\int_0^{r_2} e^{-4\, r_1/a}\, \frac{a}{r_2}\, r_1^2\, dr_1 + \int_{r_2}^{\infty} e^{-4\, r_1/a} a\, r_1\, dr_1 \right] \\
&= 2\, |E_1|\, \frac{32}{a^3} \left(\frac{a}{4}\right)^3 \left[\frac{a}{r_2} \int_0^{4\, r_2/a} z^2\, e^{-z}\, dz + 4 \int_{4\, r_2/a}^{\infty} z\, e^{-z}\, dz \right] \\
&= |E_1| \left\{ \frac{a}{r_2} \left[2 - \left(2 + \frac{8\, r_2}{a} + \left(\frac{4\, r_2}{a}\right)^2 \right) e^{-4\, r_2/a} \right] \right. \\
&\quad \left. +4 \left(1 + \frac{4\, r_2}{a} \right) e^{-4\, r_2/a} \right\} \\
&= 2\, |E_1| \left[\frac{a}{r_2} - \left(2 + \frac{a}{r_2} \right) e^{-4\, r_2/a} \right] .
\end{aligned}$$

Now since V_1 and ψ_{200} depend only on r_2, not θ_2, ϕ_2 we have

$$\begin{aligned}
K &= 8\,\pi \int_0^{\infty} |\psi_{200}(r_2)|^2\, V_1(r_2)\, r_2^2\, dr_2 \\
&= 8\,\pi\, 2\, |E_1| \int_0^{\infty} \frac{1}{\pi\, a^3} \left(1 - \frac{r_2}{a}\right)^2 e^{-2\, r_2/a} \left[\frac{a}{r_2} - \left(2 + \frac{a}{r_2} \right) e^{-4\, r_2/a} \right] r_2^2\, dr_2 \\
&= \frac{16}{a^3}\, |E_1| \left[\int_0^{\infty} a\, r_2 \left(1 - \frac{r_2}{a}\right)^2 e^{-2\, r_2/a}\, dr_2 \right. \\
&\quad \left. - \int_0^{\infty} \left(2\, r_2^2 + a\, r_2\right) \left(1 - \frac{r_2}{a}\right)^2 e^{-6\, r_2/a}\, dr_2 \right]
\end{aligned}$$

Now we'll perform a variable substitution where $z = 2\, r_2/a$ in the first integral and $z = 6\, r_2/a$ in the second integral. We then have

$$\begin{aligned}
K &= \frac{16}{a^3}\, |E_1| \left[\int_0^{\infty} \frac{a^2\, z}{2} \left(1 - \frac{z}{2}\right)^2 e^{-z}\, \frac{a}{2}\, dz \right. \\
&\quad \left. - \int_0^{\infty} \left(\frac{1}{18} a^2\, z^2 + \frac{1}{6}\, a^2\, z \right) \left(1 - \frac{z}{6}\right)^2 e^{-z}\, \frac{a}{6}\, dz \right] \\
&= 2\, |E_1| \int_0^{\infty} \left(\frac{16}{9}\, z - 2\, z^2 + \frac{14}{27}\, z^3 - \frac{1}{486}\, z^4 \right) e^{-z}\, dz \\
&= 2\, |E_1| \left(\frac{16}{9} - 4 + \frac{42}{9} - \frac{4}{81} \right)
\end{aligned}$$

and

$$\boxed{K = \frac{136}{81}\,|E_1|\,.}$$

Next we compute

$$J = 2\int \psi_{200}(r_2)\,\psi_{100}(r_2)\,\underbrace{\int \psi_{200}(r_1)\,\psi_{100}(r_1)\,\frac{e^2}{4\,\pi\,\epsilon_0\,r}\,d^3\mathbf{r}_1}_{\equiv V_2}\,d^3\mathbf{r}_2\,.$$

Here

$$\begin{aligned}
V_2 &= \frac{e^2}{4\,\pi\,\epsilon_0\,a}\,\frac{2\sqrt{2}}{\pi\,a^3}\int\left(1-\frac{r_1}{a}\right)\,e^{-3\,r_1/a}\,\frac{a}{|\mathbf{r}_1-\mathbf{r}_2|}\,d\mathbf{r}_1\\
&= 2\,|E_1|\,\frac{2\sqrt{2}}{\pi\,a^3}\,2\,\pi\int_0^\infty\left(1-\frac{r_1}{a}\right)\,e^{-3\,r_1/a}\,Z_1(r_1)\,r_1^2\,dr_1
\end{aligned}$$

where the $2\,\pi$ is from the ϕ integral and where the function Z_1 is the same one that appeared in the computation of K. Then

$$\begin{aligned}
V_2 &= 2\,|E_1|\,\frac{8\sqrt{2}}{a^3}\left[\int_0^{r_2}\frac{a\,r_1^2}{r_2}\left(1-\frac{r_1}{a}\right)\,e^{-3\,r_1/a}\,dr_1\right.\\
&\quad\left.+\int_{r_2}^\infty a\,r_1\left(1-\frac{r_1}{a}\right)\,e^{-3\,r_1/a}\,dr_1\right]\\
&= 2\,|E_1|\,\frac{8\sqrt{2}}{a^3}\left[\int_0^{3\,r_2/a}\frac{a^3\,z^2}{9\,r_2}\left(1-\frac{z}{3}\right)\,e^{-z}\,\frac{a}{3}\,dz\right.\\
&\quad\left.+\int_{3r_2/a}^\infty\frac{a^2\,z}{3}\left(1-\frac{z}{3}\right)\,e^{-z}\,\frac{a}{3}\,dz\right]
\end{aligned}$$

with the variable change $z = 3\,r_1/a$. Then

$$\begin{aligned}
V_2 &= 2\,|E_1|\,\frac{8\sqrt{2}}{9}\left[\frac{a}{3\,r_2}\int_0^{3\,r_2/a}\left(z^2-\frac{z^3}{3}\right)\,e^{-z}\,\frac{a}{3}\,dz\right.\\
&\quad\left.+\int_{3r_2/a}^\infty\left(z-\frac{z^2}{3}\right)\,e^{-z}\,\frac{a}{3}\,dz\right]\\
&= 2\,|E_1|\,\frac{8\sqrt{2}}{9}\left(\frac{a}{3\,r_2}\left\{2-\left(2+\frac{6\,r_2}{a}+\frac{9\,r_2^2}{a^2}\right)\,e^{-3\,r_2/a}\right.\right.\\
&\quad\left.-\left[2-\left(2+\frac{6\,r_2}{a}+\frac{9\,r_2^2}{a^2}+\frac{9\,r_2^3}{a^3}\right)\,e^{-3\,r_2/a}\right]\right\}+\left(1+\frac{3\,r_1}{a}\right)\,e^{-3\,r_2/a}\\
&\quad\left.-\frac{1}{3}\left(2+\frac{6\,r_2}{a}+\frac{9\,r_2^2}{a^2}\right)\,e^{-3\,r_2/a}\right)\\
&= |E_1|\,\frac{16\sqrt{2}}{27}\left(1+\frac{3\,r_2}{a}\right)\,e^{-3\,r_2/a}\,.
\end{aligned}$$

We now plug this back into our expression for J. Once again the angular integration is trivial and

$$\begin{aligned} J &= 8\,\pi \int \psi_{200}(r_2)\ \psi_{100}(r_2)\ V_2(r_2)\ r_2^2\,dr_2 \\ &= 8\,\pi\ |E_1|\ \frac{16\sqrt{2}}{27}\ \frac{2\sqrt{2}}{\pi\,a^3} \int_0^\infty \left(1-\frac{r_2}{a}\right) e^{-3\,r_2/a} \left(1+\frac{3\,r_2}{a}\right) e^{-3\,r_2/a}\, r_2^2\,dr_2 \\ &= \frac{512}{27}\ |E_1|\ \frac{1}{a^3}\left(\frac{a^3}{6}\right) \int_0^\infty \left(1-\frac{z}{6}\right)\left(1+\frac{z}{2}\right) e^{-z}\, z^2\,dz \\ &= \frac{64}{729}\ |E_1| \int_0^\infty \left(z^2+\frac{z^3}{3}-\frac{1}{12}\,z^4\right) e^{-z}\,dz \\ &= \frac{64}{729}\ |E_1|\,(2+2-2) \end{aligned}$$

and

$$\boxed{J = \frac{128}{729}\ |E_1|\ .}$$

So the energies are

$$E^0 + \frac{1}{2}(K+J) = 4\,E_1 + 4\,\underbrace{E_2}_{E_1/4} - \frac{68}{81}\,E_1 - \frac{64}{729}\,E_1 = \frac{2969}{729}\,E_1 = -55.39\,\text{eV}$$

for the symmetric spatial state (parahelium) and

$$E^0 + \frac{1}{2}(K-J) = 4\,E_1 + 4\,\underbrace{E_2}_{E_1/4} - \frac{68}{81}\,E_1 + \frac{64}{729}\,E_1 = \frac{3097}{729}\,E_1 = -57.78\,\text{eV}$$

for the antisymmetric spatial state (orthohelium). Looking at Figure 5.1, this calculation correctly predicts that orthohelium is lower in energy, roughly by the correct amount.

Problem 7.57

(a) Setting $q = 0$ in Equation 6.14: $-\dfrac{\hbar^2}{2m}\dfrac{d^2 u_{n0}}{dx^2} + V(x)\,u_{no} = E_{n0}\,u_{n0}$, so $\boxed{H_0 = \dfrac{\hat{p}^2}{2m} + V(x).}$

Then, for $q \neq 0$, $\boxed{H' = \dfrac{\hbar q}{m}\hat{p} + \dfrac{\hbar^2 q^2}{2m}.}$

(b) From Equations 7.9 and 7.15:

$$E_{nq} \approx E_{n0} + \langle u_{n0}|H'|u_{n0}\rangle + \sum_{m\neq n} \frac{|\langle u_{m0}|H'|u_{n0}\rangle|^2}{E_{n0}-E_{m0}}.$$

Now, $\langle u_{m0}|H'|u_{n0}\rangle = \dfrac{\hbar q}{m}\langle u_{m0)}|\hat{p}|u_{n0}\rangle + \dfrac{\hbar^2 q^2}{2m}\delta_{mn}$, so

$$\boxed{E_{nq} \approx E_{n0} + \frac{\hbar q}{m}\langle u_{n0)}|\hat{p}|u_{n0}\rangle + \frac{\hbar^2 q^2}{2m} + \left(\frac{\hbar q}{m}\right)^2 \sum_{m\neq n} \frac{|\langle u_{m0}|\hat{p}|u_{n0}\rangle|^2}{E_{n0}-E_{m0}}.}$$

(c) From Problem 2.1(b), the solutions u_{n0} can be chosen to be *real*. Then

$$\langle u_{n0}|\,\hat{p}\,|u_{n0}\rangle = \int_0^a u_{n0}(x)\left(-i\hbar\frac{d}{dx}\right)u_{n0}(x)\,dx = -\frac{i\hbar}{2}\int_0^a \frac{d}{dx}\left[u_{n0}(x)\right]^2\,dx = -\frac{i\hbar}{2}\left[u_{n0}(a)^2 - u_{n0}(0)^2\right] = 0.$$

Chapter 8

The Variational Principle

Problem 8.1

(a)

$$\langle V\rangle = 2\alpha A^2\int_0^\infty x e^{-2bx^2}dx = 2\alpha A^2\left(-\frac{1}{4b}e^{-2bx^2}\right)\Big|_0^\infty = \frac{\alpha A^2}{2b} = \frac{\alpha}{2b}\sqrt{\frac{2b}{\pi}} = \frac{\alpha}{\sqrt{2b\pi}}.$$

$$\langle H\rangle = \frac{\hbar^2 b}{2m} + \frac{\alpha}{\sqrt{2\pi b}}. \quad \frac{\partial\langle H\rangle}{\partial b} = \frac{\hbar^2}{2m} - \frac{1}{2}\frac{\alpha}{\sqrt{2\pi}}b^{-3/2} = 0 \Longrightarrow b^{3/2} = \frac{\alpha}{\sqrt{2\pi}}\frac{m}{\hbar^2};\ b = \left(\frac{m\alpha}{\sqrt{2\pi}\hbar^2}\right)^{2/3}.$$

$$\langle H\rangle_{\min} = \frac{\hbar^2}{2m}\left(\frac{m\alpha}{\sqrt{2\pi}\hbar^2}\right)^{2/3} + \frac{\alpha}{\sqrt{2\pi}}\left(\frac{\sqrt{2\pi}\hbar^2}{m\alpha}\right)^{1/3} = \frac{\alpha^{2/3}\hbar^{2/3}}{m^{1/3}(2\pi)^{1/3}}\left(\frac{1}{2}+1\right) = \boxed{\frac{3}{2}\left(\frac{\alpha^2\hbar^2}{2\pi m}\right)^{1/3}.}$$

(b)

$$\langle V\rangle = 2\alpha A^2\int_0^\infty x^4 e^{-2bx^2}dx = 2\alpha A^2\frac{3}{8(2b)^2}\sqrt{\frac{\pi}{2b}} = \frac{3\alpha}{16b^2}\sqrt{\frac{\pi}{2b}}\sqrt{\frac{2b}{\pi}} = \frac{3\alpha}{16b^2}.$$

$$\langle H\rangle = \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16b^2}. \quad \frac{\partial\langle H\rangle}{\partial b} = \frac{\hbar^2}{2m} - \frac{3\alpha}{8b^3} = 0 \Longrightarrow b^3 = \frac{3\alpha m}{4\hbar^2};\ b = \left(\frac{3\alpha m}{4\hbar^2}\right)^{1/3}.$$

$$\langle H\rangle_{\min} = \frac{\hbar^2}{2m}\left(\frac{3\alpha m}{4\hbar^2}\right)^{1/3} + \frac{3\alpha}{16}\left(\frac{4\hbar^2}{3\alpha m}\right)^{2/3} = \frac{\alpha^{1/3}\hbar^{4/3}}{m^{2/3}}3^{1/3}4^{-1/3}\left(\frac{1}{2}+\frac{1}{4}\right) = \boxed{\frac{3}{4}\left(\frac{3\alpha\hbar^4}{4m^2}\right)^{1/3}.}$$

Problem 8.2

Normalize: $$1 = 2|A|^2\int_0^\infty \frac{1}{(x^2+b^2)^2}dx = 2|A|^2\frac{\pi}{4b^3} = \frac{\pi}{2b^3}|A|^2. \quad A = \sqrt{\frac{2b^3}{\pi}}.$$

Kinetic Energy: $$\langle T\rangle = -\frac{\hbar^2}{2m}|A|^2\int_{-\infty}^\infty \frac{1}{(x^2+b^2)}\frac{d^2}{dx^2}\left(\frac{1}{(x^2+b^2)}\right)dx.$$

But $\frac{d^2}{dx^2}\left(\frac{1}{(x^2+b^2)}\right) = \frac{d}{dx}\left(\frac{-2x}{(x^2+b^2)^2}\right) = \frac{-2}{(x^2+b^2)^2} + 2x\frac{4x}{(x^2+b^2)^3} = \frac{2(3x^2-b^2)}{(x^2+b^2)^3}$, so

$$\begin{aligned}\langle T\rangle &= -\frac{\hbar^2}{2m}\frac{2b^3}{\pi}4\int_0^\infty \frac{(3x^2-b^2)}{(x^2+b^2)^4}dx = -\frac{4\hbar^2b^3}{\pi m}\left[3\int_0^\infty \frac{1}{(x^2+b^2)^3}dx - 4b^2\int_0^\infty \frac{1}{(x^2+b^2)^4}dx\right] \\ &= -\frac{4\hbar^2b^3}{\pi m}\left[3\frac{3\pi}{16b^5} - 4b^2\frac{5\pi}{32b^7}\right] = \frac{\hbar^2}{4mb^2}.\end{aligned}$$

Potential Energy: $\langle V\rangle = \frac{1}{2}m\omega^2|A|^2\,2\int_0^\infty \frac{x^2}{(x^2+b^2)^2}dx = m\omega^2\frac{2b^3}{\pi}\frac{\pi}{4b} = \frac{1}{2}m\omega^2b^2.$

$$\langle H\rangle = \frac{\hbar^2}{4mb^2} + \frac{1}{2}m\omega^2b^2. \quad \frac{\partial\langle H\rangle}{\partial b} = -\frac{\hbar^2}{2mb^3} + m\omega^2 b = 0 \Longrightarrow b^4 = \frac{\hbar^2}{2m^2\omega^2} \Longrightarrow b^2 = \frac{1}{\sqrt{2}}\frac{\hbar}{m\omega}.$$

$$\langle H\rangle_{\min} = \frac{\hbar^2}{4m}\frac{\sqrt{2}m\omega}{\hbar} + \frac{1}{2}m\omega^2\frac{1}{\sqrt{2}}\frac{\hbar}{m\omega} = \hbar\omega\left(\frac{\sqrt{2}}{4} + \frac{1}{2\sqrt{2}}\right) = \boxed{\frac{\sqrt{2}}{2}\hbar\omega} = 0.707\,\hbar\omega > \frac{1}{2}\hbar\omega. \quad \checkmark$$

Problem 8.3

$$\psi(x) = \begin{cases} A(x+a/2), & (-a/2 < x < 0), \\ A(a/2-x), & (0 < x < a/2), \\ 0, & (\text{otherwise}). \end{cases}$$

$$1 = |A|^2 2\int_0^{a/2}\left(\frac{a}{2}-x\right)^2 dx = -2|A|^2\frac{1}{3}\left(\frac{a}{2}-x\right)^3\Big|_0^{a/2} = \frac{2}{3}|A|^2\left(\frac{a}{2}\right)^3 = \frac{a^3}{12}|A|^2; \quad A = \sqrt{\frac{12}{a^3}} \quad (\text{as before}).$$

$$\frac{d\psi}{dx} = \begin{cases} A, & (-a/2 < x < 0), \\ -A, & (0 < x < a/2), \\ 0, & (\text{otherwise}). \end{cases} \qquad \frac{d^2\psi}{dx^2} = A\delta\left(x+\frac{a}{2}\right) - 2A\delta(x) + A\delta\left(x-\frac{a}{2}\right).$$

$$\begin{aligned}\langle T\rangle &= -\frac{\hbar^2}{2m}\int \psi\left[A\delta\left(x+\frac{a}{2}\right) - 2A\delta(x) + A\delta\left(x-\frac{a}{2}\right)\right]dx = \frac{\hbar^2}{2m}2A\psi(0) = \frac{\hbar^2}{m}A^2\frac{a}{2} \\ &= \frac{\hbar^2 a}{2m}\frac{12}{a^3} = 6\frac{\hbar^2}{ma^2} \quad (\text{as before}). \\ \langle V\rangle &= -\alpha\int|\psi|^2\delta(x)\,dx = -\alpha|\psi(0)|^2 = -\alpha A^2\left(\frac{a}{2}\right)^2 = -3\frac{\alpha}{a}. \quad \langle H\rangle = \langle T\rangle + \langle V\rangle = 6\frac{\hbar^2}{ma^2} - 3\frac{\alpha}{a}.\end{aligned}$$

$$\frac{\partial}{\partial a}\langle H\rangle = -12\frac{\hbar^2}{ma^3} + 3\frac{\alpha}{a^2} = 0 \Rightarrow a = 4\frac{\hbar^2}{m\alpha}.$$

$$\langle H\rangle_{\min} = 6\frac{\hbar^2}{m}\left(\frac{m\alpha}{4\hbar^2}\right)^2 - 3\alpha\left(\frac{m\alpha}{4\hbar^2}\right) = \frac{m\alpha^2}{\hbar^2}\left(\frac{3}{8}-\frac{3}{4}\right) = \boxed{-\frac{3m\alpha^2}{8\hbar^2}} > -\frac{m\alpha^2}{2\hbar^2}. \quad \checkmark$$

Problem 8.4

(a) Follow the proof in §8.1: $\psi = \sum_{n=1}^{\infty} c_n\psi_n$, where ψ_1 is the ground state. Since $\langle\psi_1|\psi\rangle = 0$, we have: $\sum_{n=1}^{\infty} c_n\langle\psi_1|\psi_n\rangle = c_1 = 0$; the coefficient of the ground state is zero. So

$$\langle H\rangle = \sum_{n=2}^{\infty} E_n|c_n|^2 \geq E_{\text{fe}}\sum_{n=2}^{\infty}|c_n|^2 = E_{\text{fe}}, \text{ since } E_n \geq E_{\text{fe}} \text{ for all } n \text{ except } 1.$$

(b)

$$1 = |A|^2\int_{-\infty}^{\infty} x^2 e^{-2bx^2}dx = |A|^2\,2\frac{1}{8b}\sqrt{\frac{\pi}{2b}} \Longrightarrow |A|^2 = 4b\sqrt{\frac{2b}{\pi}}.$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}|A|^2\int_{-\infty}^{\infty} xe^{-bx^2}\frac{d^2}{dx^2}\left(xe^{-bx^2}\right)dx$$

$$\frac{d^2}{dx^2}\left(xe^{-bx^2}\right) = \frac{d}{dx}\left(e^{-bx^2} - 2bx^2e^{-bx^2}\right) = -2bxe^{-bx^2} - 4bxe^{-bx^2} + 4b^2x^3e^{-bx^2}$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}4b\sqrt{\frac{2b}{\pi}}2\int_0^{\infty}\left(-6bx^2 + 4b^2x^4\right)e^{-2bx^2}dx = -\frac{2\hbar^2 b}{m}\sqrt{\frac{2b}{\pi}}\,2\left[-6b\frac{1}{8b}\sqrt{\frac{\pi}{2b}} + 4b^2\frac{3}{32b^2}\sqrt{\frac{\pi}{2b}}\right]$$

$$= -\frac{4\hbar^2 b}{m}\left(-\frac{3}{4} + \frac{3}{8}\right) = \frac{3\hbar^2 b}{2m}.$$

$$\langle V\rangle = \frac{1}{2}m\omega^2|A|^2\int_{-\infty}^{\infty} x^2e^{-2bx^2}x^2dx = \frac{1}{2}m\omega^2 4b\sqrt{\frac{2b}{\pi}}\,2\frac{3}{32b^2}\sqrt{\frac{\pi}{2b}} = \frac{3m\omega^2}{8b}.$$

$$\langle H\rangle = \frac{3\hbar^2 b}{2m} + \frac{3m\omega^2}{8b};\quad \frac{\partial\langle H\rangle}{\partial b} = \frac{3\hbar^2}{2m} - \frac{3m\omega^2}{8b^2} = 0 \Longrightarrow b^2 = \frac{m^2\omega^2}{4\hbar^2} \Longrightarrow b = \frac{m\omega}{2\hbar}.$$

$$\langle H\rangle_{\min} = \frac{3\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{3m\omega^2}{8}\frac{2\hbar}{m\omega} = \hbar\omega\left(\frac{3}{4} + \frac{3}{4}\right) = \boxed{\frac{3}{2}\hbar\omega.}$$

This is *exact*, since the trial wave function is in the form of the true first excited state.

Problem 8.5

The trial function has to vanish at $x = 0$ and (of course) go to zero at ∞. I'll choose

$$\psi(x) = A\,x\,e^{-\lambda\,x^2}.$$

We first normalize the wave function:

$$1 = \int_0^{\infty}|\psi|^2\,dx = A^2\int_0^{\infty}x^2\,e^{-2\lambda x^2}\,dx = A^2\,\frac{1}{\sqrt{8\,\lambda^3}}\underbrace{\int_0^{\infty}u^2\,e^{-u^2}\,du}_{\sqrt{\pi}/4}$$

(where $u = \sqrt{2\,\lambda}\,x$) so that

$$A^2 = 8\sqrt{\frac{2\,\lambda^3}{\pi}}\,.$$

Now

$$\frac{d\psi}{dx} = A\,e^{-\lambda\,x^2} - 2\,\lambda\,A\,x^2\,e^{-\lambda\,x^2}$$

and exploiting the hermiticity of $\hat{p}$ we can then compute the kinetic energy as

$$\begin{aligned}
\int_0^\infty \psi^*\,\frac{\hat{p}^2}{2\,m}\,\psi\,dx &= \frac{1}{2\,m}\int_0^\infty \left|\hat{p}\,\psi\right|^2\,dx \\
&= \frac{1}{2\,m}\,A^2\,\hbar^2\int_0^\infty \left(1-2\,\lambda\,x^2\right)^2\,e^{-2\,\lambda\,x^2}\,dx \\
&= \frac{\hbar^2}{2\,m}\,8\sqrt{\frac{2\,\lambda^3}{\pi}}\,\frac{1}{\sqrt{2\,\lambda}}\,\underbrace{\int_0^\infty \left(1-u^2\right)^2\,e^{-u^2}\,du}_{3\sqrt{\pi}/8} \\
&= \frac{3}{2}\,\lambda\,\frac{\hbar^2}{m}\,.
\end{aligned}$$

The potential energy is

$$\begin{aligned}
\int_0^\infty \psi^*(x)\;V(x)\;\psi(x) &= A^2\,m\,g\int_0^\infty x^3\,e^{-2\,\lambda\,x^2}\,dx \\
&= 8\sqrt{\frac{2\,\lambda^3}{\pi}}\,m\,g\,\frac{1}{(2\,\lambda)^2}\,\underbrace{\int_0^\infty u^3\,e^{-u^2}\,du}_{1/2} \\
&= \frac{2}{\sqrt{\pi\,\lambda}}\,m\,g\,.
\end{aligned}$$

Therefore the expectation value of the energy is

$$E(\lambda) = \frac{3}{2}\,\lambda\,\frac{\hbar^2}{m} + \frac{2}{\sqrt{\pi\,\lambda}}\,m\,g\,.$$

We still need to minimize the energy to find the tightest upper bound.

$$\frac{dE}{d\lambda} = \frac{3\,\hbar^2}{2\,m} + m\,g\sqrt{\frac{2}{\pi}}\left(-\frac{1}{2}\right)\,\frac{1}{\lambda^{3/2}} = 0$$

so that

$$\lambda = \left(\frac{2\,m^4\,g^2}{9\,\pi\,\hbar^4}\right)^{1/3}$$

and evaluating E using this result for λ we get

$$\boxed{E_{\text{gs}} \le 3\left(\frac{3}{2\,\pi}\right)^{1/3}\left(\frac{m\,g^2\,\hbar^2}{2}\right)^{1/3} \approx 2.345\left(\frac{m\,g^2\,\hbar^2}{2}\right)^{1/3}\,.}$$

This is fairly close to the exact result.

Problem 8.6

(a) Use the unperturbed ground state ($\psi^0_{\rm gs}$) as the trial wave function. The variational principle says $\langle\psi^0_{\rm gs}|H|\psi^0_{\rm gs}\rangle \geq E_{\rm gs}$. But $H = H^0 + H'$, so $\langle\psi^0_{\rm gs}|H|\psi^0_{\rm gs}\rangle = \langle\psi^0_{\rm gs}|H^0|\psi^0_{\rm gs}\rangle + \langle\psi^0_{\rm gs}|H'|\psi^0_{\rm gs}\rangle$. But $\langle\psi^0_{\rm gs}|H^0|\psi^0_{\rm gs}\rangle = E^0_{\rm gs}$ (the unperturbed ground state energy), and $\langle\psi^0_{\rm gs}|H'|\psi^0_{\rm gs}\rangle$ is precisely the first order correction to the ground state energy (Eq. 7.9), so $E^0_{\rm gs} + E^1_{\rm gs} \geq E_{\rm gs}$. QED

(b) The second order correction ($E^2_{\rm gs}$) is $E^2_{\rm gs} = \displaystyle\sum_{m\neq{\rm gs}} \frac{|\langle\psi^0_m|H'|\psi_{\rm gs}\rangle|^2}{E^0_{\rm gs} - E^0_m}$. But the numerator is clearly *positive*, and the denominator is always negative (since $E^0_{\rm gs} < E^0_m$ for all m), so $E^2_{\rm gs}$ is *negative.*

Problem 8.7

He^+ is a hydrogenic ion (see Problem 4.19); its ground state energy is $(2)^2(-13.6\text{ eV})$, or -54.4 eV. It takes $79.0 - 54.4 = \boxed{24.6\text{ eV}}$ to remove one electron.

Problem 8.8

I'll do the general case of a nucleus with Z_0 protons. Ignoring electron-electron repulsion altogether gives

$$\psi_0 = \frac{Z_0^3}{\pi a^3} e^{-Z_0(r_1+r_2)/a}, \quad \text{(generalizing Eq. 8.18)}$$

and the energy is $2Z_0^2E_1$. $\langle V_{ee}\rangle$ goes like $1/a$ (Eqs. 8.21 and 8.26), so the generalization of Eq. 8.26 is $\langle V_{ee}\rangle = -\frac{5}{4}Z_0E_1$, and the generalization of Eq. 8.27 is $\langle H\rangle = (2Z_0^2 - \frac{5}{4}Z_0)E_1$.

If we include shielding, the only change is that $(Z-2)$ in Eqs. 8.29, 8.30, and 8.33 is replaced by $(Z - Z_0)$. Thus Eq. 8.33 generalizes to

$$\langle H\rangle = \left[2Z^2 - 4Z(Z-Z_0) - \frac{5}{4}Z\right]E_1 = \left[-2Z^2 + 4ZZ_0 - \frac{5}{4}Z\right]E_1.$$

$$\frac{\partial\langle H\rangle}{\partial Z} = \left[-4Z + 4Z_0 - \frac{5}{4}\right]E_1 = 0 \Longrightarrow \boxed{Z = Z_0 - \frac{5}{16}.}$$

$$\begin{aligned}
\langle H\rangle_{\rm min} &= \left[-2\left(Z_0 - \frac{5}{16}\right)^2 + 4\left(Z_0 - \frac{5}{16}\right)Z_0 - \frac{5}{4}\left(Z_0 - \frac{5}{16}\right)\right]E_1 \\
&= \left(-2Z_0^2 + \frac{5}{4}Z_0 - \frac{25}{128} + 4Z_0^2 - \frac{5}{4}Z_0 - \frac{5}{4}Z_0 + \frac{25}{64}\right)E_1 \\
&= \boxed{\left(2Z_0^2 - \frac{5}{4}Z_0 + \frac{25}{128}\right)E_1} = \frac{(16Z_0-5)^2}{128}E_1,
\end{aligned}$$

generalizing Eq. 8.35. The first term is the naive estimate ignoring electron-electron repulsion altogether; the second term is $\langle V_{ee}\rangle$ in the unscreened state, and the third term is the effect of screening.

$\underline{Z_0 = 1\ (H^-)}$: $Z = 1 - \dfrac{5}{16} = \boxed{\dfrac{11}{16} = 0.688.}$ The effective nuclear charge is less than 1, as expected.

$$\langle H\rangle_{\min} = \frac{11^2}{128}E_1 = \boxed{\frac{121}{128}E_1 = -12.9 \text{ eV.}}$$

$\underline{Z_0 = 2 \text{ (He)}}$: $Z = 2 - \frac{5}{16} = \frac{27}{16} = 1.69$ (as before); $\langle H\rangle_{\min} = \frac{27^2}{128}E_1 = \frac{729}{128}E_1 = -77.5$ eV.

$\underline{Z_0 = 3 \text{ (Li}^+)}$: $Z = 3 - \frac{5}{16} = \boxed{\frac{43}{16} = 2.69}$ (somewhat less than 3); $\langle H\rangle_{\min} = \frac{43^2}{128}E_1 = \boxed{\frac{1849}{128}E_1 = -196\,\text{eV.}}$

Problem 8.9

$$D = a\langle\psi_0(r_1)\left|\frac{1}{r_2}\right|\psi_0(r_1)\rangle = a\langle\psi_0(r_2)\left|\frac{1}{r_1}\right|\psi_0(r_2)\rangle = a\frac{1}{\pi a^3}\int e^{-2r_2/a}\frac{1}{r_1}d^3r$$

$$= \frac{1}{\pi a^2}\int e^{-\frac{2}{a}\sqrt{r^2+R^2-2rR\cos\theta}}\,\frac{1}{r}r^2\sin\theta\,dr\,d\theta\,d\phi = \frac{2\pi}{\pi a^2}\int_0^\infty r\left[\int_0^\pi e^{-\frac{2}{a}\sqrt{r^2+R^2-2rR\cos\theta}}\sin\theta\,d\theta\right]dr.$$

$$[\dots] = \frac{1}{rR}\int_{|r-R|}^{r+R} e^{-2y/a}y\,dy = -\frac{a}{2rR}\left[e^{-2(r+R)/a}\left(r+R+\frac{a}{2}\right) - e^{-2|r-R|/a}\left(|r-R|+\frac{a}{2}\right)\right]$$

$$D = \frac{2}{a^2}\left(-\frac{a}{2R}\right)\left[e^{-2R/a}\int_0^\infty e^{-2r/a}\left(r+R+\frac{a}{2}\right)dr\right.$$
$$\left. -e^{-2R/a}\int_0^R e^{2r/a}\left(R-r+\frac{a}{2}\right)dr - e^{2R/a}\int_R^\infty e^{-2r/a}\left(r-R+\frac{a}{2}\right)dr\right]$$

$$= -\frac{1}{aR}\left\{e^{-2R/a}\left[\left(\frac{a}{2}\right)^2 + \left(R+\frac{a}{2}\right)\left(\frac{a}{2}\right)\right] - e^{-2R/a}\left(R+\frac{a}{2}\right)\left(\frac{a}{2}e^{2r/a}\right)\Big|_0^R\right.$$
$$\left. +e^{-2R/a}\left(\frac{a}{2}\right)^2 e^{2r/a}\left(\frac{2r}{a}-1\right)\Big|_0^R - e^{2R/a}\left(-R+\frac{a}{2}\right)\left(-\frac{a}{2}e^{-2r/a}\right)\Big|_R^\infty - e^{2R/a}\left(\frac{a}{2}\right)^2 e^{-2r/a}\left(-\frac{2r}{a}-1\right)\Big|_R^\infty\right\}$$

$$= -\frac{1}{aR}\left\{e^{-2R/a}\left[\frac{a^2}{4}+\frac{aR}{2}+\frac{a^2}{4}+\frac{aR}{2}+\frac{a^2}{4}+\frac{a^2}{4}\right] + \left[-\frac{aR}{2}-\frac{a^2}{4}+\frac{a^2}{4}\frac{2R}{a}-\frac{a^2}{4}+\frac{aR}{2}-\frac{a^2}{4}-\frac{a^2}{4}\frac{2R}{a}-\frac{a^2}{4}\right]\right\}$$

$$= -\frac{1}{aR}\left[e^{-2R/a}\left(a^2+aR\right) + \left(-a^2\right)\right] \Longrightarrow \boxed{D = \frac{a}{R} - \left(1+\frac{a}{R}\right)e^{-2R/a}} \quad \text{(confirms Eq. 8.48).}$$

$$X = a\langle\psi_0(r_1)\left|\frac{1}{r_1}\right|\psi_0(r_2)\rangle = a\frac{1}{\pi a^3}\int e^{-r_1/a}e^{-r_2/a}\frac{1}{r_1}d^3r$$

$$= \frac{1}{\pi a^2}\int e^{-r/a}e^{-\sqrt{r^2+R^2-2rR\cos\theta}/a}\,\frac{1}{r}r^2\sin\theta\,dr\,d\theta\,d\phi = \frac{2\pi}{\pi a^2}\int_0^\infty re^{-r/a}\left[\int_0^\pi e^{-\sqrt{r^2+R^2-2rR\cos\theta}/a}\sin\theta\,d\theta\right]dr.$$

$$[\dots] = -\frac{a}{rR}\left[e^{-(r+R)/a}(r+R+a) - e^{-|r-R|/a}(|r-R|+a)\right]$$

$$X = \frac{2}{a^2}\left(-\frac{a}{R}\right)\left[e^{-R/a}\int_0^\infty e^{-2r/a}(r+R+a)dr\right.$$
$$\left. -e^{-R/a}\int_0^R (R-r+a)dr - e^{R/a}\int_R^\infty e^{-2r/a}(r-R+a)dr\right]$$

$$= -\frac{2}{aR}\left\{e^{-R/a}\left[\left(\frac{a}{2}\right)^2 + (R+a)\left(\frac{a}{2}\right)\right] - e^{-R/a}\left[(R+a)R - \frac{R^2}{2}\right]\right.$$

$$
-e^{R/a}(-R+a)\left(-\frac{a}{2}e^{-2r/a}\right)\Big|_R^\infty - e^{R/a}\left(\frac{a}{2}\right)^2 e^{-2r/a}\left(-\frac{2r}{a}-1\right)\Big|_R^\infty \Bigg\}
$$

$$
= -\frac{2}{aR}\left[e^{-R/a}\left(\frac{a^2}{4}+\frac{aR}{2}+\frac{a^2}{2}-R^2-aR+\frac{R^2}{2}+\frac{aR}{2}-\frac{a^2}{2}-\frac{a^2}{4}\frac{2R}{a}-\frac{a^2}{4}\right)\right]
$$

$$
= -\frac{2}{aR}e^{-R/a}\left(-\frac{aR}{2}-\frac{R^2}{2}\right) \Longrightarrow \boxed{X = e^{-R/a}\left(1+\frac{R}{a}\right)} \quad \text{(confirms Eq. 8.49).}
$$

Problem 8.10

There are two changes: (1) the 2 in Eq. 8.39 changes sign ... which amounts to changing the sign of I in Eq. 8.44; (2) the last term in Eq. 8.45 changes sign ... which amounts to reversing the sign of X. Thus Eq. 8.50 becomes

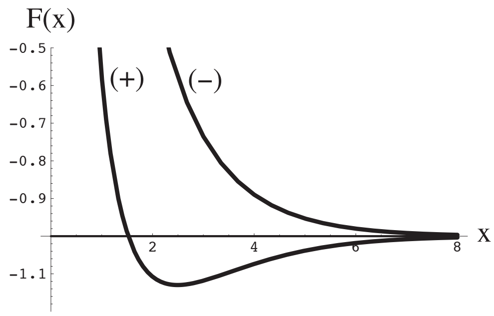
$$
\langle H\rangle = \left[1+2\frac{D-X}{1-I}\right]E_1, \qquad \text{and hence Eq. 8.52 becomes}
$$

$$
F(x) = \frac{E_{\text{tot}}}{-E_1} = \frac{2a}{R} - 1 - 2\frac{D-X}{1-I} = -1 + \frac{2}{x} - 2\frac{1/x - (1+1/x)\,e^{-2x} - (1+x)e^{-x}}{1-(1+x+x^2/3)e^{-x}}
$$

$$
= -1 + \frac{2}{x}\left[\frac{1-(1+x+x^2/3)e^{-x} - 1 + (x+1)e^{-2x} + (x+x^2)e^{-x}}{1-(1+x+x^2/3)e^{-x}}\right]
$$

$$
= \boxed{-1 + \frac{2}{x}\left[\frac{(1+x)e^{-2x} + \left(\frac{2}{3}x^2-1\right)e^{-x}}{1-(1+x+x^2/3)e^{-x}}\right]}.
$$

The graph (with plus sign for comparison) has no minimum, and remains above -1, indicating that the energy is greater than for the proton and atom dissociated. Hence, no evidence of bonding here.



Problem 8.11

According to *Mathematica*, the minimum occurs at $x = 2.493$, and at this point $F'' = 0.1257$.

$$
m\omega^2 = V'' = -\frac{E_1}{a^2}F'', \quad \text{so} \quad \omega = \frac{1}{a}\sqrt{\frac{-(0.1257)E_1}{m}}.
$$

Here m is the reduced mass of the proton: $m = \dfrac{m_p m_p}{m_p + m_p} = \dfrac{1}{2}m_p$.

$$
\omega = \frac{3\times10^8\ \text{m/s}}{(0.529\times10^{-10}\ \text{m})}\sqrt{\frac{(0.1257)(13.6\ \text{eV})}{(938\times10^6\ \text{eV})/2}} = 3.42\times10^{14}/\text{s}.
$$

$$\frac{1}{2}\hbar\omega = \frac{1}{2}(6.58\times 10^{-16}\,\text{eV}\cdot\text{s})(3.42\times 10^{14}\,/\text{s}) = \boxed{0.113\text{ eV}} \quad \text{(ground state vibrational energy).}$$

Mathematica says that at the minimum $F = -1.1297$, so the binding energy is $(0.1297)(13.6\text{ eV}) = 1.76$ eV. Since this is substantially greater than the vibrational energy, it stays bound. The highest vibrational energy is given by $(n+\frac{1}{2})\hbar\omega = 1.76$ eV, so $n = \dfrac{1.76}{0.226} - \dfrac{1}{2} = 7.29$. I estimate $\boxed{\text{eight}}$ bound vibrational states (including $n = 0$).

Problem 8.12

I'll drop the (irrelevant) normalization factors:

$$\begin{aligned}
\psi(\mathbf{r}_1,\mathbf{r}_2) &= \psi_B(\mathbf{r}_1)\psi_A(\mathbf{r}_2) - \psi_A(\mathbf{r}_1)\psi_B(\mathbf{r}_2)\\
&= [\psi_0(r_1)+\psi_0(r_1')]\,[\psi_0(r_2)-\psi_0(r_2')] - [\psi_0(r_1)-\psi_0(r_1')]\,[\psi_0(r_2)+\psi_0(r_2')]\\
&= \cancel{\psi_0(r_1)\psi_0(r_2)} - \psi_0(r_1)\psi_0(r_2') + \psi_0(r_1')\psi_0(r_2) - \cancel{\psi_0(r_1')\psi_0(r_2')}\\
&\quad - \cancel{\psi_0(r_1)\psi_0(r_2)} - \psi_0(r_1)\psi_0(r_2') + \psi_0(r_1')\psi_0(r_2) + \cancel{\psi_0(r_1')\psi_0(r_2')}\\
&= -2\,[\psi_0(r_1)\psi_0(r_2') - \psi_0(r_1')\psi_0(r_2)]\,. \quad \checkmark
\end{aligned}$$

Problem 8.13

$$\begin{aligned}
\left\langle -\frac{e^2}{4\pi\epsilon_0 r_1}\right\rangle_{\pm} &= -\left(\frac{e^2}{4\pi\epsilon_0 a}\right)A_{\pm}^2\left[\left\langle \psi_0(r_1)\left|\frac{a}{r_1}\right|\psi_0(r_1)\right\rangle \langle\psi_0(r_2')\,|\,\psi_0(r_2')\rangle\right.\\
&\quad \left. + \left\langle \psi_0(r_1')\left|\frac{a}{r_1}\right|\psi_0(r_1')\right\rangle \langle\psi_0(r_2)\,|\,\psi_0(r_2)\rangle \pm 2\left\langle \psi_0(r_1)\left|\frac{a}{r_1}\right|\psi_0(r_1')\right\rangle \langle\psi_0(r_2')\,|\,\psi_0(r_2)\rangle\right]\\
&= -\left(\frac{e^2}{4\pi\epsilon_0 a}\right)\frac{1}{2(1\pm I^2)}\,[(1)(1) + (D)(1) \pm 2(X)(I)]\\
&= -\frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0 a}\right)\frac{1+D\pm 2\,I\,X}{1\pm I^2}. \quad \checkmark
\end{aligned}$$

Problem 8.14

(a) The ϕ_1 integral is trivial:

$$\Phi(r_2) = \frac{2\pi}{\pi a^2}\int e^{-2r_1/a}\frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_1}}\,r_1^2\,dr_1\,\sin\theta_1\,d\theta_1.$$

Now do the θ_1 integral:

$$\begin{aligned}
\int_0^{\pi}\frac{\sin\theta_1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_1}}\,d\theta_1 &= \frac{-1}{r_1r_2}\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_1}\Big|_0^{\pi}\\
&= \frac{1}{r_1r_2}\left(\sqrt{(r_1+r_2)^2} - \sqrt{(r_1-r_2)^2}\right) = \frac{r_1+r_2-|r_1-r_2|}{r_1r_2}\\
&= \begin{cases} 2/r_2, & \text{if } r_1 < r_2,\\ 2/r_1 & \text{if } r_1 > r_2.\end{cases}
\end{aligned}$$

Finally, the r_1 integral:

$$\Phi(r_2) = \frac{4}{a^2}\left\{\frac{1}{r_2}\int_0^{r_2} e^{-2r_1/a}\, r_1^2\, dr_1 + \int_{r_2}^{\infty} e^{-2r_1/a}\, r_1\, dr_1\right\}$$
$$= \frac{4}{a^2}\left\{\frac{1}{r_2}\left[-\frac{a^3}{4}e^{-2r_1/a}\left(2\left(\frac{r_1}{a}\right)^2 + 2\left(\frac{r_1}{a}\right)+1\right)\right]\Bigg|_0^{r_2} + \left[-\frac{a^2}{4}e^{-2r_1/a}\left(2\frac{r_1}{a}+1\right)\right]\Bigg|_{r_2}^{\infty}\right\}$$
$$= \frac{a}{r_2} - \left(1+\frac{a}{r_2}\right)e^{-2r_2/a}. \quad \checkmark$$

(b) Again, the ϕ_2 integral is trivial:

$$D_2 = \frac{2\pi}{\pi a^3}\int e^{-2\sqrt{R^2+r_2^2-2Rr_2 cos\theta_2}/a}\left[\frac{a}{r_2} - \left(1+\frac{a}{r_2}\right)e^{-2r_2/a}\right] r_2^2\, dr_2\, \sin\theta_2\, d\theta_2.$$

For the θ_2 integral, let $u \equiv 2\sqrt{R^2+r_2^2-2Rr_2\cos\theta_2}/a$, so $du = \dfrac{4Rr_2}{P}a^2 u \sin\theta_2\, d\theta_2$. Then

$$I_\theta \equiv \int_0^{\pi} e^{-2\sqrt{R^2+r_2^2-2Rr_2\, cos\theta_2}/a}\, \sin\theta_2\, d\theta_2 = \frac{a^2}{4Rr_2}\int_{u_1}^{u_2} ue^{-u}\, du = -\frac{a^2}{4Rr_2}(u+1)e^{-u}\Big|_{u_1}^{u_2}.$$

Now, letting $\rho \equiv 2R/a$ and $x \equiv r_2/R$,

$$u_2 = \frac{2}{a}\sqrt{R^2+r_2^2+2Rr_2} = \frac{2}{a}(R+r_2) = \rho(1+x), \quad u_1 = \frac{2}{a}\sqrt{R^2+r_2^2-2Rr_2} = \frac{2}{a}|R-r_2| = \rho|1-x|.$$

Then

$$I_\theta = \frac{1}{\rho^2 x}\left\{[\rho|1-x|+1]e^{-\rho|1-x|} - [\rho(1+x)+1]e^{-\rho(1+x)}\right\}.$$

Finally, the r_2 integral becomes

$$D_2 = \frac{1}{4}\int_0^{\infty}\left\{[\rho|1-x|+1]e^{-\rho|1-x|} - [\rho(1+x)+1]e^{-\rho(1+x)}\right\}\left[2-(\rho x+2)\,e^{-\rho x}\right]\, dx$$
$$= \frac{e^{-\rho}}{4}\int_0^1 \{[\rho(1-x)+1]e^{\rho x}\}\left[2-(\rho x+2)\,e^{-\rho x}\right]\, dx$$
$$+ \frac{e^{\rho}}{4}\int_1^{\infty}\{[\rho(x-1)+1]e^{-\rho x}\}\left[2-(\rho x+2)\,e^{-\rho x}\right]\, dx$$
$$- \frac{e^{-\rho}}{4}\int_0^{\infty}\{[\rho(1+x)+1]e^{-\rho x}\}\left[2-(\rho x+2)\,e^{-\rho x}\right]\, dx$$
$$= \frac{e^{-\rho}}{4}\left\{2\int_0^1[(\rho+1)-\rho x]e^{\rho x}\, dx - \int_0^1[2(\rho+1)+(\rho-1)\rho x-(\rho x)^2]\, dx\right\}$$
$$+ \frac{e^{\rho}}{4}\left\{2\int_1^{\infty}[(1-\rho)+\rho x]e^{-\rho x}\, dx - \int_1^{\infty}\left[2(1-\rho)+\rho x(3-\rho)+(\rho x)^2\right]e^{-2\rho x}\, dx\right\}$$
$$- \frac{e^{-\rho}}{4}\left\{2\int_0^{\infty}[(1+\rho)+\rho x]e^{-\rho x}\, dx - \int_0^{\infty}\left[2(1+\rho)+(3+\rho)\rho x+(\rho x)^2\right]e^{-2\rho x}\, dx\right\}$$
$$= \frac{e^{-\rho}}{4}\left\{\frac{2}{\rho}(2e^{\rho}-\rho-2) - \left[2+\frac{3}{2}\rho+\frac{1}{6}\rho^2\right]\right\} + \frac{e^{\rho}}{4}\left\{\frac{4}{\rho}e^{-\rho} - \left[\frac{3}{4}+\frac{2}{\rho}\right]e^{-2\rho}\right\}$$
$$- \frac{e^{-\rho}}{4}\left\{2\left[1+\frac{2}{\rho}\right] - \left[\frac{5}{4}+\frac{2}{\rho}\right]\right\} = \frac{2}{\rho} - \frac{1}{8}\left(11+3\rho+\frac{16}{\rho}+\frac{\rho^2}{3}\right)e^{-\rho}.$$

Or, puitting back $\rho \equiv 2R/a$:

$$D_2 = \frac{a}{R} - \left(\frac{11}{8} + \frac{3R}{4a} + \frac{a}{R} + \frac{R^2}{6a^2} \right) e^{-2R/a}. \quad \checkmark$$

Problem 8.15

```
DInt[ρ_] := 1 / ρ - (1 + 1 / ρ) Exp[-2 ρ];

XInt[ρ_] := (1 + ρ) Exp[-ρ];

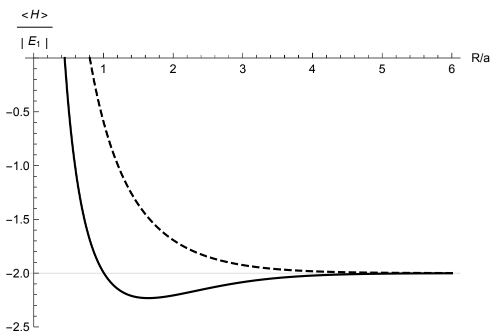
IInt[ρ_] := Exp[-ρ] (1 + ρ + 1 / 3 ρ^2);

D2Int[ρ_] := 1 / ρ - Exp[-2 ρ] / ρ (1 + 11 / 8 ρ + 3 / 4 ρ^2 + 1 / 6 ρ^3);

X2Int[ρ_] := 1 / 5 (Exp[-2 ρ] (25 / 8 - 23 / 4 ρ - 3 ρ^2 - 1 / 3 ρ^3) +
    6 / ρ (IInt[ρ]^2 (EulerGamma + Log[ρ]) + IInt[-ρ]^2 ExpIntegralEi[-4 ρ] -
       2 IInt[ρ] IInt[-ρ] ExpIntegralEi[-2 ρ]))

H[pm_, ρ_] := - 2 (1 - 1 / ρ +
    (2 DInt[ρ] - D2Int[ρ] + pm (2 IInt[ρ] XInt[ρ] - X2Int[ρ])) / (1 + pm IInt[ρ]^2))

Plot[{H[1, ρ], H[-1, ρ]}, {ρ, 0, 6},
 PlotRange → {-2.5, 0}, AxesLabel → {"R/a", "<H>/|E₁|"},
 PlotStyle → {{Black}, {Black, Dashed}}, GridLines → {None, {-2}}]
```

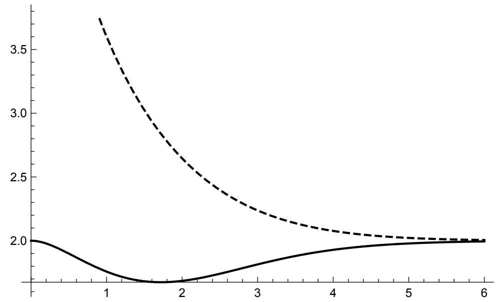



```
Kinetic[pm_, ρ_] := -2 (1 - 2 (1 + pm XInt[ρ] IInt[ρ]) / (1 + pm IInt[ρ]^2))

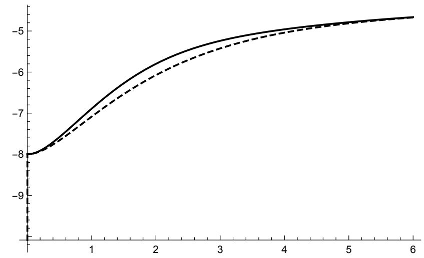
IonPotential[pm_, ρ_] := -4 (1 + DInt[ρ] + pm 2 XInt[ρ] IInt[ρ]) / (1 + pm IInt[ρ]^2)

ElectronPotential[pm_, ρ_] := (2 D2Int[ρ]) / (1 + pm IInt[ρ]^2) + (2 pm X2Int[ρ]) / (1 + pm IInt[ρ]^2)
```

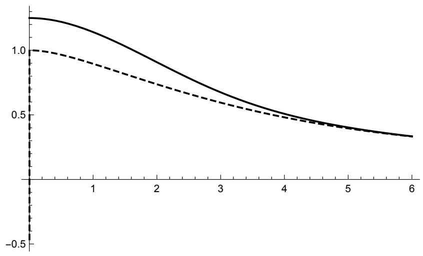
```
Plot[{Kinetic[1, ρ] , Kinetic[-1, ρ]},
 {ρ, 0, 6}, PlotStyle → {{Black}, {Black, Dashed}}]
```




```
Plot[{IonPotential[1, ρ] , IonPotential[-1, ρ]},
 {ρ, 0, 6}, PlotStyle → {{Black}, {Black, Dashed}}]
```




```
Plot[{ElectronPotential[1, ρ], ElectronPotential[-1, ρ]},
 {ρ, 0, 6}, PlotStyle → {{Black}, {Black, Dashed}}]
```



Problem 8.16

(a) First we normalize the function

$$\begin{aligned} 1 &= \int_0^a |\psi(x)|^2 \, dx = A^2 \int_0^a x^2 \, (a-x)^2 \, dx \\ &= A^2 \, a^5 \int_0^1 u^2 \, (1-u)^2 \, du = \frac{A^2 \, a^5}{30} \end{aligned}$$

so that $A^2 = 30/a^5$. The expectation value of the Hamiltonian is

$$\begin{aligned}
\langle H \rangle &= \int_0^a \psi^*(x) \left[-\frac{\hbar^2}{2\,m} \underbrace{\frac{d^2\psi}{dx^2}}_{2\,A} \right] dx \\
&= \frac{\hbar^2\,A^2}{m} \int_0^a x\,(a-x)\;dx \\
&= \frac{30\,\hbar^2}{m\,a^5}\,a^3 \int_0^1 u\,(1-u)\;du \\
&= 5\,\frac{\hbar^2}{m\,a^2}\,.
\end{aligned}$$

Therefore

$$\boxed{E_{\text{gs}} \leq \frac{10}{\pi^2}\,\frac{\pi^2\,\hbar^2}{2\,m\,a^2}\,.}$$

which is approximately 1.3% larger than the exact answer.

(b) Again we start by normalizing

$$1 = \int_0^a |\psi|^2\;dx = A^2 \int_0^a x^{2\,p}\,(a-x)^{2\,p}\;dx = A^2\,a^{4\,p+1} \int_0^1 |u\,(1-u)|^{2\,p}\;du\,.$$

I'll leave the integral alone for a second. The expectation value of the Hamiltonian is

$$\begin{aligned}
\langle H \rangle &= \frac{1}{2\,m} \int_0^a \psi^* \left[-\frac{\hbar^2}{2\,m}\,\frac{d^2\psi}{dx^2} \right] dx \\
&= \frac{\hbar^2}{2\,m} \int_0^a \left(\frac{d\,\psi}{dx} \right)^* \frac{d\psi}{dx}\,dx \\
&= \frac{\hbar^2}{2\,m}\,A^2 \int_0^a p^2 (a-2\,x)^2\;[x\,(a-x)]^{2\,p-2}\;dx \\
&= p^2\,\frac{\hbar^2}{2\,m}\,a^{4\,p-1}\,A^2 \int_0^1 (1-2\,u)^2\;[u\,(1-u)]^{2\,p-2}\;du \\
&= p^2\,\frac{\hbar^2}{2\,m\,a^2}\,\frac{\int_0^1 (1-2\,u)^2\;[u\,(1-u)]^{2\,p-2}\;du}{\int_0^1 |u\,(1-u)|^{2\,p}\;du}\,.
\end{aligned}$$

Now note that the integral in the numerator is

$$\begin{aligned}
\int_0^1 (1-2\,u)^2\;[u\,(1-u)]^{2\,p-2}\;du &= \frac{1}{2\,p-1} \int_0^1 (1-2\,u)\,\frac{d}{du}\,[u\,(1-u)]^{2\,p-1}\;du \\
&= \frac{1}{2\,p-1} \left[0 + 2 \int_0^1 [u\,(1-u)]^{2\,p-1}\;du \right]
\end{aligned}$$

where in the second line we've integrated by parts. Therefore

$$\langle H \rangle = \frac{2\,p^2}{2\,p-1}\,\frac{\hbar^2}{2\,m\,a^2}\,\frac{\int_0^1 [u\,(1-u)]^{2\,p-1}\;du}{\int_0^1 |u\,(1-u)|^{2\,p}\;du}$$

These integrals can be looked up in a table (for example Schaum's 18.24) to give

$$\langle H\rangle = \frac{2\,p\,(4\,p+1)}{2\,p-1}\,\frac{\hbar^2}{2\,m\,a^2}\,. \tag{8.1}$$

We can then minimize this

$$\frac{d\,\langle H\rangle}{dp} = 0$$

$$\frac{\hbar^2}{2\,m\,a^2}\,\frac{16\,p^2-16\,p-2}{(2\,p-1)^2} = 0\,.$$

The positive root of the quadratic (the other root would give a solution that diverges at 0 and a) is $p_{\min} = \left(2+\sqrt{6}\right)/4$. Plugging this into Equation 8.1 gives

$$\boxed{E_{\text{gs}} \le \frac{5+2\sqrt{6}}{\pi^2}\,\frac{\pi^2\,\hbar^2}{2\,m\,a^2}\,.}$$

This bound is approximately 0.3% greater than the exact value.

Problem 8.17

(a)

$$\begin{aligned}
1 &= \int |\psi|^2\,dx = |A|^2\int_{-a/2}^{a/2}\cos^2\left(\frac{\pi x}{a}\right)dx = |A|^2\frac{a}{2} \quad\Rightarrow\quad A=\sqrt{\frac{2}{a}}.\\
\langle T\rangle &= -\frac{\hbar^2}{2m}\int\psi\frac{d^2\psi}{dx^2}\,dx = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2\int\psi^2\,dx = \frac{\pi^2\hbar^2}{2ma^2}.\\
\langle V\rangle &= \frac{1}{2}m\omega^2\int x^2\psi^2\,dx = \frac{1}{2}m\omega^2\frac{2}{a}\int_{-a/2}^{a/2}x^2\cos^2\left(\frac{\pi x}{a}\right)dx = \frac{m\omega^2}{a}\left(\frac{a}{\pi}\right)^3\int_{-\pi/2}^{\pi/2}y^2\cos^2 y\,dy\\
&= \frac{m\omega^2a^2}{\pi^3}\left[\frac{y^3}{6}+\left(\frac{y^2}{4}-\frac{1}{8}\right)\sin 2y+\frac{y\cos 2y}{4}\right]\Bigg|_{-\pi/2}^{\pi/2} = \frac{m\omega^2a^2}{4\pi^2}\left(\frac{\pi^2}{6}-1\right).\\
\langle H\rangle &= \frac{\pi^2\hbar^2}{2ma^2}+\frac{m\omega^2a^2}{4\pi^2}\left(\frac{\pi^2}{6}-1\right); \quad \frac{\partial\langle H\rangle}{\partial a} = -\frac{\pi^2\hbar^2}{ma^3}+\frac{m\omega^2 a}{2\pi^2}\left(\frac{\pi^2}{6}-1\right)=0 \;\Rightarrow
\end{aligned}$$

$$\boxed{a = \pi\sqrt{\frac{\hbar}{m\omega}}\left(\frac{2}{\pi^2/6-1}\right)^{1/4}.}$$

$$\begin{aligned}
\langle H\rangle_{\min} &= \frac{\pi^2\hbar^2}{2m\pi^2}\frac{m\omega}{\hbar}\sqrt{\frac{\pi^2/6-1}{2}}+\frac{m\omega^2}{4\pi^2}\left(\frac{\pi^2}{6}-1\right)\pi^2\frac{\hbar}{m\omega}\sqrt{\frac{2}{\pi^2/6-1}}\\
&= \boxed{\frac{1}{2}\hbar\omega\sqrt{\frac{\pi^2}{3}-2}} = \frac{1}{2}\hbar\omega(1.136) > \frac{1}{2}\hbar\omega. \quad\checkmark
\end{aligned}$$

[We do *not* need to worry about the kink at $\pm a/2$. It is true that $d^2\psi/dx^2$ has delta functions there, but since $\psi(\pm a/2)=0$ no "extra" contribution to T comes from these points.]

(b) Because this trial function is odd, it is orthogonal to the ground state, so by Problem 8.4 $\langle H\rangle$ will give an upper bound to the first excited state.

$$\begin{aligned}
1 &= \int |\psi|^2\,dx = |B|^2\int_{-a}^{a}\sin^2\left(\frac{\pi x}{a}\right)dx = |B|^2 a \quad\Rightarrow\quad B=\frac{1}{\sqrt{a}}.\\
\langle T\rangle &= -\frac{\hbar^2}{2m}\int\psi\frac{d^2\psi}{dx^2}\,dx = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2\int\psi^2\,dx = \frac{\pi^2\hbar^2}{2ma^2}.\\
\langle V\rangle &= \frac{1}{2}m\omega^2\int x^2\psi^2\,dx = \frac{1}{2}m\omega^2\frac{1}{a}\int_{-a}^{a}x^2\sin^2\left(\frac{\pi x}{a}\right)dx = \frac{m\omega^2}{2a}\left(\frac{a}{\pi}\right)^3\int_{-\pi}^{\pi}y^2\sin^2 y\,dy\\
&= \frac{m\omega^2a^2}{2\pi^3}\left[\frac{y^3}{6}-\left(\frac{y^2}{4}-\frac{1}{8}\right)\sin 2y - \frac{y\cos 2y}{4}\right]\Bigg|_{-\pi}^{\pi} = \frac{m\omega^2a^2}{4\pi^2}\left(\frac{2\pi^2}{3}-1\right).\\
\langle H\rangle &= \frac{\pi^2\hbar^2}{2ma^2}+\frac{m\omega^2a^2}{4\pi^2}\left(\frac{2\pi^2}{3}-1\right);\quad \frac{\partial\langle H\rangle}{\partial a} = -\frac{\pi^2\hbar^2}{ma^3}+\frac{m\omega^2 a}{2\pi^2}\left(\frac{2\pi^2}{3}-1\right)=0\;\Rightarrow
\end{aligned}$$

$$\boxed{a=\pi\sqrt{\frac{\hbar}{m\omega}}\left(\frac{2}{2\pi^2/3-1}\right)^{1/4}}.$$

$$\begin{aligned}
\langle H\rangle_{\min} &= \frac{\pi^2\hbar^2}{2m\pi^2}\frac{m\omega}{\hbar}\sqrt{\frac{2\pi^2/3-1}{2}}+\frac{m\omega^2}{4\pi^2}\left(\frac{2\pi^2}{3}-1\right)\pi^2\frac{\hbar}{m\omega}\sqrt{\frac{2}{2\pi^2/3-1}}\\
&= \boxed{\frac{1}{2}\hbar\omega\sqrt{\frac{4\pi^2}{3}-2}} = \frac{1}{2}\hbar\omega(3.341) > \frac{3}{2}\hbar\omega.\quad\checkmark
\end{aligned}$$

Problem 8.18

We will need the following integral repeatedly:

$$\int_0^\infty \frac{x^k}{(x^2+b^2)^l}\,dx = \frac{1}{2b^{2l-k-1}}\frac{\Gamma\left(\frac{k+1}{2}\right)\Gamma\left(\frac{2l-k-1}{2}\right)}{\Gamma(l)}.$$

(a)

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty}|\psi|^2\,dx = 2|A|^2\int_0^\infty\frac{1}{(x^2+b^2)^{2n}}\,dx = \frac{|A|^2}{b^{4n-1}}\frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{4n-1}{2}\right)}{\Gamma(2n)} \;\Rightarrow A=\sqrt{\frac{b^{4n-1}\Gamma(2n)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{4n-1}{2}\right)}}.\\
\langle T\rangle &= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\psi\frac{d^2\psi}{dx^2}\,dx = -\frac{\hbar^2}{2m}A^2\int_{-\infty}^{\infty}\frac{1}{(x^2+b^2)^n}\frac{d}{dx}\left[\frac{-2nx}{(x^2+b^2)^{n+1}}\right]dx\\
&= \frac{n\hbar^2}{m}A^2\int_{-\infty}^{\infty}\frac{1}{(x^2+b^2)^n}\left[\frac{1}{(x^2+b^2)^{n+1}}-\frac{2(n+1)x^2}{(x^2+b^2)^{n+2}}\right]dx\\
&= \frac{2n\hbar^2}{m}A^2\left[\int_0^\infty\frac{1}{(x^2+b^2)^{2n+1}}\,dx - 2(n+1)\int_0^\infty\frac{x^2}{(x^2+b^2)^{2n+2}}\,dx\right]\\
&= \frac{2n\hbar^2}{m}\frac{b^{4n-1}\Gamma(2n)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{4n-1}{2}\right)}\left[\frac{1}{2b^{4n+1}}\frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{4n+1}{2}\right)}{\Gamma(2n+1)}-\frac{2(n+1)}{2b^{4n-1}}\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{4n+1}{2}\right)}{\Gamma(2n+2)}\right] = \frac{\hbar^2}{4mb^2}\frac{n(4n-1)}{(2n+1)}.
\end{aligned}$$

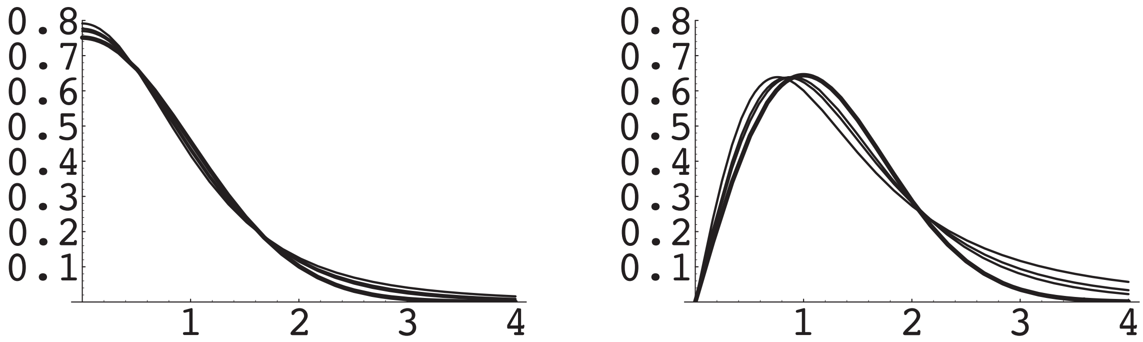
$$\begin{aligned}
\langle V\rangle &= \frac{1}{2}m\omega^2\int_{-\infty}^{\infty}\psi^2x^2\,dx = \frac{1}{2}m\omega^2 2A^2\int_0^{\infty}\frac{x^2}{(x^2+b^2)^{2n}}\,dx \\
&= m\omega^2\frac{b^{4n-1}\Gamma(2n)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{4n-1}{2}\right)}\frac{1}{2b^{4n-3}}\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{4n-3}{2}\right)}{\Gamma(2n)} = \frac{m\omega^2b^2}{2(4n-3)}. \\
\langle H\rangle &= \frac{\hbar^2}{4mb^2}\frac{n(4n-1)}{(2n+1)}+\frac{m\omega^2b^2}{(4n-3)}; \quad \frac{\partial\langle H\rangle}{\partial b} = -\frac{\hbar^2}{2mb^3}\frac{n(4n-1)}{(2n+1)}+\frac{m\omega^2 b}{(4n-3)} = 0 \;\Rightarrow \\
b &= \sqrt{\frac{\hbar}{m\omega}}\left[\frac{n(4n-1)(4n-3)}{2(2n+1)}\right]^{1/4}. \\
\langle H\rangle_{\min} &= \frac{\hbar^2}{4m}\frac{n(4n-1)}{(2n+1)}\frac{m\omega}{\hbar}\sqrt{\frac{2(2n+1)}{n(4n-1)(4n-3)}}+\frac{m\omega^2}{2(4n-3)}\frac{\hbar}{m\omega}\sqrt{\frac{n(4n-1)(4n-3)}{2(2n+1)}} \\
&= \boxed{\frac{1}{2}\hbar\omega\sqrt{\frac{2n(4n-1)}{(2n+1)(4n-3)}}} = \frac{1}{2}\hbar\omega\sqrt{\frac{8n^2-2n}{8n^2-2n-3}} \;>\; \frac{1}{2}\hbar\omega. \quad \checkmark
\end{aligned}$$

(b)

$$\begin{aligned}
1 &= 2|B|^2\int_0^{\infty}\frac{x^2}{(x^2+b^2)^{2n}}\,dx = \frac{|B|^2}{b^{4n-3}}\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{4n-3}{2}\right)}{\Gamma(2n)} \;\Rightarrow B = \sqrt{\frac{b^{4n-3}\Gamma(2n)}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{4n-3}{2}\right)}}. \\
\langle T\rangle &= -\frac{\hbar^2}{2m}B^2\int_{-\infty}^{\infty}\frac{x}{(x^2+b^2)^n}\frac{d}{dx}\left[\frac{1}{(x^2+b^2)^n}-\frac{2nx^2}{(x^2+b^2)^{n+1}}\right]dx \\
&= -\frac{\hbar^2B^2}{2m}\int_{-\infty}^{\infty}\frac{x}{(x^2+b^2)^n}\left[\frac{-2nx}{(x^2+b^2)^{n+1}}-\frac{4nx}{(x^2+b^2)^{n+1}}+\frac{4n(n+1)x^3}{(x^2+b^2)^{n+2}}\right]dx \\
&= \frac{4n\hbar^2B^2}{2m}\left[3\int_0^{\infty}\frac{x^2}{(x^2+b^2)^{2n+1}}\,dx-2(n+1)\int_0^{\infty}\frac{x^4}{(x^2+b^2)^{2n+2}}\,dx\right] \\
&= \frac{2n\hbar^2}{m}\frac{b^{4n-3}\Gamma(2n)}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{4n-3}{2}\right)}\left[\frac{3}{2b^{4n-1}}\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{4n-1}{2}\right)}{\Gamma(2n+1)}-\frac{2(n+1)}{2b^{4n-1}}\frac{\Gamma\left(\frac{5}{2}\right)\Gamma\left(\frac{4n-1}{2}\right)}{\Gamma(2n+2)}\right] = \frac{3\hbar^2}{4mb^2}\frac{n(4n-3)}{(2n+1)}.
\end{aligned}$$

$$\begin{aligned}
\langle V\rangle &= \frac{1}{2}m\omega^2 2B^2\int_0^{\infty}\frac{x^4}{(x^2+b^2)^{2n}}\,dx = \frac{1}{2}m\omega^2\frac{b^{4n-3}\Gamma(2n)}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{4n-3}{2}\right)}\frac{2}{2b^{4n-5}}\frac{\Gamma\left(\frac{5}{2}\right)\Gamma\left(\frac{4n-5}{2}\right)}{\Gamma(2n)} = \frac{3}{2}\frac{m\omega^2b^2}{(4n-5)}. \\
\langle H\rangle &= \frac{3\hbar^2}{4mb^2}\frac{n(4n-3)}{(2n+1)}+\frac{3}{2}\frac{m\omega^2b^2}{(4n-5)}; \quad \frac{\partial\langle H\rangle}{\partial b} = -\frac{3\hbar^2}{2mb^3}\frac{n(4n-3)}{(2n+1)}+\frac{3m\omega^2b}{(4n-5)} = 0 \;\Rightarrow \\
b &= \sqrt{\frac{\hbar}{m\omega}}\left[\frac{n(4n-3)(4n-5)}{2(2n+1)}\right]^{1/4}. \\
\langle H\rangle_{\min} &= \frac{3\hbar^2}{4m}\frac{n(4n-3)}{(2n+1)}\frac{m\omega}{\hbar}\sqrt{\frac{2(2n+1)}{n(4n-3)(4n-5)}}+\frac{3}{2}\frac{m\omega^2}{(4n-5)}\frac{\hbar}{m\omega}\sqrt{\frac{n(4n-3)(4n-5)}{2(2n+1)}} \\
&= \boxed{\frac{3}{2}\hbar\omega\sqrt{\frac{2n(4n-3)}{(2n+1)(4n-5)}}} = \frac{3}{2}\hbar\omega\sqrt{\frac{8n^2-6n}{8n^2-6n-5}} \;>\; \frac{3}{2}\hbar\omega. \quad \checkmark
\end{aligned}$$

(c) As $n \to \infty$, ψ becomes more and more "gaussian". In the figures I have plotted the trial wave functions for $n = 2$, $n = 3$, and $n = 4$, as well as the exact states (heavy line). Even for $n = 2$ the fit is pretty good, so it is hard to see the improvement, but the successive curves do move perceptably toward the correct result.



Analytically, for large n, $b \approx \sqrt{\frac{\hbar}{m\omega}}\left(\frac{n \cdot 4n \cdot 4n}{2 \cdot 2n}\right)^{1/4} = \sqrt{\frac{2n\hbar}{m\omega}}$, so

$$\left(x^2+b^2\right)^n = b^{2n}\left(1+\frac{x^2}{b^2}\right)^n \approx b^{2n}\left(1+\frac{m\omega x^2}{2\hbar n}\right)^n \quad \to \quad b^{2n}e^{m\omega x^2/2\hbar}.$$

Meanwhile, using Stirling's approximation in the form $\Gamma(z+1) \approx z^z e^{-z}$:

$$A^2 = \frac{b^{4n-1}\Gamma(2n)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(2n-\frac{1}{2}\right)} \approx \frac{b^{4n-1}}{\sqrt{\pi}}\frac{(2n-1)^{2n-1}e^{-(2n-1)}}{\left(2n-\frac{3}{2}\right)^{2n-3/2}e^{-(2n-3/2)}} \approx \frac{b^{4n-1}}{\sqrt{\pi}}\frac{1}{\sqrt{e}}\left(\frac{2n-1}{2n-\frac{3}{2}}\right)^{2n-1}\sqrt{2n-3/2}.$$

$$\text{But} \quad \left(\frac{1-\frac{1}{2n}}{1-\frac{3}{4n}}\right) \approx \left(1-\frac{1}{2n}\right)\left(1+\frac{3}{4n}\right) \approx 1+\frac{3}{4n}-\frac{1}{2n} = 1+\frac{1}{4n};$$

$$\text{so} \quad \left(\frac{2n-1}{2n-\frac{3}{2}}\right)^{2n-1} \approx \left[\left(1+\frac{1}{4n}\right)^n\right]^2 \frac{1}{1+1/4n} \to \left(e^{1/4}\right)^2 = \sqrt{e}.$$

$$= \frac{b^{4n-1}}{\sqrt{\pi e}}\sqrt{e}\sqrt{2n} = \sqrt{\frac{2n}{\pi}}b^{4n-1} \quad \Rightarrow \quad A \approx \left(\frac{2n}{\pi}\right)^{1/4} b^{2n-1/2}. \quad \text{So}$$

$$\psi \approx \left(\frac{2n}{\pi}\right)^{1/4} b^{2n-1/2}\frac{1}{b^{2n}}e^{-m\omega x^2/2\hbar} = \left(\frac{2n}{\pi}\right)^{1/4}\left(\frac{m\omega}{2n\hbar}\right)^{1/4}e^{-m\omega x^2/2\hbar} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-m\omega x^2/2\hbar},$$

which is precisely the ground state of the harmonic oscillator (Eq. 2.60). So it's no accident that we get the exact energies, in the limit $n \to \infty$.

Problem 8.19

$$1 = |A|^2\int e^{-2br^2}r^2\sin\theta\,dr\,d\theta\,d\phi = 4\pi|A|^2\int_0^\infty r^2e^{-2br^2}dr = |A|^2\left(\frac{\pi}{2b}\right)^{3/2} \Rightarrow A = \left(\frac{2b}{\pi}\right)^{3/4}.$$

$$\langle V\rangle = -\frac{e^2}{4\pi\epsilon_0}|A|^2 4\pi\int_0^\infty e^{-2br^2}\frac{1}{r}r^2dr = -\frac{e^2}{4\pi\epsilon_0}\left(\frac{2b}{\pi}\right)^{3/2}4\pi\frac{1}{4b} = -\frac{e^2}{4\pi\epsilon_0}2\sqrt{\frac{2b}{\pi}}.$$

$$\begin{aligned}
\langle T\rangle &= -\frac{\hbar^2}{2m}|A|^2\int e^{-br^2}(\nabla^2 e^{-br^2})\,r^2\sin\theta\,dr\,d\theta\,d\phi\\
&\qquad \text{But}\quad (\nabla^2 e^{-br^2}) = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}e^{-br^2}\right) = \frac{1}{r^2}\frac{d}{dr}\left(-2br^3e^{-br^2}\right) = \frac{-2b}{r^2}\left(3r^2-2br^4\right)e^{-br^2}.\\
&= \frac{-\hbar^2}{2m}\left(\frac{2b}{\pi}\right)^{3/2}(4\pi)(-2b)\int_0^\infty(3r^2-2br^4)e^{-2br^2}\,dr = \frac{\hbar^2}{m}\pi b4\left(\frac{2b}{\pi}\right)^{3/2}\left[3\frac{1}{8b}\sqrt{\frac{\pi}{2b}}-2b\frac{3}{32b^2}\sqrt{\frac{\pi}{2b}}\right]\\
&= \frac{\hbar^2}{m}4\pi b\left(\frac{2b}{\pi}\right)\left(\frac{3}{8b}-\frac{3}{16b}\right) = \frac{3\hbar^2 b}{2m}.
\end{aligned}$$

$$\langle H\rangle = \frac{3\hbar^2 b}{2m} - \frac{e^2}{4\pi\epsilon_0}2\sqrt{\frac{2b}{\pi}};\qquad \frac{\partial\langle H\rangle}{\partial b} = \frac{3\hbar^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{b}} = 0 \quad\Rightarrow\quad \sqrt{b} = \frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi}}\frac{2m}{3\hbar^2}.$$

$$\begin{aligned}
\langle H\rangle_{\min} &= \frac{3\hbar^2}{2m}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{2}{\pi}\frac{4m^2}{9\hbar^4} - \frac{e^2}{4\pi\epsilon_0}2\sqrt{\frac{2}{\pi}}\left(\frac{e^2}{4\pi\epsilon_0}\right)\sqrt{\frac{2}{\pi}}\frac{2m}{3\hbar^2} = \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{m}{\hbar^2}\left(\frac{4}{3\pi}-\frac{8}{3\pi}\right)\\
&= -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{8}{3\pi} = \boxed{\frac{8}{3\pi}E_1 = -11.5\text{ eV}.}
\end{aligned}$$

Problem 8.20

Adopting the variational wave function

$$\psi(r,\theta,\phi) = Ae^{-br^2}Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}Ae^{-br^2}\cos\theta,$$

$$\begin{aligned}
1 &= |A|^2\int_0^\infty e^{-2br^2}r^2\,dr\int|Y_1^0|^2\,d\Omega = |A|^2\left(\frac{1}{8b}\sqrt{\frac{\pi}{2b}}\right)(1) \Rightarrow A = 2\left(\frac{8b^3}{\pi}\right)^{1/4}.\\
\langle V\rangle &= -\frac{e^2}{4\pi\epsilon_0}|A|^2\int_0^\infty e^{-2br^2}\frac{1}{r}r^2dr = -\frac{e^2}{4\pi\epsilon_0}\left(4\sqrt{\frac{8b^3}{\pi}}\right)\frac{1}{4b} = -\frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{8b}{\pi}}.
\end{aligned}$$

$$\begin{aligned}
\nabla^2\psi &= \left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)\right\}\\
&= \sqrt{\frac{3}{4\pi}}\,A\left\{\frac{\cos\theta}{r^2}\frac{d}{dr}\left[r^2(-2br)e^{-br^2}\right] + \frac{e^{-br^2}}{r^2\sin\theta}\frac{\partial}{\partial\theta}(-\sin^2\theta)\right\}\\
&= \sqrt{\frac{3}{4\pi}}\,A\left\{-\frac{2b\cos\theta}{r^2}\left(3r^2e^{-br^2}-2br^4e^{-br^2}\right) - \frac{e^{-br^2}}{r^2\sin\theta}(2\sin\theta\cos\theta)\right\}\\
&= \sqrt{\frac{3}{\pi}}Ae^{-br^2}\frac{\cos\theta}{r^2}\left(2b^2r^4-3br^2-1\right).
\end{aligned}$$

$$\begin{aligned}\langle T\rangle &= -\frac{\hbar^2}{2m}\int \psi^*\nabla^2\psi\, d^3\mathbf{r} = -\frac{\hbar^2}{2m}\sqrt{\frac{3}{\pi}}\sqrt{\frac{3}{4\pi}}|A|^2\int e^{-br^2}\cos\theta e^{-br^2}\frac{\cos\theta}{r^2}\left(2b^2r^4-3br^2-1\right)r^2\sin\theta\, dr\, d\theta\, d\phi \\ &= -\frac{\hbar^2}{2m}\frac{3}{2\pi}|A|^2 2\pi\int_0^\infty e^{-2br^2}\left(2b^2r^4-3br^2-1\right)dr\int_0^\pi \cos^2\theta\,\sin\theta\, d\theta \\ &= -\frac{3\hbar^2}{2m}|A|^2\left\{2b^2\left(12\sqrt{\pi}\frac{1}{(2\sqrt{2b})^5}\right)-3b\left(2\sqrt{\pi}\frac{1}{(2\sqrt{2b})^3}\right)-\left(\sqrt{\pi}\frac{1}{(2\sqrt{2b})}\right)\right\}\left(\frac{2}{3}\right) \\ &= -\frac{\hbar^2}{m}|A|^2\frac{\sqrt{\pi}}{2\sqrt{2b}}\left[\frac{24b^2}{(2\sqrt{2b})^4}-\frac{6b}{(2\sqrt{2b})^2}-1\right] = \frac{\hbar^2}{m}|A|^2\sqrt{\frac{\pi}{2b}}\frac{11}{16} = \frac{11b\hbar^2}{2m}.\end{aligned}$$

$$\langle H\rangle = \frac{11\,b\hbar^2}{2m}-\frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{8b}{\pi}};\quad \frac{\partial\langle H\rangle}{\partial b} = \frac{11\hbar^2}{2m}-\frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi b}} = 0 \quad\Rightarrow\quad \sqrt{b} = \frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi}}\frac{2m}{11\hbar^2}.$$

$$\begin{aligned}\langle H\rangle_{\min} &= \frac{11\hbar^2}{2m}\frac{e^4}{16\pi^2\epsilon_0^2}\frac{2}{\pi}\frac{4m^2}{121\hbar^4}-\frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{8}{\pi}}\frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi}}\frac{2m}{11\hbar^2} = -\left(\frac{4}{11\pi}\right)\frac{me^4}{\hbar^2(4\pi\epsilon_0)^2} \\ &= \boxed{\frac{32}{11\pi}E_2 = 0.926E_2.}\end{aligned}$$

Since E_2 is negative this is indeed an upper bound, within about 7% of the exact answer.

Problem 8.21

Let $\psi = \dfrac{1}{\sqrt{\pi b^3}}e^{-r/b}$ (same as hydrogen, but with $a \to b$ adjustable). From Eq. 4.218, we have $\langle T\rangle = -E_1 = \dfrac{\hbar^2}{2ma^2}$ for hydrogen, so in this case $\langle T\rangle = \dfrac{\hbar^2}{2mb^2}$.

$$\langle V\rangle = -\frac{e^2}{4\pi\epsilon_0}\frac{4\pi}{\pi b^3}\int_0^\infty e^{-2r/b}\frac{e^{-\mu r}}{r}r^2\,dr = -\frac{e^2}{4\pi\epsilon_0}\frac{4}{b^3}\int_0^\infty e^{-(\mu+2/b)r}r\,dr = -\frac{e^2}{4\pi\epsilon_0}\frac{4}{b^3}\frac{1}{(\mu+2/b)^2} = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{b(1+\frac{\mu b}{2})^2}.$$

$$\langle H\rangle = \frac{\hbar^2}{2mb^2}-\frac{e^2}{4\pi\epsilon_0}\frac{1}{b(1+\frac{\mu b}{2})^2}.$$

$$\frac{\partial\langle H\rangle}{\partial b} = -\frac{\hbar^2}{mb^3}+\frac{e^2}{4\pi\epsilon_0}\left[\frac{1}{b^2(1+\mu b/2)^2}+\frac{\mu}{b(1+\mu b/2)^3}\right] = -\frac{\hbar^2}{mb^3}+\frac{e^2}{4\pi\epsilon_0}\frac{(1+3\mu b/2)}{b^2(1+\mu b/2)^3} = 0 \quad\Rightarrow$$

$$\frac{\hbar^2}{m}\left(\frac{4\pi\epsilon_0}{e^2}\right) = b\frac{(1+3\mu b/2)}{(1+\mu b/2)^3},\quad \text{or}\quad b\frac{(1+3\mu b/2)}{(1+\mu b/2)^3} = a.$$

This determines b, but unfortunately it's a cubic equation. So we use the fact that μ is small to obtain a suitable approximate solution. If $\mu = 0$, then $b = a$ (of course), so $\mu a \ll 1 \Longrightarrow \mu b \ll 1$ too. We'll expand in powers of μb:

$$a \approx b\left(1+\frac{3\mu b}{2}\right)\left[1-\frac{3\mu b}{2}+6\left(\frac{\mu b}{2}\right)^2\right] \approx b\left[1-\frac{9}{4}(\mu b)^2+\frac{6}{4}(\mu b)^2\right] = b\left[1-\frac{3}{4}(\mu b)^2\right].$$

Since the $\frac{3}{4}(\mu b)^2$ term is *already* a second-order correction, we can replace b by a:

$$b \approx \frac{a}{\left[1-\frac{3}{4}(\mu b)^2\right]} \approx a\left[1+\frac{3}{4}(\mu a)^2\right].$$

$$\begin{aligned}
\langle H\rangle_{\min} &= \frac{\hbar^2}{2ma^2\left[1+\frac{3}{4}(\mu a)^2\right]^2} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{a\left[1+\frac{3}{4}(\mu a)^2\right]\left[1+\frac{1}{2}(\mu a)\right]^2} \\
&\approx \frac{\hbar^2}{2ma^2}\left[1-2\frac{3}{4}(\mu a)^2\right] - \frac{e^2}{4\pi\epsilon_0}\frac{1}{a}\left[1-\frac{3}{4}(\mu a)^2\right]\left[1-2\frac{\mu a}{2}+3\left(\frac{\mu a}{2}\right)^2\right] \\
&= -E_1\left[1-\frac{3}{2}(\mu a)^2\right] + 2E_1\left[1-\mu a+\frac{3}{4}(\mu a)^2-\frac{3}{4}(\mu a)^2\right] = \boxed{E_1\left[1-2(\mu a)+\frac{3}{2}(\mu a)^2\right].}
\end{aligned}$$

Problem 8.22

(a)

$$\mathsf{H} = \begin{pmatrix} E_a & h \\ h & E_b \end{pmatrix}; \ \det(\mathsf{H}-\lambda) = (E_a-\lambda)(E_b-\lambda) - h^2 = 0 \Longrightarrow \lambda^2 - \lambda(E_a+E_b) + E_aE_b - h^2 = 0.$$

$$\lambda = \frac{1}{2}\left(E_a+E_b \pm \sqrt{E_a^2+2E_aE_b+E_b^2-4E_aE_b+4h^2}\right) \Rightarrow \boxed{E_\pm = \tfrac{1}{2}\left[E_a+E_b\pm\sqrt{(E_a-E_b)^2+4h^2}\right].}$$

(b) Zeroth order: $E_a^0 = E_a$, $E_b^0 = E_b$. First order: $E_a^1 = \langle\psi_a|H'|\psi_a\rangle = 0$, $E_b^1 = \langle\psi_b|H'|\psi_b\rangle = 0$. Second order:

$$E_a^2 = \frac{|\langle\psi_b|H'|\psi_a\rangle|^2}{E_a-E_b} = -\frac{h^2}{E_b-E_a}; \qquad E_b^2 = \frac{|\langle\psi_a|H'|\psi_b\rangle|^2}{E_b-E_a} = \frac{h^2}{E_b-E_a};$$

$$\boxed{E_- \approx E_a - \frac{h^2}{(E_b-E_a)}; \quad E_+ \approx E_b + \frac{h^2}{(E_b-E_a)}.}$$

(c)

$$\begin{aligned}
\langle H\rangle &= \langle\cos\phi\,\psi_a+\sin\phi\,\psi_b|(H^0+H')|\cos\phi\,\psi_a+\sin\phi\,\psi_b\rangle \\
&= \cos^2\phi\,\langle\psi_a|H^0|\psi_a\rangle + \sin^2\phi\,\langle\psi_b|H^0|\psi_b\rangle + \sin\phi\cos\phi\,\langle\psi_b|H'|\psi_a\rangle + \sin\phi\cos\phi\,\langle\psi_a|H'|\psi_b\rangle \\
&= E_a\cos^2\phi + E_b\sin^2\phi + 2h\sin\phi\cos\phi. \\
\frac{\partial\langle H\rangle}{\partial\phi} &= -E_a2\cos\phi\sin\phi + E_b2\sin\phi\cos\phi + 2h(\cos^2\phi-\sin^2\phi) = (E_b-E_a)\sin2\phi + 2h\cos2\phi = 0.
\end{aligned}$$

$$\tan2\phi = -\frac{2h}{E_b-E_a} = -\epsilon \quad \text{where} \quad \epsilon \equiv \frac{2h}{E_b-E_a}. \quad \frac{\sin2\phi}{\sqrt{1-\sin^2 2\phi}} = -\epsilon; \quad \sin^2 2\phi = \epsilon^2(1-\sin^2 2\phi);$$

$$\text{or} \quad \sin^2 2\phi(1+\epsilon^2) = \epsilon^2; \quad \sin2\phi = \frac{\pm\epsilon}{\sqrt{1+\epsilon^2}}; \quad \cos^2 2\phi = 1-\sin^2 2\phi = 1-\frac{\epsilon^2}{1+\epsilon^2} = \frac{1}{1+\epsilon^2};$$

$$\cos2\phi = \frac{\mp1}{\sqrt{1+\epsilon^2}} \quad \text{(sign dictated by } \tan2\phi = \frac{\sin2\phi}{\cos2\phi} = -\epsilon).$$

$$\cos^2\phi = \frac{1}{2}(1+\cos2\phi) = \frac{1}{2}\left(1\mp\frac{1}{\sqrt{1+\epsilon^2}}\right); \quad \sin^2\phi = \frac{1}{2}(1-\cos2\phi) = \frac{1}{2}\left(1\pm\frac{1}{\sqrt{1+\epsilon^2}}\right).$$

$$\langle H\rangle_{\min} = \frac{1}{2}E_a\left(1\mp\frac{1}{\sqrt{1+\epsilon^2}}\right) + \frac{1}{2}E_b\left(1\pm\frac{1}{\sqrt{1+\epsilon^2}}\right) \pm h\frac{\epsilon}{\sqrt{1+\epsilon^2}} = \frac{1}{2}\left[E_a+E_b\pm\frac{(E_b-E_a+2h\epsilon)}{\sqrt{1+\epsilon^2}}\right]$$

But $\dfrac{(E_b - E_a + 2h\epsilon)}{\sqrt{1+\epsilon^2}} = \dfrac{(E_b - E_a) + 2h\frac{2h}{(E_b-E_a)}}{\sqrt{1+\frac{4h^2}{(E_b-E_a)^2}}} = \dfrac{(E_b-E_a)^2 + 4h^2}{\sqrt{(E_b-E_a)^2+4h^2}} = \sqrt{(E_b-E_a)^2+4h^2},$ So

$$\langle H\rangle_{\min} = \frac{1}{2}\left[E_a + E_b \pm \sqrt{(E_b-E_a)^2+4h^2}\right] \quad \text{we want the minus sign (+ is maximum)}$$
$$= \boxed{\tfrac{1}{2}\left[E_a + E_b - \sqrt{(E_b-E_a)^2+4h^2}\right].}$$

(d) If h is small, the exact result (a) can be expanded: $E_\pm = \frac{1}{2}\left[(E_a+E_b) \pm (E_b - E_a)\sqrt{1+\frac{4h^2}{(E_b-E_a)^2}}\right]$.

$$\Longrightarrow E_\pm \approx \frac{1}{2}\left\{E_a + E_b \pm (E_b - E_a)\left[1 + \frac{2h^2}{(E_b-E_a)^2}\right]\right\} = \frac{1}{2}\left[E_a + E_b \pm (E_b - E_a) \pm \frac{2h^2}{(E_b-E_a)}\right],$$

so $\quad E_+ \approx E_b + \dfrac{h^2}{(E_b-E_a)}, \quad E_- \approx E_a - \dfrac{h^2}{(E_b-E_a)},$

confirming the perturbation theory results in (b). The variational principle (c) gets the ground state (E_-) *exactly* right—not too surprising since the trial wave function Eq. 8.75 is *almost* the most general state (there could be a relative phase factor $e^{i\theta}$).

Problem 8.23

For the electron, $\gamma = -e/m$, so $E_\pm = \pm eB_z\hbar/2m$ (Eq. 4.161). For consistency with Problem 8.22, $E_b > E_a$, so $\chi_b = \chi_+ = \begin{pmatrix}1\\0\end{pmatrix}, \quad \chi_a = \chi_- = \begin{pmatrix}0\\1\end{pmatrix}, \quad E_b = E_+ = \dfrac{eB_z\hbar}{2m}, \quad E_a = E_- = -\dfrac{eB_z\hbar}{2m}.$

(a)

$$\langle\chi_a|H'|\chi_a\rangle = \frac{eB_x}{m}\frac{\hbar}{2}\,(0\ 1)\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \frac{eB_x\hbar}{2m}\,(0\ 1)\begin{pmatrix}1\\0\end{pmatrix} = 0;$$

$$\langle\chi_b|H'|\chi_b\rangle = \frac{eB_x\hbar}{2m}\,(1\ 0)\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0; \quad \langle\chi_b|H'|\chi_a\rangle = \frac{eB_x\hbar}{2m}\,(1\ 0)\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \frac{eB_x\hbar}{2m};$$

$$\langle\chi_a|H'|\chi_b\rangle = \frac{eB_x\hbar}{2m}\,(0\ 1)\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{eB_x\hbar}{2m}\,(0\ 1)\begin{pmatrix}0\\1\end{pmatrix} = \frac{eB_x\hbar}{2m}. \quad \text{So} \quad \boxed{h = \frac{eB_x\hbar}{2m},}$$

and the conditions of Problem 8.22 are met.

(b) From Problem 8.22(b),

$$E_{\text{gs}} \approx E_a - \frac{h^2}{(E_b-E_a)} = -\frac{eB_z\hbar}{2m} - \frac{(eB_x\hbar/2m)^2}{(eB_z\hbar/m)} = \boxed{-\frac{e\hbar}{2m}\left(B_z + \frac{B_x^2}{2B_z}\right).}$$

(c) From Problem 8.22(c), $E_{\text{gs}} = \frac{1}{2}\left[E_a + E_b - \sqrt{(E_b-E_a)^2+4h^2}\right]$ (it's actually the *exact* ground state).

$$E_{\text{gs}} = -\frac{1}{2}\sqrt{\left(\frac{eB_z\hbar}{m}\right)^2 + 4\left(\frac{eB_x\hbar}{2m}\right)^2} = \boxed{-\frac{e\hbar}{2m}\sqrt{B_z^2+B_x^2}}$$

(which was obvious from the start, since the square root is simply the magnitude of the total field).

Problem 8.24

(a)

$$\mathbf{r_1} = \frac{1}{\sqrt{2}}(\mathbf{u}+\mathbf{v});\ \mathbf{r_2} = \frac{1}{\sqrt{2}}(\mathbf{u}-\mathbf{v});\ r_1^2 + r_2^2 = \frac{1}{2}(u^2 + 2\mathbf{u}\cdot\mathbf{v} + v^2 + u^2 - 2\mathbf{u}\cdot\mathbf{v} + v^2) = u^2 + v^2.$$

$$(\nabla_1^2 + \nabla_2^2) f(\mathbf{r_1}, \mathbf{r_2}) = \left(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial y_1^2} + \frac{\partial^2 f}{\partial z_1^2} + \frac{\partial^2 f}{\partial x_2^2} + \frac{\partial^2 f}{\partial y_2^2} + \frac{\partial^2 f}{\partial z_2^2}\right).$$

$$\frac{\partial f}{\partial x_1} = \frac{\partial f}{\partial u_x}\frac{\partial u_x}{\partial x_1} + \frac{\partial f}{\partial v_x}\frac{\partial v_x}{\partial x_1} = \frac{1}{\sqrt{2}}\left(\frac{\partial f}{\partial u_x} + \frac{\partial f}{\partial v_x}\right);\ \frac{\partial f}{\partial x_2} = \frac{\partial f}{\partial u_x}\frac{\partial u_x}{\partial x_2} + \frac{\partial f}{\partial v_x}\frac{\partial v_x}{\partial x_2} = \frac{1}{\sqrt{2}}\left(\frac{\partial f}{\partial u_x} - \frac{\partial f}{\partial v_x}\right).$$

$$\begin{aligned}
\frac{\partial^2 f}{\partial x_1^2} &= \frac{1}{\sqrt{2}}\frac{\partial}{\partial x_1}\left(\frac{\partial f}{\partial u_x} + \frac{\partial f}{\partial v_x}\right) = \frac{1}{\sqrt{2}}\left(\frac{\partial^2 f}{\partial u_x^2}\frac{\partial u_x}{\partial x_1} + \frac{\partial^2 f}{\partial u_x \partial v_x}\frac{\partial v_x}{\partial x_1} + \frac{\partial^2 f}{\partial v_x \partial u_x}\frac{\partial u_x}{\partial x_1} + \frac{\partial^2 f}{\partial v_x^2}\frac{\partial v_x}{\partial x_1}\right)\\
&= \frac{1}{2}\left(\frac{\partial^2 f}{\partial u_x^2} + 2\frac{\partial^2 f}{\partial u_x \partial v_x} + \frac{\partial^2 f}{\partial v_x^2}\right);\\
\frac{\partial^2 f}{\partial x_2^2} &= \frac{1}{\sqrt{2}}\frac{\partial}{\partial x_2}\left(\frac{\partial f}{\partial u_x} - \frac{\partial f}{\partial v_x}\right) = \frac{1}{\sqrt{2}}\left(\frac{\partial^2 f}{\partial u_x^2}\frac{\partial u_x}{\partial x_2} + \frac{\partial^2 f}{\partial u_x \partial v_x}\frac{\partial v_x}{\partial x_2} - \frac{\partial^2 f}{\partial v_x \partial u_x}\frac{\partial u_x}{\partial x_2} - \frac{\partial^2 f}{\partial v_x^2}\frac{\partial v_x}{\partial x_2}\right)\\
&= \frac{1}{2}\left(\frac{\partial^2 f}{\partial u_x^2} - 2\frac{\partial^2 f}{\partial u_x \partial v_x} + \frac{\partial^2 f}{\partial v_x^2}\right).
\end{aligned}$$

So $\left(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2}\right) = \left(\frac{\partial^2 f}{\partial u_x^2} + \frac{\partial^2 f}{\partial v_x^2}\right)$, and likewise for y and z: $\nabla_1^2 + \nabla_2^2 = \nabla_u^2 + \nabla_v^2$.

$$\begin{aligned}
H &= -\frac{\hbar^2}{2m}(\nabla_u^2 + \nabla_v^2) + \frac{1}{2}m\omega^2(u^2+v^2) - \frac{\lambda}{4}m\omega^2 2v^2\\
&= \left[-\frac{\hbar^2}{2m}\nabla_u^2 + \frac{1}{2}m\omega^2 u^2\right] + \left[-\frac{\hbar^2}{2m}\nabla_v^2 + \frac{1}{2}m\omega^2 v^2 - \frac{1}{2}\lambda m\omega^2 v^2\right]. \quad \text{QED}
\end{aligned}$$

(b) The energy is $\frac{3}{2}\hbar\omega$ (for the u part) and $\frac{3}{2}\hbar\omega\sqrt{1-\lambda}$ (for the v part): $\boxed{E_{\text{gs}} = \frac{3}{2}\hbar\omega\left(1+\sqrt{1-\lambda}\right).}$

(c) The ground state for a *one*-dimensional oscillator is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} \quad \text{(Eq. 2.60).}$$

So, for a 3-D oscillator, the ground state is $\psi_0(\mathbf{r}) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar}$, and for two particles

$$\psi(\mathbf{r_1}, \mathbf{r_2}) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} e^{-\frac{m\omega}{2\hbar}(r_1^2 + r_2^2)}. \quad \text{(This is the analog to Eq. 8.18.)}$$

$$\langle H\rangle = \frac{3}{2}\hbar\omega + \frac{3}{2}\hbar\omega + \langle V_{ee}\rangle = 3\hbar\omega + \langle V_{ee}\rangle \quad \text{(the analog to Eq. 8.20).}$$

$$\langle V_{ee}\rangle = -\frac{\lambda}{4}m\omega^2\left(\frac{m\omega}{\pi\hbar}\right)^3 \int e^{-\frac{m\omega}{\hbar}(r_1^2+r_2^2)} \underbrace{(\mathbf{r_1} - \mathbf{r_2})^2}_{r_1^2 - 2\mathbf{r_1}\cdot\mathbf{r_2} + r_2^2} d^3\mathbf{r}_1\, d^3\mathbf{r}_2 \quad \text{(the analog to Eq. 8.21).}$$

The $\mathbf{r_1}\cdot\mathbf{r_2}$ term integrates to zero, by symmetry, and the r_2^2 term is the same as the r_1^2 term, so

$$\begin{aligned}
\langle V_{ee}\rangle &= -\frac{\lambda}{4}m\omega^2\left(\frac{m\omega}{\pi\hbar}\right)^3 2\int e^{-\frac{m\omega}{\hbar}(r_1^2+r_2^2)}\,r_1^2\,d^3\mathbf{r}_1\,d^3\mathbf{r}_2 \\
&= -\frac{\lambda}{2}m\omega^2\left(\frac{m\omega}{\pi\hbar}\right)^3(4\pi)^2\int_0^\infty e^{-m\omega r_2^2/\hbar}\,r_2^2\,dr_2\int_0^\infty e^{-m\omega r_1^2/\hbar}\,r_1^4\,dr_1 \\
&= -\lambda\frac{8m^4\omega^5}{\pi\hbar^3}\left[\frac{1}{4}\frac{\hbar}{m\omega}\sqrt{\frac{\pi\hbar}{m\omega}}\right]\left[\frac{3}{8}\left(\frac{\hbar}{m\omega}\right)^2\sqrt{\frac{\pi\hbar}{m\omega}}\right] = -\frac{3}{4}\lambda\hbar\omega. \\
\langle H\rangle &= 3\hbar\omega-\frac{3}{4}\lambda\hbar\omega = \boxed{3\hbar\omega\left(1-\frac{\lambda}{4}\right).}
\end{aligned}$$

The variational principle says this must *exceed* the exact ground-state energy (b); let's check it:

$$3\hbar\omega\left(1-\frac{\lambda}{4}\right) > \frac{3}{2}\hbar\omega\left(1+\sqrt{1-\lambda}\right) \;\Leftrightarrow\; 2-\frac{\lambda}{2} > 1+\sqrt{1-\lambda} \;\Leftrightarrow\; 1-\frac{\lambda}{2} > \sqrt{1-\lambda} \;\Leftrightarrow\; 1-\lambda+\frac{\lambda^2}{4} > 1-\lambda.$$

It checks. In fact, expanding the exact answer in powers of λ, $E_{\text{gs}}\approx\frac{3}{2}\hbar\omega(1+1-\frac{1}{2}\lambda) = 3\hbar\omega\left(1-\frac{\lambda}{4}\right)$, we recover the variational result.

Problem 8.25

$$\begin{aligned}
1 &= \int|\psi|^2 d^3\mathbf{r}_1\,d^3\mathbf{r}_2 = |A|^2\left[\int\psi_1^2\,d^3\mathbf{r}_1\int\psi_2^2\,d^3\mathbf{r}_2 + 2\int\psi_1\psi_2\,d^3\mathbf{r}_1\int\psi_1\psi_2\,d^3\mathbf{r}_2 + \int\psi_2^2\,d^3\mathbf{r}_1\int\psi_1^2\,d^3\mathbf{r}_2\right] \\
&= |A|^2(1+2S^2+1),
\end{aligned}$$

where

$$S\equiv\int\psi_1(r)\psi_2(r)\,d^3\mathbf{r} = \frac{\sqrt{(Z_1Z_2)^3}}{\pi a^3}\int e^{-(Z_1+Z_2)r/a}4\pi r^2 dr = \frac{4}{a^3}\left(\frac{y}{2}\right)^3\left[\frac{2a^3}{(Z_1+Z_2)^3}\right] = \left(\frac{y}{x}\right)^3.$$

$$\boxed{A^2 = \frac{1}{2\left[1+(y/x)^6\right]}.}$$

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_1}+\frac{1}{r_2}\right) + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|},$$

$$\begin{aligned}
H\psi = A\Bigg\{&\left[-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)-\frac{e^2}{4\pi\epsilon_0}\left(\frac{Z_1}{r_1}+\frac{Z_2}{r_2}\right)\right]\psi_1(r_1)\psi_2(r_2) \\
&+\left[-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)-\frac{e^2}{4\pi\epsilon_0}\left(\frac{Z_1}{r_1}+\frac{Z_2}{r_2}\right)\right]\psi_2(r_1)\psi_1(r_2)\Bigg\} \\
&+A\frac{e^2}{4\pi\epsilon_0}\left\{\left[\frac{Z_1-1}{r_1}+\frac{Z_2-1}{r_2}\right]\psi_1(r_1)\psi_2(r_2)+\left[\frac{Z_2-1}{r_1}+\frac{Z_1-1}{r_2}\right]\psi_2(r_1)\psi_1(r_2)\right\}+V_{ee}\psi,
\end{aligned}$$

where $V_{ee}\equiv\dfrac{e^2}{4\pi\epsilon_0}\dfrac{1}{|\mathbf{r_1}-\mathbf{r_2}|}$.

The term in first curly brackets is $(Z_1^2 + Z_2^2)E_1\psi_1(r_1)\psi_2(r_2) + (Z_2^2 + Z_1^2)E_1\psi_2(r_1)\psi_1(r_2)$, so

$$H\psi = (Z_1^2 + Z_2^2)E_1\psi + A\frac{e^2}{4\pi\epsilon_0}\left\{\left[\frac{Z_1 - 1}{r_1} + \frac{Z_2 - 1}{r_2}\right]\psi_1(r_1)\psi_2(r_2) + \left[\frac{Z_2 - 1}{r_1} + \frac{Z_1 - 1}{r_2}\right]\psi_2(r_1)\psi_1(r_2)\right\} + V_{ee}\psi$$

$$\langle H\rangle = (Z_1^2 + Z_2^2)E_1 + \langle V_{ee}\rangle + A^2\left(\frac{e^2}{4\pi\epsilon_0}\right)$$
$$\times\left\{\langle\psi_1(r_1)\psi_2(r_2) + \psi_2(r_1)\psi_1(r_2)\left|\left(\left[\frac{Z_1 - 1}{r_1} + \frac{Z_2 - 1}{r_2}\right]\right|\psi_1(r_1)\psi_2(r_2)\rangle + \left[\frac{Z_2 - 1}{r_1} + \frac{Z_1 - 1}{r_2}\right]\right|\psi_2(r_1)\psi_1(r_2)\rangle\right)\right\}.$$

$$\begin{aligned}
\Big\{\Big\} &= (Z_1 - 1)\langle\psi_1(r_1)\left|\frac{1}{r_1}\right|\psi_1(r_1)\rangle + (Z_2 - 1)\langle\psi_2(r_2)\left|\frac{1}{r_2}\right|\psi_2(r_2)\rangle \\
&\quad + (Z_2 - 1)\langle\psi_1(r_1)\left|\frac{1}{r_1}\right|\psi_2(r_1)\rangle\langle\psi_2(r_2)|\psi_1(r_2)\rangle \\
&\quad + (Z_1 - 1)\langle\psi_1(r_1)|\psi_2(r_1)\rangle\langle\psi_2(r_2)\left|\frac{1}{r_2}\right|\psi_1(r_2)\rangle + (Z_1 - 1)\langle\psi_2(r_1)\left|\frac{1}{r_1}\right|\psi_1(r_1)\rangle\langle\psi_1(r_2)|\psi_2(r_2)\rangle \\
&\quad + (Z_2 - 1)\langle\psi_2(r_1)|\psi_1(r_1)\rangle\langle\psi_1(r_2)\left|\frac{1}{r_2}\right|\psi_2(r_2)\rangle + (Z_2 - 1)\langle\psi_2(r_1)\left|\frac{1}{r_1}\right|\psi_2(r_1)\rangle \\
&\quad + (Z_1 - 1)\langle\psi_1(r_2)\left|\frac{1}{r_2}\right|\psi_1(r_2)\rangle \\
&= 2(Z_1 - 1)\left\langle\frac{1}{r}\right\rangle_1 + 2(Z_2 - 1)\left\langle\frac{1}{r}\right\rangle_2 + 2(Z_1 - 1)\langle\psi_1|\psi_2\rangle\langle\psi_1\left|\frac{1}{r}\right|\psi_2\rangle + 2(Z_2 - 1)\langle\psi_1|\psi_2\rangle\langle\psi_1\left|\frac{1}{r}\right|\psi_2\rangle.
\end{aligned}$$

But $\left\langle\frac{1}{r}\right\rangle_1 = \langle\psi_1(r)\left|\frac{1}{r}\right|\psi_1(r)\rangle = \frac{Z_1}{a}$; $\left\langle\frac{1}{r}\right\rangle_2 = \frac{Z_2}{a}$, so $\langle H\rangle = (Z_1^2 + Z_2^2)E_1$

$$+ A^2\left(\frac{e^2}{4\pi\epsilon_0}\right)2\left[\frac{1}{a}(Z_1 - 1)Z_1 + \frac{1}{a}(Z_2 - 1)Z_2 + (Z_1 + Z_2 - 2)\langle\psi_1|\psi_2\rangle\langle\psi_1\left|\frac{1}{r}\right|\psi_2\rangle\right] + \langle V_{ee}\rangle.$$

And $\langle\psi_1|\psi_2\rangle = S = (y/x)^3$, so

$$\langle\psi_1\left|\frac{1}{r}\right|\psi_2\rangle = \frac{\sqrt{(Z_1Z_2)^3}}{\pi a^3}4\pi\int e^{-(Z_1+Z_2)r/a}\,r\,dr = \frac{y^3}{2a^3}\left[\frac{a}{Z_1 + Z_2}\right]^2 = \frac{y^3}{2ax^2}.$$

$$\begin{aligned}
\langle H\rangle &= (x^2 - \frac{1}{2}y^2)E_1 + A^2\left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{2}{a}\left\{\left[Z_1^2 + Z_2^2 - (Z_1 + Z_2)\right] + (x - 2)\left(\frac{y}{x}\right)^3\frac{y^3}{2x^2}\right\} + \langle V_{ee}\rangle \\
&= (x^2 - \frac{1}{2}y^2)E_1 - 4E_1A^2\left[x^2 - \frac{1}{2}y^2 - x + \frac{1}{2}(x - 2)\frac{y^6}{x^5}\right] + \langle V_{ee}\rangle.
\end{aligned}$$

$$\begin{aligned}
\langle V_{ee}\rangle &= \frac{e^2}{4\pi\epsilon_0}\langle\psi\left|\frac{1}{|\mathbf{r_1} - \mathbf{r_2}|}\right|\psi\rangle \\
&= \left(\frac{e^2}{4\pi\epsilon_0}\right)A^2\langle\psi_1(r_1)\psi_2(r_2) + \psi_2(r_1)\psi_1(r_2)\left|\frac{1}{|\mathbf{r_1} - \mathbf{r_2}|}\right|\psi_1(r_1)\psi_2(r_2) + \psi_2(r_1)\psi_1(r_2)\rangle \\
&= \left(\frac{e^2}{4\pi\epsilon_0}\right)A^2\left[2\langle\psi_1(r_1)\psi_2(r_2)\left|\frac{1}{|\mathbf{r_1} - \mathbf{r_2}|}\right|\psi_1(r_1)\psi_2(r_2)\rangle + 2\langle\psi_1(r_1)\psi_2(r_2)\left|\frac{1}{|\mathbf{r_1} - \mathbf{r_2}|}\right|\psi_2(r_1)\psi_1(r_2)\rangle\right] \\
&= 2\left(\frac{e^2}{4\pi\epsilon_0}\right)A^2(B + C), \text{ where}
\end{aligned}$$

$$B \equiv \langle\psi_1(r_1)\psi_2(r_2)\left|\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}\right|\psi_1(r_1)\psi_2(r_2)\rangle; \quad C \equiv \langle\psi_1(r_1)\psi_2(r_2)\left|\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}\right|\psi_2(r_1)\psi_1(r_2)\rangle.$$

$$B = \frac{Z_1^3 Z_2^3}{(\pi a^3)^2}\int e^{-2Z_1r_1/a}e^{-2Z_2r_2/a}\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}\,d^3\mathbf{r}_1\,d^3\mathbf{r}_2.$$ As on page 334, the $\mathbf{r}_2$ integral is

$$\int e^{-2Z_2r_2/a}\frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}}\,d^3\mathbf{r}_2$$
$$= \frac{\pi a^3}{Z_2^3 r_1}\left[1-\left(1+\frac{Z_2r_1}{a}\right)e^{-2Z_2r_1/a}\right] \quad \text{(Eq. 8.25, but with } a\to\frac{2}{Z_2}a).$$

$$B = \frac{Z_1^3Z_2^3}{(\pi a^3)^2}\frac{(\pi a^3)}{Z_2^3}4\pi\int_0^\infty e^{-2Z_1r_1/a}\frac{1}{r_1}\left[1-\left(1+\frac{Z_2r_1}{a}\right)e^{-2Z_2r_1/a}\right]r_1^2\,dr_1$$
$$= \frac{4Z_1^3}{a^3}\int_0^\infty\left[r_1e^{-2Z_1r_1/a}-r_1e^{-2(Z_1+Z_2)r_1/a}-\frac{Z_2}{a}r_1^2e^{-2(Z_1+Z_2)r_1/a}\right]dr_1$$
$$= \frac{4Z_1^3}{a^3}\left[\left(\frac{a}{2Z_1}\right)^2-\left(\frac{a}{2(Z_1+Z_2)}\right)^2-\frac{Z_2}{a}2\left(\frac{a}{2(Z_1+Z_2)}\right)^3\right] = \frac{Z_1^3}{a}\left(\frac{1}{Z_1^2}-\frac{1}{(Z_1+Z_2)^2}-\frac{Z_2}{(Z_1+Z_2)^3}\right)$$
$$= \frac{Z_1Z_2}{a(Z_1+Z_2)}\left[1+\frac{Z_1Z_2}{(Z_1+Z_2)^2}\right] = \frac{y^2}{4ax}\left(1+\frac{y^2}{4x^2}\right).$$

$$C = \frac{Z_1^3Z_2^3}{(\pi a^3)^2}\int e^{-Z_1r_1/a}e^{-Z_2r_2/a}e^{-Z_2r_1/a}e^{-Z_1r_2/a}\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}\,d^3\mathbf{r}_1\,d^3\mathbf{r}_2$$
$$= \frac{(Z_1Z_2)^3}{(\pi a^3)^2}\int e^{-(Z_1+Z_2)(r_1+r_2)/a}\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}\,d^3\mathbf{r}_1\,d^3\mathbf{r}_2.$$

The integral is the same as in Eq. 8.21, only with $a\to\frac{4}{Z_1+Z_2}a$. Comparing Eqs. 8.21 and 8.26, we see that the integral itself was

$$\frac{5}{4a}\left(\frac{\pi a^3}{8}\right)^2 = \frac{5}{256}\pi^2a^5. \quad \text{So} \quad C = \frac{(Z_1Z_2)^3}{(\pi a^3)^2}\frac{5\pi^2}{256}\frac{4^5a^5}{(Z_1+Z_2)^5} = \frac{20}{a}\frac{(Z_1Z_2)^3}{(Z_1+Z_2)^5} = \frac{5}{16a}\frac{y^6}{x^5}.$$

$$\langle V_{ee}\rangle = 2\left(\frac{e^2}{4\pi\epsilon_0}\right)A^2\left[\frac{y^2}{4ax}\left(1+\frac{y^2}{4x^2}\right)+\frac{5}{16a}\frac{y^6}{x^5}\right] = 2A^2(-2E_1)\frac{y^2}{4x}\left(1+\frac{y^2}{4x^2}+\frac{5y^4}{4x^4}\right).$$

$$\langle H\rangle = E_1\left\{x^2-\frac{1}{2}y^2-\frac{2}{[1+(y/x)^6]}\left[x^2-\frac{1}{2}y^2-x+\frac{1}{2}(x-2)\frac{y^6}{x^5}\right]-\frac{2}{[1+(y/x)^6]}\frac{y^2}{4x}\left(1+\frac{y^2}{4x^2}+\frac{5y^4}{4x^4}\right)\right\}$$
$$= \frac{E_1}{(x^6+y^6)}\left\{(x^2-\frac{1}{2}y^2)(x^6+y^6)-2x^6\left[x^2-\frac{1}{2}y^2-x+\frac{1}{2}\frac{y^6}{x^4}-\frac{y^6}{x^5}+\frac{y^2}{4x}+\frac{y^4}{16x^3}+\frac{5y^6}{16x^5}\right]\right\}$$
$$= \frac{E_1}{(x^6+y^6)}\left(x^8+x^2y^6-\frac{1}{2}x^6y^2-\frac{1}{2}y^8-2x^8+x^6y^2+2x^7-x^2y^6+2xy^6-\frac{1}{2}x^5y^2-\frac{1}{8}x^3y^4-\frac{5}{8}xy^6\right)$$
$$= \boxed{\frac{E_1}{(x^6+y^6)}\left(-x^8+2x^7+\frac{1}{2}x^6y^2-\frac{1}{2}x^5y^2-\frac{1}{8}x^3y^4+\frac{11}{8}xy^6-\frac{1}{2}y^8\right).}$$

Mathematica finds the minimum of $\langle H\rangle$ at $x = 1.32245,\ y = 1.08505$, corresponding to $Z_1 = 1.0392,\ Z_2 = 0.2832$. At this point, $\boxed{\langle H\rangle_{\min} = 1.0266E_1 = -13.962 \text{ eV},}$ which *is* less than -13.6 eV—but not by much!

Problem 8.26

The calculation is the same as before, but with $m_e \to m_r$, the reduced mass of the muon:

$$m_r = \frac{m_\mu m_d}{m_\mu + m_d} = \frac{m_\mu 2m_p}{m_\mu + 2m_p} = \frac{m_\mu}{1 + m_\mu/2m_p}.$$

From Problem 7.32, $m_\mu = 207m_e$, so

$$1 + \frac{m_\mu}{2m_p} = 1 + \frac{207}{2}\frac{(9.11 \times 10^{-31})}{(1.67 \times 10^{-27})} = 1.056; \quad m_r = \frac{207m_e}{1.056} = 196m_e.$$

This shrinks the muonic "Bohr radius" down by a factor of nearly 200. Equation 8.50 is still valid, but now E_1 is the ground state energy of the muonic "atom." The potential energy associated with the deuteron-deuteron repulsion is the same as V_{pp} (Eq. 8.51), and since the product aE_1 is independent of mass, it doesn't matter whether we write it using the electron values or the muon values. Thus Eq. 8.52 still holds, and the entire molecule shrinks by that same factor of 196. The equilibrium separation for the electron case was $2.493a$ (Problem 8.11), so for muons

$$R = \frac{2.493}{196}(0.529 \times 10^{-10}\,\text{m}) = \boxed{6.73 \times 10^{-13}\,\text{m}.}$$

Problem 8.27

(a)

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}\right) = E\psi. \quad \text{Let } \psi(x,y) = X(x)Y(y).$$

$$Y\frac{d^2X}{dx^2} + X\frac{d^2Y}{dy^2} = -\frac{2mE}{\hbar^2}XY; \quad \frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} = -\frac{2mE}{\hbar^2}.$$

$\displaystyle\frac{d^2X}{dx^2} = -k_x^2X; \quad \frac{d^2Y}{dy^2} = -k_y^2Y, \quad \text{with} \quad k_x^2 + k_y^2 = \frac{2mE}{\hbar^2}.$ The general solution to the y equation is

$Y(y) = A\cos k_y y + B\sin k_y y$; the boundary conditions $Y(\pm a) = 0$ yield $k_y = \dfrac{n\pi}{2a}$ with minimum $\dfrac{\pi}{2a}$.

[Note that k_y^2 has to be positive, or you cannot meet the boundary conditions at all.] So

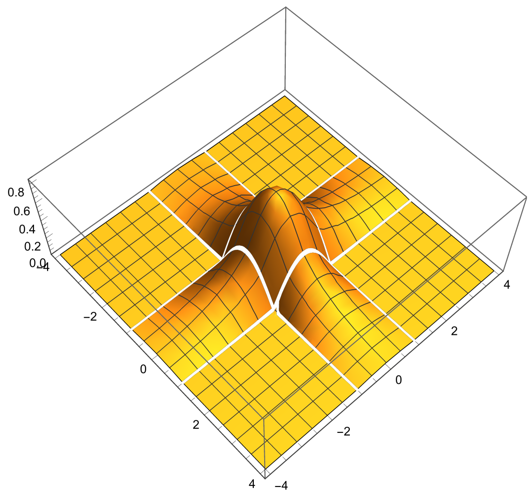
$E \geq \dfrac{\hbar^2}{2m}\left(k_x^2 + \dfrac{\pi^2}{4a^2}\right)$. For a traveling wave k_x^2 has to be positive. *Conclusion:* Any solution with $E <$ $\boxed{\dfrac{\pi^2\hbar^2}{8ma^2}}$ will be a bound state.

(b) Here's a graph of $\psi(x,y)$:

```
a = 0.9
0.9

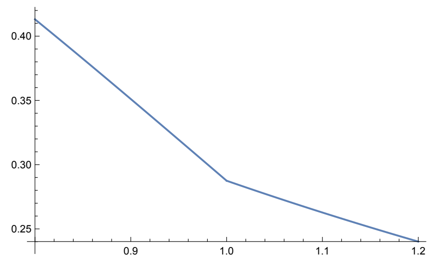
g[x_, y_] :=
 Piecewise[{{(Cos[π x/2] + Cos[π y/2]) ⅇ^(-a), Abs[x] < 1 && Abs[y] < 1},
   {(Cos[π x/2]) ⅇ^(-a Abs[y]) , Abs[x] < 1 && Abs[y] > 1},
   {(Cos[π y/2]) ⅇ^(-a Abs[x]), Abs[x] > 1 && Abs[y] < 1}}]

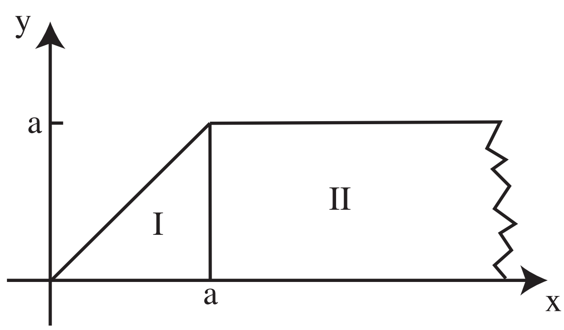
Plot3D[g[x, y], {x, -4, 4}, {y, -4, 4}, PlotRange -> {0, .85}]
```



It has roof-lines along the edges of the central square, as you can see by plotting $g[x, 0.5]$ across the kink:

```
j[x_] := g[x, .5]
Plot[j[x], {x, .8, 1.2}]
```





To normalize, we integrate $|\psi(x, y)|^2$ over regions I and II (in the figure), and multiply by 8.

$$
\begin{aligned}
I_{II} &= A^2 \int_{x=a}^{\infty} \int_{y=0}^{a} \cos^2\left(\frac{\pi y}{2a}\right) e^{-2\alpha x/a} dx\, dy \\
&= A^2 \left\{ -\frac{a}{2\alpha} e^{-2\alpha x/a} \Big|_a^{\infty} \right\} \left\{ \frac{1}{2(\pi/2a)} \sin\left(\frac{\pi y}{2a}\right) \cos\left(\frac{\pi y}{2a}\right) + \frac{1}{2} y \Big|_0^a \right\} \\
&= A^2 \left\{ \frac{a}{2\alpha} e^{-2\alpha} \right\} \left\{ 0 + \frac{1}{2} a \right\} = A^2 \frac{a^2}{4\alpha} e^{-2\alpha}.
\end{aligned}
$$

$$
\begin{aligned}
I_I &= \frac{1}{2}A^2\int_{x=0}^{a}\int_{y=0}^{a}\left[\cos\left(\frac{\pi x}{2a}\right)+\cos\left(\frac{\pi y}{2a}\right)\right]^2 e^{-2\alpha}dx\,dy \\
&= \frac{1}{2}A^2e^{-2\alpha}\left\{2\int_0^a \cos^2\left(\frac{\pi x}{2a}\right)\,dx\int_0^a dy + 2\int_0^a \cos\left(\frac{\pi x}{2a}\right)\,dx\int_0^a \cos\left(\frac{\pi y}{2a}\right)\,dy\right\} \\
&= A^2e^{-2\alpha}\left\{\left(\frac{a}{2}\right)a+\left[\frac{2a}{\pi}\sin\left(\frac{\pi x}{2a}\right)\Big|_0^a\right]^2\right\} = A^2\frac{a^2}{2}e^{-2\alpha}\left(1+\frac{8}{\pi^2}\right).
\end{aligned}
$$

Normalizing:

$$
1 = 8(I_I+I_{II}) = 8A^2a^2e^{-2\alpha}\left[\frac{1}{4\alpha}+\frac{1}{2}\left(1+\frac{8}{\pi^2}\right)\right] = 4A^2a^2e^{-2\alpha}\left(1+\frac{8}{\pi^2}+\frac{1}{2\alpha}\right),
$$

so

$$
A^2 = \frac{e^{2\alpha}}{4a^2\left(1+\frac{8}{\pi^2}+\frac{1}{2\alpha}\right)}.
$$

Next, ignoring the roof-lines for the moment, we calculate $\langle H\rangle_a = -8\frac{\hbar^2}{2m}(J_I+J_{II})$, where

$$
\begin{aligned}
J_{II} &= A^2\int_{x=a}^{\infty}\int_{y=0}^{a}\left[\cos\left(\frac{\pi y}{2a}\right)e^{-\alpha x/a}\right]\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\left[\cos\left(\frac{\pi y}{2a}\right)e^{-\alpha x/a}\right]\,dx\,dy \\
&= \left[\left(\frac{\alpha}{a}\right)^2-\left(\frac{\pi}{2a}\right)^2\right]I_{II} = A^2\frac{1}{4\alpha}\left(\alpha^2-\frac{\pi^2}{4}\right)e^{-2\alpha}.
\end{aligned}
$$

$$
\begin{aligned}
J_I &= \frac{1}{2}A^2\int_{x=0}^{a}\int_{y=0}^{a}\left[\cos\left(\frac{\pi x}{2a}\right)+\cos\left(\frac{\pi y}{2a}\right)\right]e^{-\alpha}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\left[\cos\left(\frac{\pi x}{2a}\right)+\cos\left(\frac{\pi y}{2a}\right)\right]e^{-\alpha}\,dx\,dy \\
&= -\frac{\pi^2}{4a^2}I_I = -A^2\left(1+\frac{\pi^2}{8}\right)e^{-2\alpha}.
\end{aligned}
$$

So far, then,

$$
\begin{aligned}
\langle H\rangle_a &= -8\frac{\hbar^2}{2m}\left[-A^2\left(1+\frac{\pi^2}{8}\right)e^{-2\alpha}+A^2\frac{1}{4\alpha}\left(\alpha^2-\frac{\pi^2}{4}\right)e^{-2\alpha}\right] \\
&= \frac{\hbar^2}{2m}A^2e^{-2\alpha}\left(8+\pi^2-2\alpha+\frac{\pi^2}{2\alpha}\right).
\end{aligned}
$$

Now the roof-lines, along the four sides of the central square: $\langle H\rangle_b = -8\frac{\hbar^2}{2m}J_{III}$, where

$$
\begin{aligned}
J_{III} &= \int_{x=a-\epsilon}^{a+\epsilon}\int_{y=0}^{a}\psi(x,y)\left(\frac{\partial^2}{\partial x^2}\right)\psi(x,y)\,dx\,dy \\
&= A\int_{y=0}^{a}\psi(a,y)\left\{\frac{\partial}{\partial x}\left[\cos\left(\frac{\pi y}{2a}\right)e^{-\alpha x/a}\right]\Big|_{x=a} - \frac{\partial}{\partial x}\left[\cos\left(\frac{\pi x}{2a}\right)e^{-\alpha}\right]\Big|_{x=a}\right\}dy \\
&= A^2\int_{y=0}^{a}\left[\cos\left(\frac{\pi y}{2a}\right)e^{-\alpha}\right]\left\{-\frac{\alpha}{a}\cos\left(\frac{\pi y}{2a}\right)e^{-\alpha}+\frac{\pi}{2a}\sin\left(\frac{\pi}{2}\right)e^{-\alpha}\right\}dy \\
&= A^2\frac{1}{a}e^{-2\alpha}\int_0^a\left[\frac{\pi}{2}\cos\left(\frac{\pi y}{2a}\right)-\alpha\cos^2\left(\frac{\pi y}{2a}\right)\right]\,dy = A^2e^{-2\alpha}\left(1-\frac{\alpha}{2}\right),
\end{aligned}
$$

so

$$\langle H\rangle_b = -8\frac{\hbar^2}{2m}A^2e^{-2\alpha}\left(1-\frac{\alpha}{2}\right) = \frac{\hbar^2}{2m}A^2e^{-2\alpha}4(\alpha-2).$$

Putting it all together,

$$\begin{aligned}
\langle H\rangle = \langle H\rangle_a + \langle H\rangle_b &= \frac{\hbar^2}{2m}A^2e^{-2\alpha}\left(8+\pi^2-2\alpha+\frac{\pi^2}{2\alpha}\right) + \frac{\hbar^2}{2m}A^2e^{-2\alpha}(4\alpha-8)\\
&= \frac{\hbar^2}{2m}A^2e^{-2\alpha}\left(\pi^2+\frac{\pi^2}{2\alpha}+2\alpha\right) = \frac{\hbar^2}{2m}\left[\frac{\pi^2+\frac{\pi^2}{2\alpha}+2\alpha}{4a^2\left(1+\frac{8}{\pi^2}+\frac{1}{2\alpha}\right)}\right]\\
&= \frac{\hbar^2}{ma^2}\left[\frac{\pi^2}{8}-\left(\frac{1-(\alpha/4)}{1+(8/\pi^2)+(1/2\alpha)}\right)\right].
\end{aligned}$$

Minimizing:

$$\frac{d\langle H\rangle}{d\alpha} = 0 \quad\Rightarrow\quad \frac{d}{d\alpha}\left(\frac{4-\alpha}{1+(8/\pi^2)+(1/2\alpha)}\right) = 0;$$

$$\frac{-1}{1+(8/\pi^2)+(1/2\alpha)} - \frac{4-\alpha}{(1+(8/\pi^2)+(1/2\alpha))^2}\left(\frac{-1}{2\alpha^2}\right) = 0;$$

$$1+(8/\pi^2)+(1/2\alpha) - \frac{4-\alpha}{2\alpha^2} = 0\,; \quad \alpha^2\left(1+\frac{8}{\pi^2}\right)+\alpha-2 = 0;$$

$$\alpha = \frac{-1\pm\sqrt{1+8[1+(8/\pi^2)]}}{2[1+(8/\pi^2)]} = \frac{-1+\sqrt{9+(8/\pi)^2}}{2[1+(8/\pi^2)]} = 0.81053$$

(note that α must be *positive*). Putting this value of α into the expression for $\langle H\rangle$, we get

$$\boxed{\langle H\rangle_{\min} = 0.905221\frac{\hbar^2}{ma^2}.}$$

But $E_{\text{threshold}} = \dfrac{\pi^2}{8}\dfrac{\hbar^2}{ma^2} = 1.2337\dfrac{\hbar^2}{ma^2}$, so E_0 is definitely *less* than $E_{\text{threshold}}$.

Problem 8.28

(a) To normalize the variational state

$$\begin{aligned}
1 &= \int |\psi_\beta(\mathbf{r})|^2\, d^3\mathbf{r}\\
&= A^2\,4\,\pi\int_0^\infty e^{-2\,\beta\,r/r_0}\,r^2\,dr\\
&= A^2\,4\,\pi\left(\frac{r_0}{2\,\beta}\right)^3\int_0^\infty e^{-z}\,z^2\,dz\\
&= A^2\,\frac{\pi\,r_0^3}{\beta^3}
\end{aligned}$$

and

$$\boxed{A = \sqrt{\frac{\beta^3}{\pi\, r_0^3}}\,.}$$

(b) Now we calculate the expectation value of the Hamiltonian:

$$\begin{aligned}
\langle H \rangle &= \int\!\!\int \psi_\beta^*(r) \left[-\frac{\hbar^2}{2\,\mu} \frac{1}{r^2} \left(r^2 \frac{\partial \psi_\beta}{\partial r} \right) - r_0\, V_0\, \frac{e^{-r/r_0}}{r}\, \psi_\beta(r) \right] r^2\, dr\, d\Omega \\
&= 4\,\pi\, A^2 \left(\int_0^\infty e^{-\beta\, r/r_0} \left[\frac{\hbar^2}{2\,\mu} \frac{\beta}{r_0^2} \left(\frac{2\, r_0}{r} - \beta \right) e^{-\beta\, r/r_0} \right] r^2\, dr \right. \\
&\quad \left. - r_0\, V_0 \int e^{-(2\,\beta+1)\, r/r_0}\, r\, dr \right) .
\end{aligned}$$

In the first integral we let $z = 2\,\beta\, r/r_0$ and in the second integral we let $z = (2\,\beta + 1)\ r/r_0$ to get

$$\begin{aligned}
\langle H \rangle &= \frac{4\,\beta^3}{r_0^3} \left[\frac{\hbar^2\, r_0}{4\,\mu\,\beta} \int_0^\infty \left(z - \frac{1}{4}\, z^2 \right) e^{-z}\, dz - \frac{r_0^3\, V_0}{(2\,\beta+1)^2} \int_0^\infty z\, e^{-z}\, dz \right] \\
&= \frac{4\,\beta^3}{r_0^3} \left[\frac{\hbar^2\, r_0}{4\,\mu\,\beta} \left(1 - \frac{1}{2} \right) - \frac{r_0^3\, V_0}{(2\,\beta+1)^2} \right] \\
&= \frac{\hbar^2\, \beta^2}{2\,\mu\, r_0^2} - \frac{4\,\beta^3}{(2\,\beta+1)^2} \frac{\hbar^2\, \gamma}{2\,\mu\, r_0^2}
\end{aligned}$$

which can be put in the desired form:

$$\boxed{E(\beta) = \frac{\hbar^2}{2\,\mu\, r_0^2}\, \beta^2 \left[1 - \frac{4\,\beta\,\gamma}{(2\,\beta+1)^2} \right] .}$$

(c)] Finding the value of β that minimizes the energy:

$$\begin{aligned}
\frac{dE(\beta)}{d\beta} &= 0 \\
\frac{\hbar^2}{2\,\mu\, r_0^2} \left[2\,\beta - \frac{12\,\beta^2\,\gamma}{(2\,\beta+1)^2} + 2\, \frac{4\,\beta^3\,\gamma}{(2\,\beta+1)^3}\, 2 \right] &= 0 \\
(2\,\beta+1)^3 - 6\,\beta\,(2\,\beta+1)\ \gamma + 8\,\beta^2\,\gamma &= 0 \\
(2\,\beta+1)^3 - 2\,\beta\,(3 + 2\,\beta)\ \gamma &= 0\,.
\end{aligned}$$

Solving this for γ,

$$\gamma = \frac{(2\,\beta+1)^3}{2\,\beta\,(3+2\,\beta)}\,,$$

and plugging back into our expression for the energy we have

$$\begin{aligned}
E_{\text{min}} &= \frac{\hbar^2}{2\,\mu\, r_0^2}\, \beta^2 \left[1 - \frac{4\,\beta}{(2\,\beta+1)^2} \frac{(2\,\beta+1)^3}{2\,\beta} \right] \\
&= \frac{\hbar^2}{2\,\mu\, r_0^2}\, \beta^2 \left[1 - \frac{4\,\beta}{(2\,\beta+1)^2} \frac{(2\,\beta+1)^3}{2\,\beta\,(3+2\,\beta)} \right]
\end{aligned}$$

which simplifies to

$$\boxed{E_{\text{min}} = \frac{\hbar^2\,\beta^2}{2\,\mu\,r_0^2}\,\frac{1-2\,\beta}{3+2\,\beta}\,.}$$

(d) From our plot we see that $E_{\text{min}} < 0$ for $\beta > 1/2$. We can turn this into a value for γ; there will be a negative-energy (or bound) state when

$$\gamma > \frac{(2\cdot 1/2 + 1)^3}{2\cdot 1/2\,(3 + 2\cdot 1/2)} = 2$$

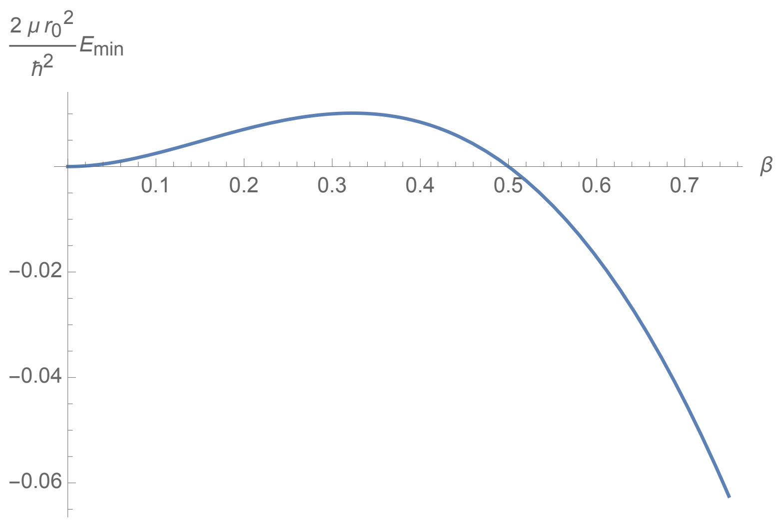
which in turn means

$$\frac{2\,\mu_0\,r_0^2}{\hbar^2}\,V_0 > 2$$

or

$$\boxed{V_0 > \frac{\hbar^2}{\mu r_0^2} = 2\,\frac{\left(m_\pi\,c^2\right)^2}{m_p\,c^2} = 42\,\text{MeV}\,.}$$

So we know there is a bound state for $V_0 > 42\,\text{MeV}$ but a better variational wave function could show a bound state for a smaller value of V_0.



Problem 8.29

(a) Let ψ_1 be the true ground state (with energy E_1) of the Hamiltonian with potential V_1 and use it as the variational wave function for the Hamiltonian with potential V_2. The true ground state energy of this second Hamiltonian then satisfies

$$\begin{aligned}
E_2 &\le \int_{-\infty}^{\infty} \psi_1^*(x) \left[-\frac{\hbar^2}{2\,m} + V_2(x)\right] \psi_1(x)\;dx \\
&= \int_{-\infty}^{\infty} \psi_1^*(x) \left[-\frac{\hbar^2}{2\,m} + V_1(x)\right] \psi_1(x)\;dx \\
&\quad + \int_{-\infty}^{\infty} \psi_1^*(x)\;[V_2(x) - V_1(x)]\;\psi_1(x)\;dx \\
&= E_1 + \int_{-\infty}^{\infty} |\psi_1(x)|^2\;[V_2(x) - V_1(x)]\;dx\,.
\end{aligned}$$

Now since $V_2(x) < V_1(x)$ for all x we have

$$E_2 \le E_1 - \int_{-\infty}^{\infty} |\psi_1(x)|^2\;|V_2(x) - V_1(x)|\;dx \le E_1$$

since the remaining integral is clearly non-negative in this expression. That means that if the ground state of E_1 is negative (meaning it has a bound state), then so is the ground state of E_2, and it has a bound state as well.

(b) A finite potential well of arbitrarily small width a and arbitrarily small depth V_0 has a bound state, as shown in Section 2.6. Now for any potential, one can place a finite square well inside it as long as you make it narrow and shallow enough, and since that finite well has a bound state, so does the potential of interest by part (a).

(c) The theorem of course generalizes to any dimension. Just replace dx by $d^d\mathbf{r}$, nothing else changes. The corollary though only extends to two dimensions because a finite well of arbitrarily small depth and width binds a state in two dimensions, but not in three.

Problem 8.30

(a)

$$\frac{\partial \mathcal{E}}{\partial c_j^*} = \frac{\sum_n H_{jn}\,c_n}{\sum_n |c_n|^2} - \frac{\sum_{nm} c_m^*\,H_{mn}\,c_n}{(\sum_n |c_n|^2)^2}\,c_j = 0,$$

or, multiplying by $\sum_n |c_n|^2$,

$$\sum_n H_{jn}\,c_n - \mathcal{E}\,c_j = 0. \quad \checkmark$$

(b)

$$\frac{\partial \mathcal{E}}{\partial c_j} = \frac{\sum_m c_m^*\,H_{mj}}{\sum_n |c_n|^2} - \frac{\sum_{nm} c_m^*\,H_{mn}\,c_n}{(\sum_n |c_n|^2)^2}\,c_j^* = 0, \quad \Rightarrow \quad \sum_m c_m^* H_{mj} = \mathcal{E}\,c_j^*.$$

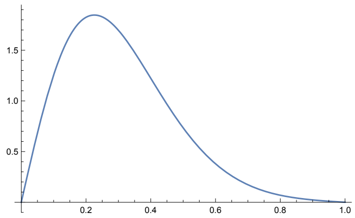
Taking the complex conjugate of both sides:

$$\sum_m c_m^* H_{mj}^* = \mathcal{E}^*\,c_j.$$

But H is Hermitian, so $H_{mj}^* = H_{jm}$, and $\mathcal{E}^* = \mathcal{E}$, and hence $\displaystyle\sum_m H_{jm}\,c_m - \mathcal{E}\,c_j = 0. \quad \checkmark$

(c) The lowest bound on the ground state energy is $39.982\,\hbar^2/ma^2$. See Mathematica output below.

```
a = ħ = m = 1;
V[x_] := 100 x;
Psi[n_, x_] := Sqrt[2/a] Sin[n Pi x / a];
f[n_, p_] = FullSimplify[Integrate[Psi[n, x] V[x] Psi[p, x], {x, 0, a}]];
fD[n_] = FullSimplify[Integrate[Psi[n, x] V[x] Psi[n, x], {x, 0, a}]];
Num = 10;
H = 1. Table[If[p == n, (n^2 π^2)/(2 m ħ^2) + fD[n], f[n, p]], {n, 1, Num}, {p, 1, Num}] // Chop;
E0 = Last[Eigenvalues[H]]
39.982
c = Normalize[Last[Eigenvectors[H]]];
c = c/Sign[c[[1]]];
ψ[x_] = Sum[c[[i]] Psi[i, x], {i, 1, Num}];
plot1 = Plot[ψ[x], {x, 0, 1}];
Show[plot1]
```



Chapter 9

The WKB Approximation

Problem 9.1

$$\int_0^a p(x)\,dx = n\pi\hbar, \quad \text{with } n = 1,2,3,\dots \text{ and } \quad p(x) = \sqrt{2m[E - V(x)]} \quad \text{(Eq. 9.17).}$$

Here $\displaystyle\int_0^a p(x)\,dx = \sqrt{2mE}\left(\frac{a}{2}\right) + \sqrt{2m(E-V_0)}\left(\frac{a}{2}\right) = \sqrt{2m}\left(\frac{a}{2}\right)\left(\sqrt{E} + \sqrt{E-V_0}\right) = n\pi\hbar$

$$\Rightarrow E + E - V_0 + 2\sqrt{E(E-V_0)} = \frac{4}{2m}\left(\frac{n\pi\hbar}{a}\right)^2 = 4E_n^0; \quad 2\sqrt{E(E-V_0)} = (4E_n^0 - 2E + V_0).$$

Square again: $4E(E-V_0) = 4E^2 - 4EV_0 = 16{E_n^0}^2 + 4E^2 + V_0^2 - 16EE_n^0 + 8E_n^0V_0 - 4EV_0$

$$\Rightarrow 16EE_n^0 = 16{E_n^0}^2 + 8E_n^0V_0 + V_0^2 \Rightarrow \boxed{E_n = E_n^0 + \frac{V_0}{2} + \frac{V_0^2}{16E_n^0}.}$$

Perturbation theory gave $E_n = E_n^0 + \dfrac{V_0}{2}$; the extra term goes to zero for very small V_0, or (since $E_n^0 \sim n^2$), for large n.

Problem 9.2

(a)

$$\frac{d\psi}{dx} = \frac{i}{\hbar}f'e^{if/\hbar}; \quad \frac{d^2\psi}{dx^2} = \frac{i}{\hbar}\left(f''e^{if/\hbar} + \frac{i}{\hbar}(f')^2e^{if/\hbar}\right) = \left[\frac{i}{\hbar}f'' - \frac{1}{\hbar^2}(f')^2\right]e^{if/\hbar}.$$

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi \Longrightarrow \left[\frac{i}{\hbar}f'' - \frac{1}{\hbar^2}(f')^2\right]e^{if/\hbar} = -\frac{p^2}{\hbar^2}e^{if/\hbar} \Longrightarrow i\hbar f'' - (f')^2 + p^2 = 0. \quad \text{QED}$$

(b) $f' = f_0' + \hbar f_1' + \hbar^2 f_2' + \cdots \Longrightarrow (f')^2 = (f_0' + \hbar f_1' + \hbar^2 f_2' + \cdots)^2 = (f_0')^2 + 2\hbar f_0'f_1' + \hbar^2[2f_0'f_2' + (f_1')^2] + \cdots$

$f'' = f_0'' + \hbar f_1'' + \hbar^2 f_2'' + \cdots$. $\quad i\hbar(f_0'' + \hbar f_1'' + \hbar^2 f_2'') - (f_0')^2 - 2\hbar f_0'f_1' - \hbar^2[2f_0'f_2' + (f_1')^2] + p^2 + \cdots = 0.$

$\hbar^0:\ (f_0')^2 = p^2; \quad \hbar^1:\ if_0'' = 2f_0'f_1'; \quad \hbar^2:\ if_1'' = 2f_0'f_2' + (f_1')^2; \quad \dots$

(c) $\dfrac{df_0}{dx} = \pm p \Longrightarrow f_0 = \pm\displaystyle\int p(x)dx + \text{constant}$; $\dfrac{df_1}{dx} = \dfrac{i}{2}\dfrac{f_0''}{f_0'} = \dfrac{i}{2}\left(\dfrac{\pm p'}{\pm p}\right) = \dfrac{i}{2}\dfrac{d}{dx}\ln p \Longrightarrow f_1 = \dfrac{i}{2}\ln p + \text{ const.}$

$$\psi = \exp\left(\frac{if}{\hbar}\right) = \exp\left[\frac{i}{\hbar}\left(\pm\int p(x)\,dx + \hbar\frac{i}{2}\ln p + K\right)\right] = \exp\left(\pm\frac{i}{\hbar}\int p\,dx\right)p^{-1/2}e^{iK/\hbar}$$
$$= \frac{C}{\sqrt{p}}\exp\left(\pm\frac{i}{\hbar}\int p\,dx\right). \quad \text{QED}$$

Problem 9.3

$$\gamma = \frac{1}{\hbar}\int |p(x)|\,dx = \frac{1}{\hbar}\int_0^{2a}\sqrt{2m(V_0-E)}\,dx = \frac{2a}{\hbar}\sqrt{2m(V_0-E)}. \quad \boxed{T \approx e^{-4a\sqrt{2m(V_0-E)}/\hbar}.}$$

From Problem 2.33, the *exact* answer is

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)}\sinh^2\gamma}.$$

Now, the WKB approximation assumes the tunneling probability is small (p. 359)—which is to say that γ is *large*. In this case, $\sinh\gamma = \frac{1}{2}(e^\gamma - e^{-\gamma}) \approx \frac{1}{2}e^\gamma$, and $\sinh^2\gamma \approx \frac{1}{4}e^{2\gamma}$, and the exact result reduces to

$$T \approx \frac{1}{1 + \frac{V_0^2}{16E(V_0-E)}e^{2\gamma}} \approx \left\{\frac{16E(V_0-E)}{V_0^2}\right\}e^{-2\gamma}.$$

The coefficient in { } is of order 1; the dominant dependence on E is in the exponential factor. In this sense $T \approx e^{-2\gamma}$ (the WKB result).

Problem 9.4

I take the masses from Thornton and Rex, *Modern Physics*, Appendix 8. They are all *atomic* masses, but the electron masses subtract out in the calculation of E. All masses are in atomic units (u): 1 u = 931 MeV/c^2. The mass of He^4 is 4.002602 u, and that of the α-particle is 3727 MeV/c^2.

$\text{U}^{238}: \ Z = 92,\ A = 238,\ m = 238.050784 \text{ u} \to \text{Th}^{234}: m = 234.043593 \text{ u}.$

$r_1 = (1.07 \times 10^{-15}\text{ m})(238)^{1/3} = 6.63 \times 10^{-15}\text{ m}.$

$E = (238.050784 - 234.043593 - 4.002602)(931)\text{ MeV} = 4.27\text{ MeV}.$

$$V = \sqrt{\frac{2E}{m}} = \sqrt{\frac{(2)(4.27)}{3727}} \times 3 \times 10^8\text{ m/s} = 1.44 \times 10^7\text{ m/s}.$$

$$\gamma = 1.980\frac{90}{\sqrt{4.27}} - 1.485\sqrt{90(6.63)} = 86.19 - 36.28 = 49.9.$$

$$\tau = \frac{(2)(6.63\times10^{-15})}{1.44\times10^7}e^{98.8}\text{ s} = 7.46\times10^{21}\text{ s} = \frac{7.46\times10^{21}}{3.15\times10^7}\text{ yr} = \boxed{2.4\times10^{14}\text{ yrs.}}$$

$\text{Po}^{212}: \ Z = 84,\ A = 212,\ m = 211.988842 \text{ u} \to \text{Pb}^{208}: m = 207.976627 \text{ u}.$

$$r_1 = (1.07 \times 10^{-15}\ \text{m})(212)^{1/3} = 6.38 \times 10^{-15}\ \text{m}.$$

$$E = (211.988842 - 207.976627 - 4.002602)(931)\ \text{MeV} = 8.95\ \text{MeV}.$$

$$V = \sqrt{\frac{2E}{m}} = \sqrt{\frac{(2)(8.95)}{3727}} \times 3 \times 10^8\ \text{m/s} = 2.08 \times 10^7\ \text{m/s}.$$

$$\gamma = 1.980\frac{82}{\sqrt{8.95}} - 1.485\sqrt{82(6.38)} = 54.37 - 33.97 = 20.4.$$

$$\tau = \frac{(2)(6.38 \times 10^{-15})}{2.08 \times 10^7} e^{40.8}\ \text{s} = \boxed{3.2 \times 10^{-4}\ \text{s.}}$$

These results are *way* off—but note the extraordinary sensitivity to nuclear masses: a tiny change in E produces enormous changes in τ.

Much more impressive results are obtained when you plot the logarithm of lifetimes against $1/\sqrt{E}$, as in Figure 9.6. Thanks to David Rubin for pointing this out. Some experimental values are listed below (all energies in MeV):

Uranium ($Z = 92$):

A	E	τ
238	4.198	4.468×10^9 yr
236	4.494	2.342×10^7 yr
234	4.775	2.455×10^5 yr
232	5.320	68.9 yr
230	5.888	20.8 day
228	6.680	9.1 min
226	7.570	0.35 s

Protactinium ($Z = 91$):

A	E	τ
224	7.488	0.79 s
222	8.540	2.9 ms
220	9.650	0.78 μs
218	9.614	0.12 ms

Thorium ($Z = 90$):

A	E	τ
232	4.012	1.405×10^{10} yr
230	4.687	7.538×10^4 yr
228	5.423	1.912 yr
226	6.337	30.57 min

Radium ($Z = 88$):

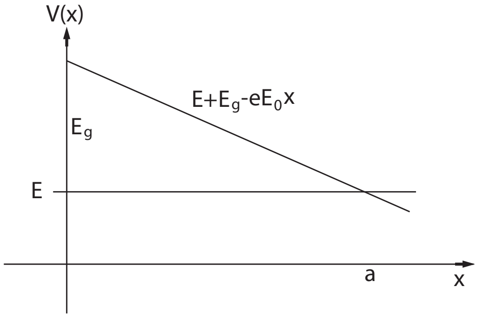
A	E	τ
226	4.784	1600 yr
224	5.685	3.66 day
222	6.559	38 s
220	7.455	18 ms
218	8.389	25.6 μs

Problem 9.5

From Equation 9.23, the tunneling probability is (approximately)

$$T = e^{-2\gamma}, \quad \text{where} \quad \gamma = \frac{1}{\hbar}\int_0^a |p(x)|\, dx, \quad \text{and} \quad p(x) = \sqrt{2m(E - V(x))}\,.$$

An electron in the lower band, with energy E, has to tunnel through the barrier shown here:



$$|p(x)| = \left|\sqrt{2m[E-(E+E_g-eE_0x)]}\right| = \left|\sqrt{-2m(E_g-eE_0x)}\right| = \sqrt{2m(E_g-eE_0x)}.$$

Then (letting $u \equiv eE_0x/E_g$)

$$\gamma = \frac{1}{\hbar}\int_0^a \sqrt{2m(E_g-eE_0x)}\,dx = \frac{\sqrt{2mE_g}}{\hbar}\int_0^a \sqrt{1-\frac{eE_0x}{E_g}}\,dx$$
$$= \frac{E_g}{eE_0}\frac{\sqrt{2mE_g}}{\hbar}\int_0^1 \sqrt{1-u}\,du = \frac{2}{3}\frac{E_g^{3/2}}{eE_0}\frac{\sqrt{2m}}{\hbar},$$

and the probability of tunneling is

$$\boxed{T = \exp\left(-\frac{4}{3}\frac{E_g^{3/2}}{eE_0}\frac{\sqrt{2m}}{\hbar}\right).}$$

Problem 9.6

(a) $\boxed{V(x) = mgx.}$

(b)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + mgx\psi = E\psi \Longrightarrow \frac{d^2\psi}{dx^2} = \frac{2m^2g}{\hbar^2}\left(x-\frac{E}{mg}\right). \quad \text{Let } y \equiv x - \frac{E}{mg}, \text{ and } \alpha \equiv \left(\frac{2m^2g}{\hbar^2}\right)^{1/3}.$$

Then $\dfrac{d^2\psi}{dy^2} = \alpha^3 y\psi$. Let $z \equiv \alpha y = \alpha(x - \dfrac{E}{mg})$, so $\dfrac{d^2\psi}{dz^2} = z\psi$. This is the Airy equation (Eq. 9.37), and the general solution is $\psi = aAi(z) + bBi(z)$. However, $Bi(z)$ blows up for large z, so $b = 0$ (to make ψ normalizable). Hence $\boxed{\psi(x) = aAi\left[\alpha(x - \frac{E}{mg})\right].}$

(c) Since $V(x) = \infty$ for $x < 0$, we require $\psi(0) = 0$; hence $Ai\left[\alpha(-E/mg)\right] = 0$. Now, the zeros of Ai are a_n $(n = 1, 2, 3, \ldots)$. Abramowitz and Stegun list $a_1 = -2.338$, $a_2 = -4.088$, $a_3 = -5.521$, $a_4 = -6.787$, etc. Here $-\dfrac{\alpha E_n}{mg} = a_n$, or $E_n = -\dfrac{mg}{\alpha}a_n = -mg\left(\dfrac{\hbar^2}{2m^2g}\right)^{1/3} a_n$, or $\boxed{E_n = -(\frac{1}{2}mg^2\hbar^2)^{1/3}a_n.}$ In this case $\frac{1}{2}mg^2\hbar^2 = \frac{1}{2}(0.1\text{ kg})(9.8\text{ m/s}^2)^2(1.055\times10^{-34}\text{J}\cdot\text{s})^2 = 5.34\times10^{-68}\text{ J}^3$; $(\frac{1}{2}mg^2\hbar^2)^{1/3} = 3.77\times10^{-23}$ J.

$$\boxed{E_1 = 8.81\times10^{-23}\text{ J},\quad E_2 = 1.54\times10^{-22}\text{ J},\quad E_3 = 2.08\times10^{-22}\text{ J},\quad E_4 = 2.56\times10^{-22}\text{ J}.}$$

(d)

$$2\langle T\rangle = \langle x\frac{dV}{dX}\rangle \text{ (Eq. 3.113);}\quad \text{here}\quad \frac{dV}{dx} = mg,\quad \text{so}\quad \langle x\frac{dV}{dx}\rangle = \langle mgx\rangle = \langle V\rangle,\quad \text{so}\quad \langle T\rangle = \frac{1}{2}\langle V\rangle.$$

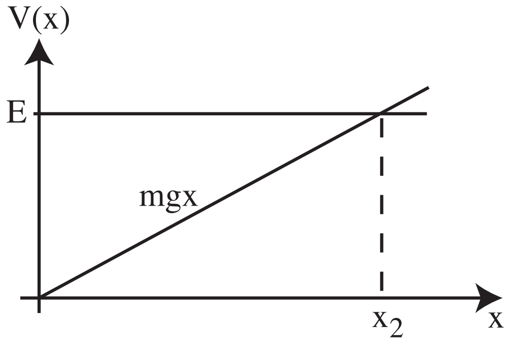
But $\langle T\rangle + \langle V\rangle = \langle H\rangle = E_n$, so $\dfrac{3}{2}\langle V\rangle = E_n$, or $\langle V\rangle = \dfrac{2}{3}E_n$. But $\langle V\rangle = mg\langle x\rangle$, so $\langle x\rangle = \dfrac{2E_n}{3mg}$.

$$\text{For the electron, } \left(\frac{1}{2}mg^2\hbar^2\right)^{1/3} = \left[\frac{1}{2}(9.11\times10^{-31})(9.8)^2(1.055\times10^{-34})^2\right]^{1/3} = 7.87\times10^{-33}\text{ J}.$$

$$E_1 = 1.84\times10^{-32}\text{ J} = \boxed{1.15\times10^{-13}\text{ eV.}}\quad \langle x\rangle = \frac{2(1.84\times10^{-32})}{3(9.11\times10^{-31})(9.8)} = 1.37\times10^{-3} = \boxed{1.37\text{ mm.}}$$

Problem 9.7

(a)



Eq. 9.48 $\Longrightarrow \int_0^{x_2} p(x)\,dx = (n-\frac{1}{4})\pi\hbar$, where $p(x) = \sqrt{2m(E-mgx)}$ and $E = mgx_2 \Longrightarrow x_2 = E/mg$.

$$\int_0^{x_2} p(x)\,dx = \sqrt{2m}\int_0^{x_2}\sqrt{E-mgx}\,dx = \sqrt{2m}\left[-\frac{2}{3mg}(E-mgx)^{3/2}\right]\Bigg|_0^{x_2}$$
$$= -\frac{2}{3}\sqrt{\frac{2}{m}}\frac{1}{g}\left[(E-mgx_2)^{3/2} - E^{3/2}\right] = \frac{2}{3}\sqrt{\frac{2}{m}}\frac{1}{g}E^{3/2}.$$

$$\frac{1}{3\sqrt{mg}}(2E)^{3/2} = (n-\frac{1}{4})\pi\hbar, \quad \text{or} \quad \boxed{E_n = \left[\tfrac{9}{8}\pi^2 mg^2\hbar^2(n-\tfrac{1}{4})^2\right]^{1/3}.}$$

(b)

$$\left(\frac{9}{8}\pi^2 mg^2\hbar^2\right)^{1/3} = \left[\frac{9}{8}\pi^2(0.1)(9.8)^2(1.055\times10^{-34})^2\right]^{1/3} = 1.0588\times10^{-22}\text{ J}.$$

$$E_1 = (1.0588\times10^{-22})\left(\frac{3}{4}\right)^{2/3} = \boxed{8.74\times10^{-23}\text{ J},}$$
$$E_2 = (1.0588\times10^{-22})\left(\frac{7}{4}\right)^{2/3} = \boxed{1.54\times10^{-22}\text{ J},}$$
$$E_3 = (1.0588\times10^{-22})\left(\frac{11}{4}\right)^{2/3} = \boxed{2.08\times10^{-22}\text{ J},}$$
$$E_4 = (1.0588\times10^{-22})\left(\frac{15}{4}\right)^{2/3} = \boxed{2.56\times10^{-22}\text{ J}.}$$

These are in very close agreement with the exact results (Problem 9.6(c)). In fact, they agree precisely (to 3 significant digits), except for E_1 (for which the exact result was 8.81×10^{-23} J).

(c) From Problem 9.6(d),

$$\langle x\rangle = \frac{2E_n}{3mg}, \quad \text{so} \quad 1 = \frac{2}{3}\frac{(1.0588\times10^{-22})}{(0.1)(9.8)}\left(n-\frac{1}{4}\right)^{2/3}, \text{ or } \left(n-\frac{1}{4}\right)^{2/3} = 1.388\times10^{22}.$$

$$n = \frac{1}{4} + (1.388\times10^{22})^{3/2} = \boxed{1.64\times10^{33}.}$$

Problem 9.8

$$\int_{x_1}^{x_2} p(x)\,dx = \left(n-\frac{1}{2}\right)\pi\hbar; \quad p(x) = \sqrt{2m\left(E-\frac{1}{2}m\omega^2x^2\right)}; \quad x_2 = -x_1 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}.$$

$$\left(n-\frac{1}{2}\right)\pi\hbar = m\omega\int_{-x_2}^{x_2}\sqrt{\frac{2E}{m\omega^2}-x^2}\,dx = 2m\omega\int_0^{x_2}\sqrt{x_2^2-x^2}\,dx = m\omega\left[x\sqrt{x_2^2-x^2}+x_2^2\sin^{-1}(x/x_2)\right]_0^{x_2}$$

$$= m\omega x_2^2\sin^{-1}(1) = \frac{\pi}{2}m\omega x_2^2 = \frac{\pi}{2}m\omega\frac{2E}{m\omega^2} = \frac{\pi E}{\omega}. \quad \boxed{E_n = \left(n-\tfrac{1}{2}\right)\hbar\omega} \; (n=1,2,3,\dots)$$

Since the WKB numbering starts with $n = 1$, whereas for oscillator states we traditionally start with $n = 0$, letting $n \to n+1$ converts this to the usual formula $E_n = (n+\frac{1}{2})\hbar\omega$. In this case the WKB approximation yields the *exact* results.

Problem 9.9

(a)

$$\frac{1}{2}m\omega^2x_2^2 = E_n = \left(n+\frac{1}{2}\right)\hbar\omega \quad (\text{counting } n = 0,1,2,\dots); \quad \boxed{x_2 = \sqrt{\frac{(2n+1)\hbar}{m\omega}}.}$$

(b)

$$V_{\text{lin}}(x) = \frac{1}{2}m\omega^2x_2^2 + (m\omega^2x_2)(x-x_2) \Longrightarrow V_{\text{lin}}(x_2+d) = \frac{1}{2}m\omega^2x_2^2 + m\omega^2x_2d.$$

$$\frac{V(x_2+d)-V_{\text{lin}}(x_2+d)}{V(x_2)} = \frac{\frac{1}{2}m\omega^2(x_2+d)^2 - \frac{1}{2}m\omega^2x_2^2 - m\omega^2x_2d}{\frac{1}{2}m\omega^2x_2^2}$$

$$= \frac{x_2^2+2x_2d+d^2-x_2^2-2x_2d}{x_2^2} = \left(\frac{d}{x_2}\right)^2 = 0.01. \quad \boxed{d = 0.1\,x_2.}$$

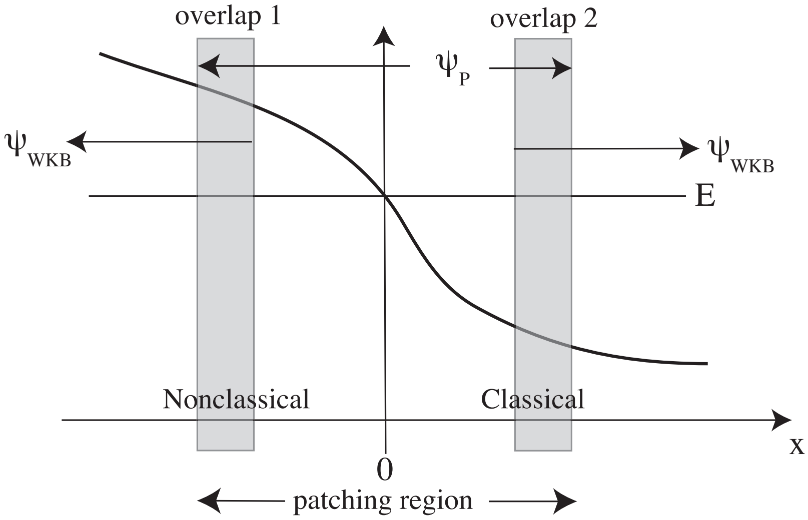
(c)

$$\alpha = \left[\frac{2m}{\hbar^2}m\omega^2x_2\right]^{1/3} \quad (\text{Eq. 9.35}), \quad \text{so} \quad 0.1\,x_2\left[\frac{2m^2\omega^2}{\hbar^2}x_2\right]^{1/3} \geq 5 \Longrightarrow \left[\frac{2m^2\omega^2}{\hbar^2}x_2^4\right]^{1/3} \geq 50.$$

$$\frac{2m^2\omega^2}{\hbar^2}\frac{(2n+1)^2\hbar^2}{m^2\omega^2} \geq (50)^3; \quad \text{or} \quad (2n+1)^2 \geq \frac{(50)^3}{2} = 62500; \quad 2n+1 \geq 250; \quad n \geq \frac{249}{2} = 124.5.$$

$\boxed{n_{\min} = 125.}$ However, as we saw in Problems 9.7 and 9.8, WKB may be valid at much smaller n.

Problem 9.10



Shift origin to the turning point.

$$\psi_{\text{WKB}} = \begin{cases} \dfrac{1}{\sqrt{|p(x)|}} D e^{-\frac{1}{\hbar}\int_x^0 |p(x')|\,dx'} & (x<0) \\ \dfrac{1}{\sqrt{p(x)}}\left[Be^{\frac{i}{\hbar}\int_0^x p(x')\,dx'} + Ce^{-\frac{i}{\hbar}\int_0^x p(x')\,dx'}\right] & (x>0) \end{cases}$$

Linearized potential in the patching region:

$V(x) \approx E + V'(0)x$. Note : $V'(0)$ is *negative*. $\dfrac{d^2\psi_p}{dx^2} = \dfrac{2mV'(0)}{\hbar^2}x\psi_p = -\alpha^3 x\psi_p$, where $\alpha \equiv \left(\dfrac{2m|V'(0)|}{\hbar^2}\right)^{1/3}$.

$\psi_p(x) = aAi(-\alpha x) + bBi(-\alpha x)$. (Note change of sign, as compared with Eq. 9.38).

$p(x) = \sqrt{2m[E - E - V'(0)x]} = \sqrt{-2mV'(0)x} = \sqrt{2m|V'(0)|x} = \sqrt{\alpha^3\hbar^2 x} = \hbar\alpha^{3/2}\sqrt{x}$.

Overlap region 1 ($x < 0$):

$$\int_x^0 |p(x')|\,dx' = \hbar\alpha^{3/2}\int_x^0 \sqrt{-x'}\,dx' = \hbar\alpha^{3/2}\left(-\frac{2}{3}(-x')^{3/2}\right)\Big|_x^0 = \frac{2}{3}\hbar\alpha^{3/2}(-x)^{3/2} = \frac{2}{3}\hbar(-\alpha x)^{3/2}.$$

$$\psi_{\text{WKB}} \approx \frac{1}{\hbar^{1/2}\alpha^{3/4}(-x)^{1/4}} De^{-\frac{2}{3}(-\alpha x)^{3/2}}.$$ For large positive argument ($-\alpha x \gg 1$) :

$$\psi_p \approx a\frac{1}{2\sqrt{\pi}(-\alpha x)^{1/4}}e^{-\frac{2}{3}(-\alpha x)^{3/2}} + b\frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}}e^{\frac{2}{3}(-\alpha x)^{3/2}}.$$ Comparing $\Rightarrow a = 2D\sqrt{\dfrac{\pi}{\alpha\hbar}}$; $b = 0$.

Overlap region 2 ($x > 0$):

$$\int_0^x p(x')\,dx' = \hbar\alpha^{3/2}\int_0^x \sqrt{x'}\,dx' = \hbar\alpha^{3/2}\left[\frac{2}{3}(x')^{3/2}\right]\Big|_0^x = \frac{2}{3}\hbar(\alpha x)^{3/2}.$$

$$\psi_{\text{WKB}} \approx \frac{1}{\hbar^{1/2}\alpha^{3/4}x^{1/4}}\left[Be^{i\frac{2}{3}(\alpha x)^{3/2}} + Ce^{-i\frac{2}{3}(\alpha x)^{3/2}}\right].$$ For large negative argument ($-\alpha x \ll -1$) :

$$\psi_p(x) \approx a\frac{1}{\sqrt{\pi}(\alpha x)^{1/4}}\sin\left[\frac{2}{3}(\alpha x)^{3/2}+\frac{\pi}{4}\right] = \frac{a}{\sqrt{\pi}(\alpha x)^{1/4}}\frac{1}{2i}\left[e^{i\pi/4}e^{i\frac{2}{3}(\alpha x)^{3/2}} - e^{-i\pi/4}e^{-i\frac{2}{3}(\alpha x)^{3/2}}\right] \text{ (remember : } b=0).$$

Comparing the two: $B = \frac{a}{2i}\sqrt{\frac{\alpha\hbar}{\pi}}e^{i\pi/4},\ C = -\frac{a}{2i}\sqrt{\frac{\alpha\hbar}{\pi}}e^{-i\pi/4}.$

Inserting the expression for a from overlap region 1 : $B = -ie^{i\pi/4}D;\ C = ie^{-i\pi/4}D.$ For $x > 0$, then,

$$\psi_{\text{WKB}} = \frac{-iD}{\sqrt{p(x)}}\left[e^{\frac{i}{\hbar}\int_0^x p(x')\,dx' + i\frac{\pi}{4}} - e^{-\frac{i}{\hbar}\int_0^x p(x')\,dx' - i\frac{\pi}{4}}\right] = \frac{2D}{\sqrt{p(x)}}\sin\left[\frac{1}{\hbar}\int_0^x p(x')\,dx' + \frac{\pi}{4}\right].$$

Finally, switching the origin back to x_1:

$$\psi_{\text{WKB}}(x) = \left\{\begin{array}{ll} \frac{D}{\sqrt{|p(x)|}}e^{-\frac{1}{\hbar}\int_x^{x_1}|p(x')|\,dx'}, & (x < x_1)\ ; \\ \frac{2D}{\sqrt{p(x)}}\sin\left[\frac{1}{\hbar}\int_{x_1}^x p(x')dx' + \frac{\pi}{4}\right], & (x > x_1). \end{array}\right\} \quad \text{QED}$$

Problem 9.11

At x_1, we have an upward-sloping turning point. Follow the method in the book. Shifting origin to x_1:

$$\psi_{\text{WKB}}(x) = \left\{\begin{array}{ll} \frac{1}{\sqrt{p(x)}}\left[Ae^{-\frac{i}{\hbar}\int_x^0 p(x')\,dx'} + Be^{\frac{i}{\hbar}\int_x^0 p(x')\,dx'}\right] & (x < 0) \\ \frac{1}{\sqrt{|p(x)|}}\left[Ce^{\frac{1}{\hbar}\int_0^x |p(x')|\,dx'} + De^{-\frac{1}{\hbar}\int_0^x |p(x')|\,dx'}\right] & (x > 0) \end{array}\right.$$

In overlap region 2, Eq. 9.40 becomes $\psi_{\text{WKB}} \approx \frac{1}{\hbar^{1/2}\alpha^{3/4}x^{1/4}}\left[Ce^{\frac{2}{3}(\alpha x)^{3/2}} + De^{-\frac{2}{3}(\alpha x)^{3/2}}\right]$,

whereas Eq. 9.41 is unchanged. Comparing them $\Longrightarrow a = 2D\sqrt{\frac{\pi}{\alpha\hbar}},\quad b = C\sqrt{\frac{\pi}{\alpha\hbar}}.$

In overlap region 1, Eq. 9.44 becomes $\psi_{\text{WKB}} \approx \frac{1}{\hbar^{1/2}\alpha^{3/4}(-x)^{1/4}}\left[Ae^{-i\frac{2}{3}(-\alpha x)^{3/2}} + Be^{i\frac{2}{3}(-\alpha x)^{3/2}}\right]$,

and Eq. 9.45 (with $b \neq 0$) generalizes to

$$\psi_p(x) \approx \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}}\sin\left[\frac{2}{3}(-\alpha x)^{3/2}+\frac{\pi}{4}\right] + \frac{b}{\sqrt{\pi}(-\alpha x)^{1/4}}\cos\left[\frac{2}{3}(-\alpha x)^{3/2}+\frac{\pi}{4}\right]$$

$$= \frac{1}{2\sqrt{\pi}(-\alpha x)^{1/4}}\left[(-ia+b)e^{i\frac{2}{3}(-\alpha x)^{3/2}}e^{i\pi/4} + (ia+b)e^{-i\frac{2}{3}(-\alpha x)^{3/2}}e^{-i\pi/4}\right].\ \text{Comparing them} \Longrightarrow$$

$A = \sqrt{\frac{\hbar\alpha}{\pi}}\left(\frac{ia+b}{2}\right)e^{-i\pi/4};\quad B = \sqrt{\frac{\hbar\alpha}{\pi}}\left(\frac{-ia+b}{2}\right)e^{i\pi/4}.$ Putting in the expressions above for a and b :

$A = \left(\frac{C}{2}+iD\right)e^{-i\pi/4};\quad B = \left(\frac{C}{2}-iD\right)e^{i\pi/4}.$

These are the connection formulas relating A, B, C, and D, at x_1.

At x_2, we have a downward-sloping turning point, and follow the method of Problem 9.10. First rewrite the middle expression in Eq. 9.53:

$$\psi_{\rm WKB} = \frac{1}{\sqrt{|p(x)|}}\left[Ce^{\frac{1}{\hbar}\int_{x_1}^{x_2}|p(x')|\,dx' + \frac{1}{\hbar}\int_{x_2}^{x}|p(x')|\,dx'} + De^{-\frac{1}{\hbar}\int_{x_1}^{x_2}|p(x')|\,dx' - \frac{1}{\hbar}\int_{x_2}^{x}|p(x')|\,dx'}\right].$$

Let $\gamma \equiv \int_{x_1}^{x_2}|p(x)|\,dx/\hbar$, as before (Eq. 9.23), and let $C' \equiv De^{-\gamma}$, $D' \equiv Ce^{\gamma}$. Then (shifting the origin to x_2):

$$\psi_{\rm WKB} = \begin{cases} \dfrac{1}{\sqrt{|p(x)|}}\left[C'e^{\frac{1}{\hbar}\int_x^0|p(x')|\,dx'} + D'e^{-\frac{1}{\hbar}\int_x^0|p(x')|\,dx'}\right], & (x<0); \\ \dfrac{1}{\sqrt{p(x)}}Fe^{\frac{i}{\hbar}\int_0^x p(x')\,dx'}, & (x>0). \end{cases}$$

In the patching region $\psi_p(x) = aAi(-\alpha x) + bBi(-\alpha x)$, where $\alpha \equiv \left(\dfrac{2m|V'(0)|}{\hbar^2}\right)^{1/3}$; $\quad p(x) = \hbar\alpha^{3/2}\sqrt{x}$.

<u>In overlap region 1</u> ($x<0$): $\displaystyle\int_x^0 |p(x')|\,dx' = \frac{2}{3}\hbar(-\alpha x)^{3/2}$, so

$$\left.\begin{aligned} \psi_{\rm WKB} &\approx \frac{1}{\hbar^{1/2}\alpha^{3/4}(-x)^{1/4}}\left[C'e^{\frac{2}{3}(-\alpha x)^{3/2}} + D'e^{-\frac{2}{3}(-\alpha x)^{3/2}}\right] \\ \psi_p &\approx \frac{a}{2\sqrt{\pi}(-\alpha x)^{1/4}}e^{-\frac{2}{3}(-\alpha x)^{3/2}} + \frac{b}{\sqrt{\pi}(-\alpha x)^{1/4}}e^{\frac{2}{3}(-\alpha x)^{3/2}} \end{aligned}\right\} \text{Comparing} \Longrightarrow \begin{cases} a = 2\sqrt{\dfrac{\pi}{\hbar\alpha}}D' \\ b = \sqrt{\dfrac{\pi}{\hbar\alpha}}C' \end{cases}$$

<u>In overlap region 2</u> ($x>0$): $\displaystyle\int_0^x p(x')\,dx' = \frac{2}{3}\hbar(\alpha x)^{3/2} \Longrightarrow \psi_{\rm WKB} \approx \frac{1}{\hbar^{1/2}\alpha^{3/4}x^{1/4}}Fe^{i\frac{2}{3}(\alpha x)^{3/2}}$.

$$\begin{aligned} \psi_p &\approx \frac{a}{\sqrt{\pi}(\alpha x)^{1/4}}\sin\left[\frac{2}{3}(\alpha x)^{3/2} + \frac{\pi}{4}\right] + \frac{b}{\sqrt{\pi}(\alpha x)^{1/4}}\cos\left[\frac{2}{3}(\alpha x)^{3/2} + \frac{\pi}{4}\right] \\ &= \frac{1}{2\sqrt{\pi}(\alpha x)^{1/4}}\left[(-ia+b)e^{i\frac{\pi}{4}}e^{i\frac{2}{3}(\alpha x)^{3/2}} + (ia+b)e^{-i\frac{\pi}{4}}e^{-i\frac{2}{3}(\alpha x)^{3/2}}\right]. \quad \text{Comparing} \Longrightarrow (ia+b)=0; \end{aligned}$$

$$F = \sqrt{\frac{\hbar\alpha}{\pi}}\left(\frac{-ia+b}{2}\right)e^{i\pi/4} = b\sqrt{\frac{\hbar\alpha}{\pi}}e^{i\pi/4}. \quad b = \sqrt{\frac{\pi}{\hbar\alpha}}e^{-i\pi/4}F; \quad a = i\sqrt{\frac{\pi}{\hbar\alpha}}e^{-i\pi/4}F.$$

$$C' = \sqrt{\frac{\hbar\alpha}{\pi}}b = e^{-i\pi/4}F, \quad D' = \frac{1}{2}\sqrt{\frac{\hbar\alpha}{\pi}}a = \frac{i}{2}e^{-i\pi/4}F. \quad D = e^{\gamma}e^{-i\pi/4}F; \quad C = \frac{i}{2}e^{-\gamma}e^{-i\pi/4}F.$$

These are the connection formulas at x_2. Putting them into the equation for A:

$$A = \left(\frac{C}{2} + iD\right)e^{-i\pi/4} = \left(\frac{i}{4}e^{-\gamma}e^{-i\pi/4}F + ie^{\gamma}e^{-i\pi/4}F\right)e^{-i\pi/4} = \left(\frac{e^{-\gamma}}{4} + e^{\gamma}\right)F.$$

$$T = \left|\frac{F}{A}\right|^2 = \frac{1}{(e^{\gamma} + \frac{e^{-\gamma}}{4})^2} = \boxed{\frac{e^{-2\gamma}}{\left[1 + (e^{-2\gamma}/4)\right]^2}.}$$

If $\gamma \gg 1$, the denominator is essentially 1, and we recover $T = e^{-2\gamma}$ (Eq. 9.23).

Problem 9.12

In the plot below the blue and red curves make up the piecewise WKB solution, and the black dashed line is the exact result. I chose the width of the patching region to be $0.3\,x_2$, centered at x_2.

```
$Assumptions = m > 0 && En > 0 && ω > 0;
```

Analytical Integral

$$\texttt{p[x\_] := Sqrt}\left[2\,\texttt{m}\,\left(\texttt{En} - \texttt{V[x]}\right)\right];$$

$$\texttt{V[x\_] :=}\ \frac{1}{2}\,\texttt{m}\,\omega^2\,\texttt{x}^2;$$

$$\texttt{x2} = \frac{\sqrt{2}\,\sqrt{\texttt{En}}}{\sqrt{\texttt{m}}\,\omega};$$

Numerical Method

$$\texttt{n} = 3;$$

$$\texttt{En} = \left(2\,\texttt{n} - \frac{1}{2}\right)\hbar\,\omega;$$

$$\hbar = \texttt{m} = \omega = 1;$$

$$\psi\texttt{1[x\_] :=}\ \frac{2}{\sqrt{\texttt{p[x]}}}\,\texttt{Sin}\left[\frac{1}{\hbar}\,\texttt{NIntegrate[p[xp], \{xp, x, x2\}]} + \frac{\pi}{4}\right]$$

$$\psi\texttt{3[x\_] :=}\ \frac{1}{\sqrt{\texttt{Abs[p[x]]}}}\,\texttt{Exp}\left[-\frac{1}{\hbar}\,\texttt{NIntegrate[Abs[p[xp]], \{xp, x2, x\}]}\right]$$

$$\alpha = \left(\frac{2\,\texttt{m}}{\hbar^2}\,\texttt{V'[x2]}\right)^{1/3};$$

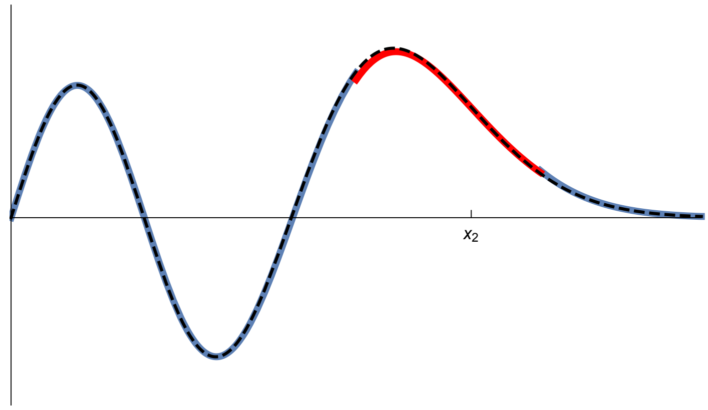
$$\psi\texttt{2[x\_] :=}\ \sqrt{\frac{4\,\pi}{\alpha\,\hbar}}\,\texttt{AiryAi}\left[\alpha\,\left(\texttt{x} - \texttt{x2}\right)\right]$$

```
ψWKB[x_] := If[x < .85 x2, ψ1[x], If[x < 1.15 x2, ψ2[x], ψ3[x]]];
```

$$\texttt{norm} = \frac{1}{\sqrt{\texttt{NIntegrate[}\psi\texttt{WKB[x]\^{}2, \{x, 0, 2 x2\}]}}};$$

$$\psi\texttt{exact[n\_, x\_] :=}\ \sqrt{2}\,\left(\frac{\texttt{m}\,\omega}{\pi\,\hbar}\right)^{1/4}\frac{1}{\sqrt{2^{\texttt{n}}\,\texttt{n!}}}\,\texttt{HermiteH}\left[\texttt{n},\ \sqrt{\frac{\texttt{m}\,\omega}{\hbar}}\,\texttt{x}\right]\,\texttt{Exp}\left[-\frac{1}{2}\left(\sqrt{\frac{\texttt{m}\,\omega}{\hbar}}\,\texttt{x}\right)^2\right]$$

```
Show[
 Plot[normψ1[x], {x, 0, .75 x2}, PlotRange → {{0, 1.5 x2}, {-1, 1}},
  Ticks → {{{x2, "x2"}}, None}, PlotStyle → Thickness[0.01]],
 Plot[normψ3[x], {x, 1.15 x2, 1.5 x2}, PlotRange → All,
  PlotStyle → Thickness[0.01]],
 Plot[normψ2[x], {x, .75 x2, 1.15 x2}, PlotRange → {{0, 2 x2}, {-2, 2}},
  PlotStyle → {Red, Thickness[0.01]}],
 Plot[ψexact[2 n - 1, x], {x, 0, 1.5 x2}, PlotStyle → {Black, Dashed}]
]
```



Problem 9.13

Equation 9.52 $\Rightarrow \left(n-\frac{1}{2}\right)\pi\hbar = 2\int_0^{x_2}\sqrt{2m(E-\alpha x^\nu)}\,dx = 2\sqrt{2mE}\int_0^{x_2}\sqrt{1-\frac{\alpha}{E}x^\nu}\,dx; \quad E=\alpha x_2^\nu.$ Let $z\equiv\frac{\alpha}{E}x^\nu$, so $x=\left(\frac{zE}{\alpha}\right)^{1/\nu}; \quad dx=\left(\frac{E}{\alpha}\right)^{1/\nu}\frac{1}{\nu}z^{\frac{1}{\nu}-1}\,dz$. Then

$$\begin{aligned}\left(n-\frac{1}{2}\right)\pi\hbar &= 2\sqrt{2mE}\left(\frac{E}{\alpha}\right)^{1/\nu}\frac{1}{\nu}\int_0^1 z^{\frac{1}{\nu}-1}\sqrt{1-z}\,dz = 2\sqrt{2mE}\left(\frac{E}{\alpha}\right)^{1/\nu}\frac{1}{\nu}\frac{\Gamma(1/\nu)\Gamma(3/2)}{\Gamma(\frac{1}{\nu}+\frac{3}{2})}\\ &= 2\sqrt{2mE}\left(\frac{E}{\alpha}\right)^{1/\nu}\frac{\Gamma(\frac{1}{\nu}+1)\frac{1}{2}\sqrt{\pi}}{\Gamma(\frac{1}{\nu}+\frac{3}{2})} = \sqrt{2\pi mE}\left(\frac{E}{\alpha}\right)^{1/\nu}\frac{\Gamma(\frac{1}{\nu}+1)}{\Gamma(\frac{1}{\nu}+\frac{3}{2})}.\end{aligned}$$

$$E^{\frac{1}{\nu}+\frac{1}{2}} = \frac{(n-\frac{1}{2})\pi\hbar}{\sqrt{2\pi m}}\alpha^{1/\nu}\frac{\Gamma(\frac{1}{\nu}+\frac{3}{2})}{\Gamma(\frac{1}{\nu}+1)}; \quad \boxed{E_n = \left[\left(n-\frac{1}{2}\right)\hbar\sqrt{\frac{\pi}{2m\alpha}}\frac{\Gamma(\frac{1}{\nu}+\frac{3}{2})}{\Gamma(\frac{1}{\nu}+1)}\right]^{\left(\frac{2\nu}{\nu+2}\right)}\alpha.}$$

For $\nu=2$: $\quad E_n = \left[\left(n-\frac{1}{2}\right)\hbar\sqrt{\frac{\pi}{2m\alpha}}\frac{\Gamma(2)}{\Gamma(3/2)}\right]\alpha = (n-\frac{1}{2})\hbar\sqrt{\frac{2\alpha}{m}}.$

For a harmonic oscillator, with $\alpha=\frac{1}{2}m\omega^2$, $\quad E_n=\left(n-\frac{1}{2}\right)\hbar\omega\ (n=1,2,3,\ldots)$. ✓

Problem 9.14

$$V(x) = -\frac{\hbar^2 a^2}{m}\text{sech}^2(ax). \quad \text{Eq. 9.52} \Longrightarrow \left(n - \frac{1}{2}\right)\pi\hbar = 2\int_0^{x_2}\sqrt{2m\left[E + \frac{\hbar^2 a^2}{m}\text{sech}^2(ax)\right]}\,dx$$

$$= 2\sqrt{2}\hbar a\int_0^{x_2}\sqrt{\text{sech}^2(ax) + \frac{mE}{\hbar^2 a^2}}\,dx.$$

$E = -\frac{\hbar^2 a^2}{m}\text{sech}^2(ax_2)$ defines x_2. Let $b \equiv -\frac{mE}{\hbar^2 a^2}$, $z \equiv \text{sech}^2(ax)$, so that $x = \frac{1}{a}\text{sech}^{-1}\sqrt{z}$, and hence

$$dx = \frac{1}{a}\left(\frac{-1}{\sqrt{z}\sqrt{1-z}}\right)\frac{1}{2\sqrt{z}}\,dz = -\frac{1}{2a}\frac{1}{z\sqrt{1-z}}\,dz. \quad \text{Then } \left(n - \frac{1}{2}\right)\pi = 2\sqrt{2}\,a\left(-\frac{1}{2a}\right)\int_{z_1}^{z_2}\frac{\sqrt{z-b}}{z\sqrt{1-z}}\,dz.$$

$$\text{Limits}: \left\{\begin{array}{l} x = 0 \;\;\; \Longrightarrow z_1 = \text{sech}^2(0) = 1 \\ x = x_2 \Longrightarrow z_2 = \text{sech}^2(ax_2) = -\frac{mE}{\hbar^2 a^2} = b \end{array}\right\}. \quad \left(n - \frac{1}{2}\right)\pi = \sqrt{2}\int_b^1 \frac{1}{z}\sqrt{\frac{z-b}{1-z}}\,dz.$$

$$\frac{1}{z}\sqrt{\frac{z-b}{1-z}} = \frac{1}{z}\frac{(z-b)}{\sqrt{(1-z)(z-b)}} = \frac{1}{\sqrt{(1-z)(z-b)}} - \frac{b}{z\sqrt{(1-z)(z-b)}}.$$

$$\begin{aligned}\left(n - \frac{1}{2}\right)\pi &= \sqrt{2}\left[\int_b^1 \frac{1}{\sqrt{(1-z)(z-b)}}\,dz - b\int_b^1 \frac{1}{z\sqrt{-b+(1+b)z-z^2}}\,dz\right] \\ &= \sqrt{2}\left\{-2\tan^{-1}\sqrt{\frac{1-z}{z-b}} - \sqrt{b}\sin^{-1}\left[\frac{(1+b)z-2b}{z(1-b)}\right]\right\}\Bigg|_b^1 \\ &= \sqrt{2}\left[-2\tan^{-1}(0) + 2\tan^{-1}(\infty) - \sqrt{b}\sin^{-1}(1) + \sqrt{b}\sin^{-1}(-1)\right] = \sqrt{2}\left(0 + 2\frac{\pi}{2} - \sqrt{b}\frac{\pi}{2} - \sqrt{b}\frac{\pi}{2}\right) \\ &= \sqrt{2}\pi(1-\sqrt{b}); \quad \frac{(n-\frac{1}{2})}{\sqrt{2}} = 1 - \sqrt{b}; \quad \sqrt{b} = 1 - \frac{1}{\sqrt{2}}\left(n - \frac{1}{2}\right).\end{aligned}$$

Since the left side is positive, the right side must also be: $(n - \frac{1}{2}) < \sqrt{2}$, $\quad n < \frac{1}{2} + \sqrt{2} = 0.5 + 1.414 = 1.914$. So the only possible n is 1; there is only *one* bound state (which is correct—see Problem 2.52).

$$\text{For } n = 1,\ \sqrt{b} = 1 - \frac{1}{2\sqrt{2}}; \quad b = 1 - \frac{1}{\sqrt{2}} + \frac{1}{8} = \frac{9}{8} - \frac{1}{\sqrt{2}}; \quad \boxed{E_1 = -\frac{\hbar^2 a^2}{m}\left(\frac{9}{8} - \frac{1}{\sqrt{2}}\right)} = -0.418\frac{\hbar^2 a^2}{m}.$$

The *exact* answer (Problem 2.52(c)) is $-0.5\frac{\hbar^2 a^2}{m}$. Not bad.

Problem 9.15

$$\begin{aligned}\left(n - \frac{1}{4}\right)\pi\hbar &= \int_0^{r_0}\sqrt{2m\left[E - V_0\ln(r/a)\right]}\,dr; \quad E = V_0\ln(r_0/a) \text{ defines } r_0. \\ &= \sqrt{2m}\int_0^{r_0}\sqrt{V_0\ln(r_0/a) - V_0\ln(r/a)}\,dr = \sqrt{2mV_0}\int_0^{r_0}\sqrt{\ln(r_0/r)}\,dr.\end{aligned}$$

Let $x \equiv \ln(r_0/r)$, so $e^x = r_0/r$, or $r = r_0 e^{-x} \Longrightarrow dr = -r_0 e^{-x}dx$.

$$\left(n - \frac{1}{4}\right)\pi\hbar = \sqrt{2mV_0}(-r_0)\int_{x_1}^{x_2}\sqrt{x}e^{-x}\,dx. \quad \text{Limits}: \left\{\begin{array}{l} r = 0 \Longrightarrow \;\; x_1 = \infty \\ r = r_0 \Longrightarrow x_2 = 0 \end{array}\right\}.$$

$$\left(n-\frac{1}{4}\right)\pi\hbar = \sqrt{2mV_0}\,r_0\int_0^\infty \sqrt{x}e^{-x}\,dx = \sqrt{2mV_0}\,r_0\Gamma(3/2) = \sqrt{2mV_0}\,r_0\frac{\sqrt{\pi}}{2}.$$

$$r_0 = \sqrt{\frac{2\pi}{mV_0}}\hbar\left(n-\frac{1}{4}\right) \quad\Rightarrow\quad \boxed{E_n = V_0\ln\left[\frac{\hbar}{a}\sqrt{\frac{2\pi}{mV_0}}\left(n-\frac{1}{4}\right)\right]} = V_0\ln\left(n-\frac{1}{4}\right)+V_0\ln\left[\frac{\hbar}{a}\sqrt{\frac{2\pi}{mV_0}}\right].$$

$$E_{n+1}-E_n = V_0\ln\left(n+\frac{3}{4}\right)-V_0\ln\left(n-\frac{1}{4}\right) = V_0\ln\left(\frac{n+3/4}{n-1/4}\right),$$ which is indeed independent of m (and a).

Problem 9.16

$$\left(n'-\frac{1}{2}\right)\pi\hbar = \int_{r_1}^{r_2}\sqrt{2m\left(E+\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}-\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right)}\,dr = \sqrt{-2mE}\int_{r_1}^{r_2}\sqrt{-1+\frac{A}{r}-\frac{B}{r^2}}\,dr,$$

where $A \equiv -\frac{e^2}{4\pi\epsilon_0}\frac{1}{E}$ and $B \equiv -\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{E}$ are positive constants, since E is negative.

$$\left(n'-\frac{1}{2}\right)\pi\hbar = \sqrt{-2mE}\int_{r_1}^{r_2}\frac{\sqrt{-r^2+Ar-B}}{r}\,dr.$$

Let r_1 and r_2 be the roots of the polynomial in the numerator: $-r^2+Ar-B = (r-r_1)(r_2-r)$.

$$\left(n'-\frac{1}{2}\right)\pi\hbar = \sqrt{-2mE}\int_{r_1}^{r_2}\frac{\sqrt{(r-r_1)(r_2-r)}}{r}\,dr = \sqrt{-2mE}\,\frac{\pi}{2}\left(\sqrt{r_2}-\sqrt{r_1}\right)^2.$$

$2\left(n'-\frac{1}{2}\right)\hbar = \sqrt{-2mE}\left(r_2+r_1-2\sqrt{r_1r_2}\right)$. But $-r^2+Ar-B = -r^2+(r_1+r_2)r-r_1r_2$
$\Longrightarrow r_1+r_2 = A;\ r_1r_2 = B$. Therefore

$$2\left(n'-\frac{1}{2}\right)\hbar = \sqrt{-2mE}\left(A-2\sqrt{B}\right) = \sqrt{-2mE}\left(-\frac{e^2}{4\pi\epsilon_0}\frac{1}{E}-2\sqrt{-\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{E}}\right)$$

$$= -\frac{e^2}{4\pi\epsilon_0}\sqrt{-\frac{2m}{E}}-2\hbar\sqrt{\ell(\ell+1)}.$$

$$-\frac{e^2}{4\pi\epsilon_0}\sqrt{-\frac{2m}{E}} = 2\hbar\left[n'-\frac{1}{2}+\sqrt{\ell(\ell+1)}\right]; \quad -\frac{E}{2m} = \frac{(e^2/4\pi\epsilon_0)^2}{4\hbar^2\left[n'-\frac{1}{2}+\sqrt{\ell(\ell+1)}\right]^2}.$$

$$E_{n'\ell} = \frac{-(m/2\hbar^2)(e^2/4\pi\epsilon_0)^2}{\left[n'-\frac{1}{2}+\sqrt{\ell(\ell+1)}\right]^2} = \boxed{\frac{-13.6\text{ eV}}{\left(n'-\frac{1}{2}+\sqrt{\ell(\ell+1)}\right)^2}.}$$

$$\sqrt{\ell(\ell+1)} = \ell\sqrt{1+\frac{1}{\ell}} = \ell\left(1+\frac{1}{2\ell}-\frac{1}{8\ell^2}+\dots\right) \approx \ell+\frac{1}{2}-\frac{1}{8\ell},$$

so

$$\left[n'-(1/2)+\sqrt{\ell(\ell+1)}\right] = \left[n-\ell-(1/2)+\sqrt{\ell(\ell+1)}\right] \approx [n-\ell-(1/2)+\ell+(1/2)-(1/8\ell)] = n-(1/8\ell),$$

and hence

$$E_{n\ell} \approx \frac{-13.6\text{ eV}}{[n-(1/8\ell)]^2} \approx \frac{-13.6\text{ eV}}{n^2},$$

which is the Bohr formula.

Problem 9.17

(a) (i) $\boxed{\psi_{\text{WKB}}(x) = \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_{x_2}^{x} |p(x')|\,dx'}}$ $\quad (x > x_2)$;

(ii) $\psi_{\text{WKB}}(x) = \frac{1}{\sqrt{p(x)}}\left[B e^{\frac{i}{\hbar}\int_x^{x_2} p(x')\,dx'} + C e^{-\frac{i}{\hbar}\int_x^{x_2} p(x')\,dx'}\right]$ $\quad (x_1 < x < x_2)$;

(iii) $\psi_{\text{WKB}}(x) = \frac{1}{\sqrt{|p(x)|}}\left[F e^{\frac{1}{\hbar}\int_x^{x_1} |p(x')|\,dx'} + G e^{-\frac{1}{\hbar}\int_x^{x_1} |p(x')|\,dx'}\right]$ $\quad (0 < x < x_1)$.

Equation 9.47 $\Longrightarrow$ $\boxed{\text{(ii) } \psi_{\text{WKB}} = \frac{2D}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4}\right]}$ $\quad (x_1 < x < x_2)$.

To effect the join at x_1, first rewrite (ii):

$$\text{(ii) } \psi_{\text{WKB}} = \frac{2D}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_{x_1}^{x_2} p(x')\,dx' - \frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' + \frac{\pi}{4}\right] = -\frac{2D}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' - \theta - \frac{\pi}{4}\right],$$

where θ is defined in Eq. 9.59. Now shift the origin to x_1:

$$\psi_{\text{WKB}} = \left\{\begin{array}{ll} \frac{1}{\sqrt{|p(x)|}}\left[F e^{\frac{1}{\hbar}\int_x^0 |p(x')|\,dx'} + G e^{-\frac{1}{\hbar}\int_x^0 |p(x')|\,dx'}\right] & (x < 0) \\ -\frac{2D}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_0^x p(x')\,dx' - \theta - \frac{\pi}{4}\right] & (x > 0) \end{array}\right\}.$$

Following Problem 9.10: $\psi_p(x) = aAi(-\alpha x) + bBi(-\alpha x)$, with $\alpha \equiv \left(\frac{2m|V'(0)|}{\hbar^2}\right)^{1/3}$; $p(x) = \hbar\alpha^{3/2}\sqrt{x}$.

<u>Overlap region 1 ($x < 0$):</u> $\int_x^0 |p(x')|\,dx' = \frac{2}{3}\hbar(-\alpha x)^{3/2}$.

$$\left.\begin{array}{ll} \psi_{\text{WKB}} & \approx \frac{1}{\hbar^{1/2}\alpha^{3/4}(-x)^{1/4}}\left[F e^{\frac{2}{3}(-\alpha x)^{3/2}} + G e^{-\frac{2}{3}(-\alpha x)^{3/2}}\right] \\ \psi_p & \approx \frac{a}{2\sqrt{\pi}(-\alpha x)^{1/4}} e^{-\frac{2}{3}(-\alpha x)^{3/2}} + \frac{b}{\sqrt{\pi}(-\alpha x)^{1/4}} e^{\frac{2}{3}(-\alpha x)^{3/2}} \end{array}\right\} \Longrightarrow a = 2G\sqrt{\frac{\pi}{\hbar\alpha}}; \quad b = F\sqrt{\frac{\pi}{\hbar\alpha}}.$$

<u>Overlap region 2 ($x > 0$):</u> $\int_0^x p(x')\,dx' = \frac{2}{3}\hbar(\alpha x)^{3/2}$.

$$\Longrightarrow \psi_{\text{WKB}} \approx -\frac{2D}{\hbar^{1/2}\alpha^{3/4}x^{1/4}} \sin\left[\frac{2}{3}(\alpha x)^{3/2} - \theta - \frac{\pi}{4}\right],$$

$$\psi_p \approx \frac{a}{\sqrt{\pi}(\alpha x)^{1/4}} \sin\left[\frac{2}{3}(\alpha x)^{3/2} + \frac{\pi}{4}\right] + \frac{b}{\sqrt{\pi}(\alpha x)^{1/4}} \cos\left[\frac{2}{3}(\alpha x)^{3/2} + \frac{\pi}{4}\right].$$

Equating the two expressions: $\frac{-2D}{\hbar^{1/2}\alpha^{3/4}}\frac{1}{2i}\left[e^{i\frac{2}{3}(\alpha x)^{3/2}} e^{-i\theta} e^{-i\pi/4} - e^{-i\frac{2}{3}(\alpha x)^{3/2}} e^{i\theta} e^{i\pi/4}\right]$

$$= \frac{1}{\sqrt{\pi}\alpha^{1/4}}\left\{\frac{a}{2i}\left[e^{i\frac{2}{3}(\alpha x)^{3/2}} e^{i\pi/4} - e^{-i\frac{2}{3}(\alpha x)^{3/2}} e^{-i\pi/4}\right] + \frac{b}{2}\left[e^{i\frac{2}{3}(\alpha x)^{3/2}} e^{i\pi/4} + e^{-i\frac{2}{3}(\alpha x)^{3/2}} e^{-i\pi/4}\right]\right\}$$

$$\Longrightarrow \left\{\begin{array}{lll} -2D\sqrt{\frac{\pi}{\alpha\hbar}} e^{-i\theta} e^{-i\pi/4} = (a + ib)e^{i\pi/4}, & \text{or} & (a + ib) = 2D\sqrt{\frac{\pi}{\alpha\hbar}} i e^{-i\theta} \\ 2D\sqrt{\frac{\pi}{\alpha\hbar}} e^{i\theta} e^{i\pi/4} = (-a + ib)e^{-i\pi/4}, & \text{or} & (a - ib) = -2D\sqrt{\frac{\pi}{\alpha\hbar}} i e^{i\theta} \end{array}\right\}$$

$$\Longrightarrow \left\{ \begin{array}{l} 2a = \; 2D\sqrt{\frac{\pi}{\alpha\hbar}} i(e^{-i\theta} - e^{i\theta}) \Rightarrow a = 2D\sqrt{\frac{\pi}{\alpha\hbar}} \sin\theta, \\ 2ib = 2D\sqrt{\frac{\pi}{\alpha\hbar}} i(e^{-i\theta} + e^{i\theta}) \Rightarrow b = 2D\sqrt{\frac{\pi}{\alpha\hbar}} \cos\theta. \end{array} \right\}$$

Combining these with the results from overlap region 1 $\Longrightarrow$

$$2G\sqrt{\frac{\pi}{\alpha\hbar}} = 2D\sqrt{\frac{\pi}{\alpha\hbar}}\sin\theta, \quad \text{or} \quad G = D\sin\theta; \quad F\sqrt{\frac{\pi}{\alpha\hbar}} = 2D\sqrt{\frac{\pi}{\alpha\hbar}}\cos\theta, \quad \text{or} \quad F = 2D\cos\theta.$$

Putting these into (iii) : $\boxed{\psi_{\text{WKB}}(x) = \frac{D}{\sqrt{|p(x)|}}\left[2\cos\theta e^{\frac{1}{\hbar}\int_x^{x_1}|p(x')|\,dx'} + \sin\theta e^{-\frac{1}{\hbar}\int_x^{x_1}|p(x')|\,dx'}\right]}$ $(0 < x < x_1)$.

(b)

Odd(−) case: (iii) $\Longrightarrow \psi(0) = 0 \Rightarrow 2\cos\theta e^{\frac{1}{\hbar}\int_0^{x_1}|p(x')|\,dx'} + \sin\theta e^{-\frac{1}{\hbar}\int_0^{x_1}|p(x')|\,dx'} = 0.$

$\frac{1}{\hbar}\int_0^{x_1}|p(x')|\,dx' = \frac{1}{2}\phi$, with ϕ defined by Eq. 8.60. So $\sin\theta e^{-\phi/2} = -2\cos\theta e^{\phi/2}$, or $\tan\theta = -2e^{\phi}$.

$$\text{Even(+) case: (iii)} \Longrightarrow \psi'(0) = 0 \Rightarrow -\frac{1}{2}\frac{D}{(|p(x)|)^{3/2}}\left.\frac{d|p(x)|}{dx}\right|_0 \left[2\cos\theta e^{\phi/2} + \sin\theta e^{-\phi/2}\right]$$

$$+\frac{D}{\sqrt{|p(x)|}}\left[2\cos\theta e^{\frac{1}{\hbar}\int_0^{x_1}|p(x')|\,dx'}\left(-\frac{1}{\hbar}|p(0)|\right) + \sin\theta e^{-\frac{1}{\hbar}\int_0^{x_1}|p(x')|\,dx'}\left(\frac{1}{\hbar}|p(0)|\right)\right] = 0.$$

Now $\frac{d|p(x)|}{dx} = \frac{d}{dx}\sqrt{2m[V(x)-E]} = \sqrt{2m}\frac{1}{2}\frac{1}{\sqrt{V-E}}\frac{dV}{dx}$, and $\left.\frac{dV}{dx}\right|_0 = 0$, so $\left.\frac{d|p(x)|}{dx}\right|_0 = 0.$

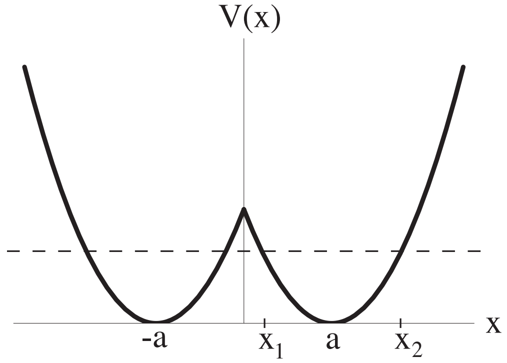
$2\cos\theta e^{\phi/2} = \sin\theta e^{-\phi/2}$, or $\tan\theta = 2e^{\phi}$. Combining the two results: $\tan\theta = \pm 2e^{\phi}$. QED

(c)

$$\tan\theta = \tan\left[\left(n+\frac{1}{2}\right)\pi + \epsilon\right] = \frac{\sin\left[\left(n+\frac{1}{2}\right)\pi+\epsilon\right]}{\cos\left[\left(n+\frac{1}{2}\right)\pi+\epsilon\right]} = \frac{(-1)^n\cos\epsilon}{(-1)^{n+1}\sin\epsilon} = -\frac{\cos\epsilon}{\sin\epsilon} \approx -\frac{1}{\epsilon}.$$

So $-\frac{1}{\epsilon} \approx \pm 2e^{\phi}$, or $\epsilon \approx \mp\frac{1}{2}e^{-\phi}$, or $\theta - \left(n+\frac{1}{2}\right)\pi \approx \mp\frac{1}{2}e^{-\phi}$, so $\theta \approx \left(n+\frac{1}{2}\right)\pi \mp \frac{1}{2}e^{-\phi}$. QED

[Note: Since θ (Eq. 9.59) is positive, n must be a *non-negative* integer: $n = 0, 1, 2, \ldots$. This is like harmonic oscillator (conventional) numbering, since it starts with $n = 0$.]



(d)

$$\begin{aligned}
\theta &= \frac{1}{\hbar}\int_{x_1}^{x_2}\sqrt{2m\left[E-\frac{1}{2}m\omega^2(x-a)^2\right]}\,dx. \quad \text{Let } z = x-a \text{ (shifts the origin to a).}\\
&= \frac{2}{\hbar}\int_0^{z_2}\sqrt{2m\left[E-\frac{1}{2}m\omega^2 z^2\right]}\,dz, \quad \text{where} \quad E = \frac{1}{2}m\omega^2 z_2^2.\\
&= \frac{2}{\hbar}m\omega\int_0^{z_2}\sqrt{z_2^2-z^2}\,dz = \frac{m\omega}{\hbar}\left[z\sqrt{z_2^2-z^2}+z_2^2\sin^{-1}(z/z_2)\right]\Bigg|_0^{z_2} = \frac{m\omega}{\hbar}z_2^2\sin^{-1}(1) = \frac{\pi}{2}\frac{m\omega}{\hbar}z_2^2,\\
&= \frac{\pi}{2}\frac{m\omega}{\hbar}\frac{2E}{m\omega^2} = \boxed{\frac{\pi E}{\hbar\omega}.}
\end{aligned}$$

Putting this into Eq. 9.62 yields $\dfrac{\pi E}{\hbar\omega} \approx \left(n+\dfrac{1}{2}\right)\pi \mp \dfrac{1}{2}e^{-\phi}$, or $E_n^{\pm} \approx \left(n+\dfrac{1}{2}\right)\hbar\omega \mp \dfrac{\hbar\omega}{2\pi}e^{-\phi}$. QED

(e)

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_n^+ e^{-iE_n^+ t/\hbar} + \psi_n^- e^{-iE_n^- t/\hbar}\right) \Longrightarrow$$

$$|\Psi(x,t)|^2 = \frac{1}{2}\left[|\psi_n^+|^2 + |\psi_n^-|^2 + \psi_n^+\psi_n^-\left(e^{i(E_n^- - E_n^+)t/\hbar} + e^{-i(E_n^- - E_n^+)t/\hbar}\right)\right].$$

(Note that the wave functions (i), (ii), (iii) are *real*). But $\dfrac{E_n^- - E_n^+}{\hbar} \approx \dfrac{1}{\hbar}2\dfrac{\hbar\omega}{2\pi}e^{-\phi} = \dfrac{\omega}{\pi}e^{-\phi}$, so

$$|\Psi(x,t)|^2 = \frac{1}{2}\left[\psi_n^+(x)^2 + \psi_n^-(x)^2\right] + \psi_n^+(x)\psi_n^-(x)\cos\left(\frac{\omega}{\pi}e^{-\phi}t\right).$$

It oscillates back and forth, with period $\tau = \dfrac{2\pi}{(\omega/\pi)\,e^{-\phi}} = \dfrac{2\pi^2}{\omega}e^{\phi}$. QED

(f)

$$\phi = 2\frac{1}{\hbar}\int_0^{x_1}\sqrt{2m\left[\frac{1}{2}m\omega^2(x-a)^2 - E\right]}\,dx = \frac{2}{\hbar}\sqrt{2mE}\int_0^{x_1}\sqrt{\frac{m\omega^2}{2E}(x-a)^2 - 1}\,dx.$$

Let $z \equiv \sqrt{\dfrac{m}{2E}}\omega(a-x)$, so $dx = -\sqrt{\dfrac{2E}{m}}\dfrac{1}{\omega}dz$. Limits: $\left\{\begin{array}{l} x = 0 \Longrightarrow z = \sqrt{\dfrac{m}{2E}}\omega a \equiv z_0 \\ x = x_1 \Longrightarrow \text{radicand } = 0 \Longrightarrow z = 1 \end{array}\right\}$.

$$\begin{aligned}
\phi &= \frac{2}{\hbar}\sqrt{2mE}\sqrt{\frac{2E}{m}}\frac{1}{\omega}\int_1^{z_0}\sqrt{z^2-1}\,dz = \frac{4E}{\hbar\omega}\int_1^{z_0}\sqrt{z^2-1}\,dz = \frac{4E}{\hbar\omega}\frac{1}{2}\left[z\sqrt{z^2-1} - \ln(z+\sqrt{z^2-1})\right]\Bigg|_1^{z_0}\\
&= \boxed{\frac{2E}{\hbar\omega}\left[z_0\sqrt{z_0^2-1} - \ln\left(z_0 + \sqrt{z_0^2-1}\right)\right],}
\end{aligned}$$

where $\boxed{z_0 = a\omega\sqrt{\dfrac{m}{2E}}.}$ $V(0) = \frac{1}{2}m\omega^2 a^2$, so $V(0) \gg E \Rightarrow \dfrac{m}{2}\omega^2 a^2 \gg E \Rightarrow a\omega\sqrt{\dfrac{m}{2E}} \gg 1$, or $z_0 \gg 1$.
In that case

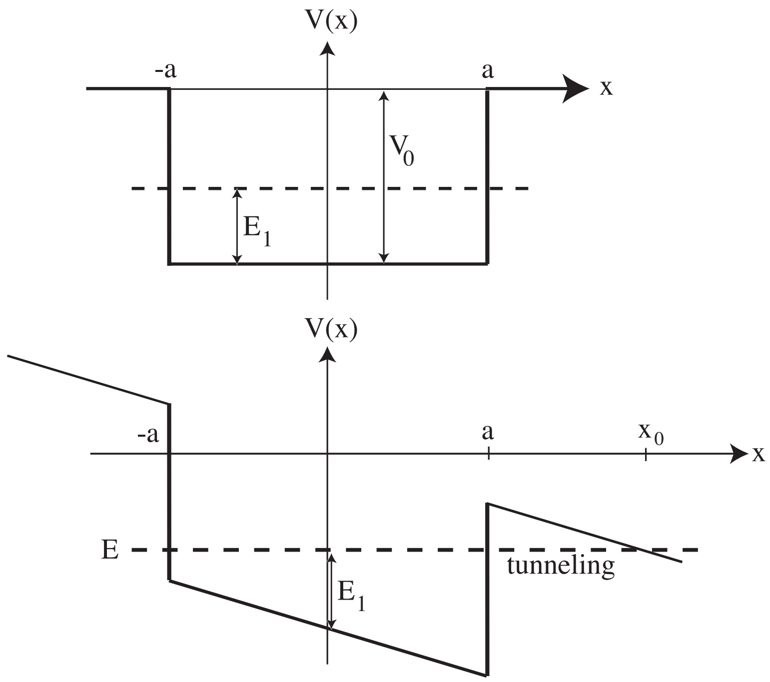
$$\phi \approx \frac{2E}{\hbar\omega}\left[z_0^2 - \ln(2z_0)\right] \approx \frac{2E}{\hbar\omega}z_0^2 = \frac{2E}{\hbar\omega}a^2\omega^2\frac{m}{2E} = \frac{m\omega a^2}{\hbar}.$$

This, together with Eq. 9.65, gives us the period of oscillation in a double well.

Problem 9.18

(a) $E_n \approx \dfrac{n^2\pi^2\hbar^2}{2m(2a)^2}$. With $n=1$, $\boxed{E_1 = \dfrac{\pi^2\hbar^2}{8ma^2}.}$

(b)



(c)

$$\begin{aligned}
\gamma &= \frac{1}{\hbar}\int_a^{x_0} |p(x)|\,dx. \quad \alpha x_0 = V_0 - E_1 \quad \Rightarrow \quad x_0 = \frac{V_0-E_1}{\alpha}. \\
p(x) &= \sqrt{2m\left[E-V(x)\right]}; \quad V(x) = -\alpha x, \quad E = E_1 - V_0. \\
&= \sqrt{2m(E_1-V_0+\alpha x)} = \sqrt{2m\alpha}\,\sqrt{x-x_0}; \quad |p(x)| = \sqrt{2m\alpha}\,\sqrt{x_0-x}. \\
\gamma &= \frac{1}{\hbar}\sqrt{2m\alpha}\int_a^{x_0}\sqrt{x_0-x}\,dx = \frac{\sqrt{2m\alpha}}{\hbar}\left[-\frac{2}{3}(x_0-x)^{3/2}\right]\Bigg|_a^{x_0} = \frac{2}{3}\frac{\sqrt{2m\alpha}}{\hbar}(x_0-a)^{3/2}.
\end{aligned}$$

Now $x_0 - a = (V_0 - E_1 - a\alpha)/\alpha$, and $\alpha a \ll \hbar^2/ma^2 \approx E_1 \ll V_0$, so we can drop E_1 and αa. Then

$$\gamma \approx \frac{2}{3}\frac{\sqrt{2m\alpha}}{\hbar}\left(\frac{V_0}{\alpha}\right)^{3/2} = \boxed{\frac{\sqrt{8mV_0^3}}{3\alpha\hbar}.}$$

Equation 9.29 $\Rightarrow$ $\tau = \dfrac{4a}{v}e^{2\gamma}$, where $\dfrac{1}{2}mv^2 \approx \dfrac{\pi^2\hbar^2}{8ma^2} \Rightarrow v^2 = \dfrac{\pi^2\hbar^2}{4m^2a^2}$, or $v = \dfrac{\pi\hbar}{2ma}$. So

$$\tau = \frac{4a}{\pi\hbar}2ma\,e^{2\gamma} = \boxed{\frac{8ma^2}{\pi\hbar}e^{2\gamma}.}$$

(d)

$$\tau = \frac{(8)\left(9.1\times 10^{-31}\right)\left(10^{-10}\right)^2}{\pi\left(1.05\times 10^{-34}\right)} e^{2\gamma} = \left(2\times 10^{-16}\right) e^{2\gamma};$$

$$\gamma = \frac{\sqrt{(8)\left(9.1\times 10^{-31}\right)\left(20\times 1.6\times 10^{-19}\right)^3}}{(3)\left(1.6\times 10^{-19}\right)\left(7\times 10^{6}\right)\left(1.05\times 10^{-34}\right)} = 4.4\times 10^4; \quad e^{2\gamma} = e^{8.8\times 10^4} = \left(10^{\log e}\right)^{8.8\times 10^4} = 10^{38{,}000}.$$

$$\tau = \left(2\times 10^{-16}\right)\times 10^{38{,}000}\ \text{s} = \boxed{10^{38{,}000}\ \text{yr.}}$$

Seconds, years ... it hardly matters; nor is the factor out front significant. This is a huge number—the age of the universe is about 10^{10} years. In any event, this is clearly *not* something to worry about.

Problem 9.19

Equation 9.23 $\Rightarrow$ the tunneling probability: $T = e^{-2\gamma}$, where

$$\gamma = \frac{1}{\hbar}\int_0^{x_0}\sqrt{2m(V-E)}\,dx. \quad \text{Here} \quad V(x) = mgx,\ E = 0,\ x_0 = \sqrt{R^2 + (h/2)^2} - h/2 \text{ (half the diagonal).}$$

$$= \frac{\sqrt{2m}}{\hbar}\sqrt{mg}\int_0^{x_0} x^{1/2}\,dx = \frac{m}{\hbar}\sqrt{2g}\frac{2}{3}x^{3/2}\Big|_0^{x_0} = \frac{2m}{3\hbar}\sqrt{2g}\,x_0^{3/2}.$$

I estimate: $h = 10$ cm, $R = 3$ cm, $m = 300$ gm; let $g = 9.8$ m/s^2. Then $x_0 = \sqrt{9+25} - 5 = 0.83$ cm, and

$$\gamma = \frac{(2)(0.3)}{(3)(1.05\times 10^{-34})}\sqrt{(2)(9.8)}\,(0.0083)^{3/2} = 6.4\times 10^{30}.$$

Frequency of "attempts": say $f = v/2R$. We want the product of the number of attempts (ft) and the probability of toppling at each attempt (T), to be 1:

$$t\frac{v}{2R}e^{-2\gamma} = 1 \quad \Rightarrow \quad t = \frac{2R}{v}e^{2\gamma}.$$

Estimating the thermal velocity: $\frac{1}{2}mv^2 = \frac{1}{2}k_BT$ (I'm done with the tunneling probability; from now on T is the temperature, 300 K) $\Rightarrow v = \sqrt{k_BT/m}$.

$$t = 2R\sqrt{\frac{m}{k_BT}}\,e^{2\gamma} = 2(0.03)\sqrt{\frac{0.3}{(1.4\times 10^{-23})(300)}}\,e^{12.8\times 10^{30}} = 5\times 10^8\left(10^{\log e}\right)^{13\times 10^{30}} = (5\times 10^8)\times 10^{5.6\times 10^{30}}\ \text{s}$$

$$= \boxed{16\times 10^{5.6\times 10^{30}}\ \text{yr.}}$$

Don't hold your breath.

[Actually, to tunnel *all the way* through the classically forbidden region, the center of mass must not only rise from 0 to x_0, but also drop back to 0. This doubles γ, and makes the final exponent 1×10^{31}.]

Problem 9.20

(a) $\phi(x) = \frac{1}{\hbar}\int_0^x p(x')\,dx'$; $\phi'(x) = \frac{1}{\hbar}p(x)$; $p(x) = \sqrt{2m(E - V(x))}$. But $V(x) = 0$ for $|x| \geq a$, so $p(\pm a) = \sqrt{2mE} = \hbar k$; $\phi'(\pm a) = k$; $p'(\pm a) = 0$ (the latter follows because $p(x)$ is constant for $|x| \geq a$ (so it's derivative is zero in that region), and by assumption $V(x)$ is smooth).

Boundary conditions at $-a$:

$$\begin{aligned}
\left(Ae^{-ika} + Be^{ika}\right) &= \frac{1}{\sqrt{p(-a)}}\left[C_+e^{i\phi(-a)} + C_-e^{-i\phi(-a)}\right], \\
ik\left(Ae^{-ika} - Be^{ika}\right) &= \frac{i}{\sqrt{p(-a)}}\left[C_+e^{i\phi(-a)} - C_-e^{-i\phi(-a)}\right]\phi'(-a).
\end{aligned}$$

(There's another term in the second equation, where $1/\sqrt{p(x)}$ is differentiated, but since $\frac{d}{dx}\left(\frac{1}{\sqrt{p(x)}}\right) = -\frac{1}{2}\frac{1}{(p(x))^{3/2}}p'(x)$, and $p'(-a) = 0$, it contributes nothing.) Meanwhile, using $\phi'(-a) = k$, the second equation simplifies to

$$\left(Ae^{-ika} - Be^{ika}\right) = \frac{1}{\sqrt{p(-a)}}\left[C_+e^{i\phi(-a)} - C_-e^{-i\phi(-a)}\right].$$

Subtracting this from the first equation, we find:

$$Be^{ika} = \frac{1}{\sqrt{p(-a)}}C_-e^{-i\phi(-a)}.$$

Boundary conditions at a:

$$\begin{aligned}
Ce^{ika} &= \frac{1}{\sqrt{p(a)}}\left[C_+e^{i\phi(a)} + C_-e^{-i\phi(a)}\right], \\
ikCe^{ika} &= \frac{i}{\sqrt{p(a)}}\left[C_+e^{i\phi(a)} - C_-e^{-i\phi(a)}\right]\phi'(a).
\end{aligned}$$

(Again, the other term in the second equation is zero.) Thus

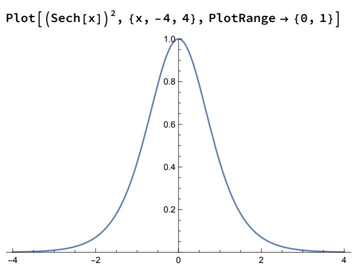
$$Ce^{ika} = \frac{1}{\sqrt{p(a)}}\left[C_+e^{i\phi(a)} - C_-e^{-i\phi(a)}\right].$$

Subtracting this from the first equation yields

$$0 = \frac{1}{\sqrt{p(a)}}C_-e^{-i\phi(a)} \quad\Rightarrow\quad C_- = 0.$$

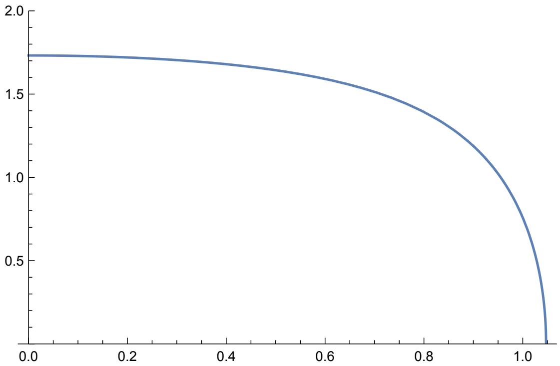
Combining the results of the boundary conditions at $-a$ and at $+a$, $B = 0$, and hence $\boxed{R = 0.}$

(b)



$\operatorname{sech}(iz) = \dfrac{1}{\cos(z)}$, so $p(iy) = \sqrt{2m\left(E - \dfrac{V_0}{\cos^2(y/a)}\right)}$. Here's the graph:

```
Plot[√(4 - (1/Cos[x])^2), {x, 0, 1.5}, PlotRange → {0, 2}]
```



$$\lambda = \frac{2}{\hbar}\int_0^{y_0} p(iy)\,dy = \frac{2}{\hbar}\int_0^{y_0}\sqrt{2m\left(E - \frac{V_0}{\cos^2(y/a)}\right)}\,dy = \frac{2a}{\hbar}\sqrt{2mV_0}\int_0^{u_0}\sqrt{\beta^2 - \frac{1}{\cos^2 u}}\,du,$$

(where $\beta \equiv \sqrt{E/V_0}$ and $u \equiv y/a$)

$$= \frac{2a}{\hbar}\sqrt{2mV_0}\int_0^{u_0}\frac{\sqrt{\beta^2\cos^2 u - 1}}{\cos u}\,du. \quad \text{Now let} \quad z \equiv \sin u, \quad \text{so} \quad dz = \cos u\,du:$$

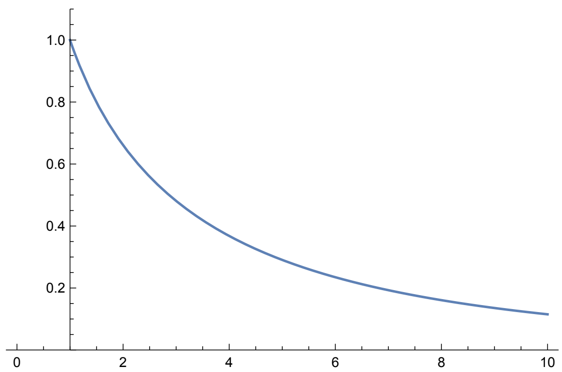
$$= \frac{2a}{\hbar}\sqrt{2mV_0}\int_0^{z_0}\frac{\sqrt{\beta^2(1-z^2)-1}}{1-z^2}\,dz = \frac{2a}{\hbar}\sqrt{2mV_0}\,\beta\int_0^{z_0}\frac{\sqrt{z_0^2 - z^2}}{1-z^2}\,dz, \quad \text{where} \quad z_0^2 \equiv 1 - (1/\beta^2).$$

Mathematica says this integral is $\dfrac{\pi}{2}\left(1 - \sqrt{1 - z_0^2}\right) = \dfrac{\pi}{2}\left(1 - \dfrac{1}{\beta}\right)$

$$= \frac{2a}{\hbar}\sqrt{2mV_0}\,\frac{\pi}{2}(\beta - 1) = \frac{\pi a}{\hbar}\sqrt{2mV_0}\left(\sqrt{\frac{E}{V_0}} - 1\right) = \frac{\pi a}{\hbar}\left(\sqrt{2mE} - \sqrt{2mV_0}\right). \quad \checkmark$$

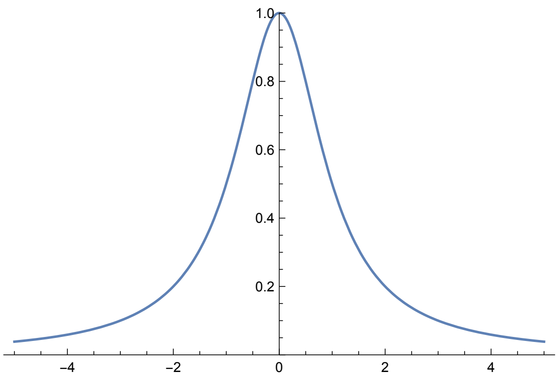
Here's the graph of $R(E)$:

```
Plot[e^(1-√x), {x, 1, 10}, PlotRange → {0, 1.1}, AxesOrigin → {1, 0}]
```



(c) Here's the plot of $V(x)$:

```
Plot[1/(1 + x^2), {x, -5, 5}, PlotRange → {0, 1}]
```



In the notation of Part (b):

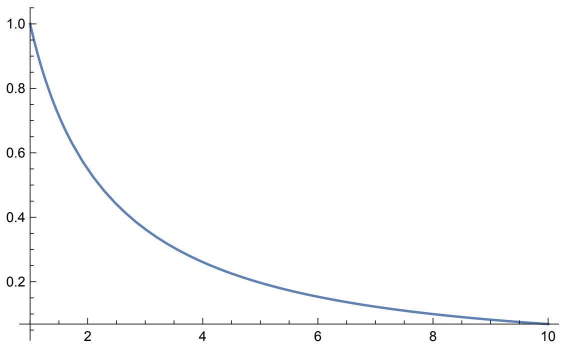
$$\begin{aligned}
\lambda &= \frac{2}{\hbar}\int_0^{y_0}\sqrt{2m\left(E-\frac{V_0}{1-(y/a)^2}\right)}\,dy = \frac{2a}{\hbar}\sqrt{2mV_0}\int_0^{u_0}\sqrt{\beta^2-\frac{1}{1-u^2}}\,du \\
&= \frac{2a\beta}{\hbar}\sqrt{2mV_0}\int_0^{u_0}\frac{\sqrt{u_0^2-u^2}}{\sqrt{1-u^2}}\,du, \quad \text{where} \quad u_0^2 = 1-(1/\beta^2); \\
&= \frac{2a\beta}{\hbar}\sqrt{2mV_0}\,u_0\int_0^{u_0}\frac{\sqrt{1-(u/u_0)^2}}{\sqrt{1-u^2}}\,du = \boxed{\frac{2a}{\hbar}\sqrt{2m(E-V_0)}E(u_0|u_0^{-2}),}
\end{aligned}$$

where $E(x|m)$ is the elliptic integral of the second kind (Arfken, third edition, Equation (5.132b)). Here's the plot of R:

```
w[x_] := 1 - 1/x

L[x_] := Sqrt[w[x]]/Sqrt[1 - w[x]] EllipticE[ArcSin[Sqrt[w[x]]], 1/w[x]]

Plot[e^(-L[x]), {x, 1, 10}]
```

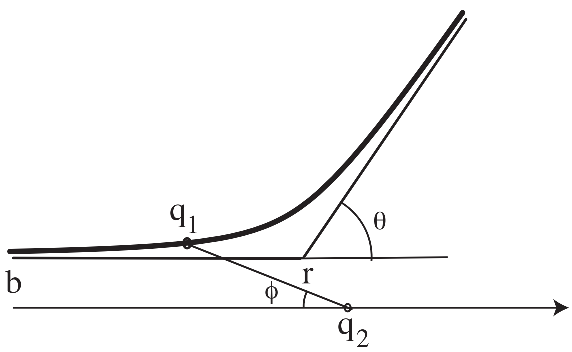


Chapter 10

Scattering

Problem 10.1

(a)



Conservation of energy: $E = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2) + V(r)$, where $V(r) = \frac{q_1 q_2}{4\pi\epsilon}\frac{1}{r}$.

Conservation of angular momentum: $J = mr^2\dot{\phi}$. So $\dot{\phi} = \frac{J}{mr^2}$.

$\dot{r}^2 + \frac{J^2}{m^2r^2} = \frac{2}{m}(E - V)$. We want r as a function of ϕ (not t). Also, let $u \equiv 1/r$. Then

$\dot{r} = \frac{dr}{dt} = \frac{dr}{du}\frac{du}{d\phi}\frac{d\phi}{dt} = \left(-\frac{1}{u^2}\right)\frac{du}{d\phi}\frac{J}{m}u^2 = -\frac{J}{m}\frac{du}{d\phi}$. Then: $\left(-\frac{J}{m}\frac{du}{d\phi}\right)^2 + \frac{J^2}{m^2}u^2 = \frac{2}{m}(E - V)$, or

$\left(\frac{du}{d\phi}\right)^2 = \frac{2m}{J^2}(E-V)-u^2$; $\frac{du}{d\phi} = \sqrt{\frac{2m}{J^2}(E - V) - u^2}$; $d\phi = \frac{du}{\sqrt{\frac{2m}{J^2}(E - V) - u^2}} = \frac{du}{\sqrt{I(u)}}$, where

$I(u) \equiv \frac{2m}{J^2}(E - V) - u^2$. Now, the particle q_1 starts out at $r = \infty$ $(u = 0)$, $\phi = 0$, and the point of closest approach is $r_{\min}$ $(u_{\max})$, Φ : $\Phi = \int_0^{u_{\max}} \frac{du}{\sqrt{I}}$. It now swings through an equal angle Φ

on the way *out*, so $\Phi + \Phi + \theta = \pi$, or $\theta = \pi - 2\Phi$. $\theta = \pi - 2\int_0^{u_{\max}} \frac{du}{\sqrt{I(u)}}$.

So far this is *general*; now we put in the specific potential:

$$I(u) = \frac{2mE}{J^2} - \frac{2m}{J^2}\frac{q_1q_2}{4\pi\epsilon_0}u - u^2 = (u_2 - u)(u - u_1), \quad \text{where } u_1 \text{ and } u_2 \text{ are the two roots.}$$

(Since $du/d\phi = \sqrt{I(u)}$, $u_{\max}$ is one of the roots; setting $u_2 > u_1$, $u_{\max} = u_2$.)

$$\begin{aligned}
\theta &= \pi - 2\int_0^{u_2} \frac{du}{\sqrt{(u_2-u)(u-u_1)}} = \pi + 2\sin^{-1}\left(\frac{-2u+u_1+u_2}{u_2-u_1}\right)\Bigg|_0^{u_2} \\
&= \pi + 2\left[\sin^{-1}(-1) - \sin^{-1}\left(\frac{u_1+u_2}{u_2-u_1}\right)\right] \\
&= \pi + 2\left[-\frac{\pi}{2} - \sin^{-1}\left(\frac{u_1+u_2}{u_2-u_1}\right)\right] = -2\sin^{-1}\left(\frac{u_1+u_2}{u_2-u_1}\right).
\end{aligned}$$

Now $J = mvb$, $E = \frac{1}{2}mv^2$, where v is the incoming velocity, so $J^2 = m^2b^2(2E/m) = 2mb^2E$, and hence $2m/J^2 = 1/b^2E$. So

$$I(u) = \frac{1}{b^2} - \frac{1}{b^2}\left(\frac{1}{E}\frac{q_1q_2}{4\pi\epsilon_0}\right)u - u^2. \quad \text{Let } A \equiv \frac{q_1q_2}{4\pi\epsilon_0 E}, \quad \text{so} \quad -I(u) = u^2 + \frac{A}{b^2}u - \frac{1}{b^2}.$$

To get the roots: $u^2 + \frac{A}{b^2}u - \frac{1}{b^2} = 0 \Longrightarrow u = \frac{1}{2}\left[-\frac{A}{b^2} \pm \sqrt{\frac{A^2}{b^4} + \frac{4}{b^2}}\right] = \frac{A}{2b^2}\left[-1 \pm \sqrt{1 + \left(\frac{2b}{A}\right)^2}\right]$.

Thus $u_2 = \frac{A}{2b^2}\left[-1 + \sqrt{1+\left(\frac{2b}{A}\right)^2}\right]$, $u_1 = \frac{A}{2b^2}\left[-1 - \sqrt{1+\left(\frac{2b}{A}\right)^2}\right]$; $\frac{u_1+u_2}{u_2-u_1} = \frac{-1}{\sqrt{1+(2b/A)^2}}$.

$$\theta = 2\sin^{-1}\left(\frac{1}{\sqrt{1+(2b/A)^2}}\right), \quad \text{or} \quad \frac{1}{\sqrt{1+(2b/A)^2}} = \sin\left(\frac{\theta}{2}\right); \quad 1 + \left(\frac{2b}{A}\right)^2 = \frac{1}{\sin^2(\theta/2)};$$

$$\left(\frac{2b}{A}\right)^2 = \frac{1-\sin^2(\theta/2)}{\sin^2(\theta/2)} = \frac{\cos^2(\theta/2)}{\sin^2(\theta/2)}; \quad \frac{2b}{A} = \cot(\theta/2), \quad \text{or} \quad \boxed{b = \frac{q_1q_2}{8\pi\epsilon_0 E}\cot(\theta/2).}$$

(b)

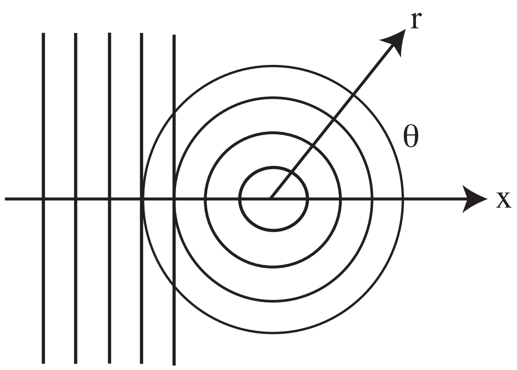
$$\begin{aligned}
D(\theta) &= \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|. \quad \text{Here } \frac{db}{d\theta} = \frac{q_1q_2}{8\pi\epsilon_0 E}\left(-\frac{1}{2\sin^2(\theta/2)}\right). \\
&= \frac{1}{2\sin(\theta/2)\cos(\theta/2)}\frac{q_1q_2}{8\pi\epsilon_0 E}\frac{\cos(\theta/2)}{\sin(\theta/2)}\frac{q_1q_2}{8\pi\epsilon_0 E}\frac{1}{2\sin^2(\theta/2)} = \boxed{\left[\frac{q_1q_2}{16\pi\epsilon_0 E\sin^2(\theta/2)}\right]^2.}
\end{aligned}$$

(c)

$$\sigma = \int D(\theta)\sin\theta\, d\theta\, d\phi = 2\pi\left(\frac{q_1q_2}{16\pi\epsilon_0 E}\right)^2 \int_0^{\pi} \frac{\sin\theta}{\sin^4(\theta/2)}\, d\theta.$$

This integral does not converge, for near $\theta = 0$ (and again near π) we have $\sin\theta \approx \theta$, $\sin(\theta/2) \approx \theta/2$, so the integral goes like $16\int_0^{\epsilon}\theta^{-3}\,d\theta = -\,8\theta^{-2}\big|_0^{\epsilon} \to \infty$.

Problem 10.2



Two dimensions: $\boxed{\psi(r,\theta) \approx A\left[e^{ikx} + f(\theta)\frac{e^{ikr}}{\sqrt{r}}\right].}$

One dimension: $\boxed{\psi(x) \approx A\left[e^{ikx} + f(x/|x|)e^{-ikx}\right].}$

Problem 10.3

Multiply Eq. 10.32 by $P_{\ell'}(\cos\theta)\sin\theta\,d\theta$ and integrate from 0 to π, exploiting the orthogonality of the Legendre polynomials (Eq. 4.34)—which, with the change of variables $x \equiv \cos\theta$, says

$$\int_0^\pi P_\ell(\cos\theta)P_{\ell'}(\cos\theta)\sin\theta\,d\theta = \left(\frac{2}{2\ell+1}\right)\delta_{\ell\ell'}.$$

The delta function collapses the sum, and we get

$$2i^{\ell'}\left[j_{\ell'}(ka) + ika_{\ell'}h_{\ell'}^{(1)}(ka)\right] = 0,$$

and hence (dropping the primes)

$$a_\ell = -\frac{j_\ell(ka)}{ikh_\ell^{(1)}(ka)}. \quad \text{QED}$$

Problem 10.4

Keeping only the $\ell = 0$ terms, Eq. 10.29 says that in the exterior region:

$$\psi \approx A\left[j_0(kr) + ika_0h_0^{(1)}(kr)\right]P_0(\cos\theta) = A\left[\frac{\sin(kr)}{kr} + ika_0\left(-i\frac{e^{ikr}}{kr}\right)\right] = A\left[\frac{\sin(kr)}{kr} + a_0\frac{e^{ikr}}{r}\right] \quad (r > a).$$

In the internal region Eq. 10.18 (with n_ℓ eliminated because it blows up at the origin) yields

$$\psi(r) \approx bj_0(kr) = b\frac{\sin(kr)}{kr} \quad (r < a).$$

The boundary conditions hold independently for each ℓ, as you can check by keeping the summation over ℓ and exploiting the orthogonality of the Legendre polynomials:

(1) ψ continuous at $r=a$: $\quad A\left[\frac{\sin ka}{ka}+a_0\frac{e^{ika}}{a}\right]=b\frac{\sin ka}{ka}.$

(2) ψ' discontinuous at $r=a$: Integrating the radial equation across the delta function gives

$$-\frac{\hbar^2}{2m}\int\frac{d^2u}{dr^2}\,dr+\int\left[\alpha\delta(r-a)+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u\,dr=E\int u\,dr\Rightarrow-\frac{\hbar^2}{2m}\Delta u'+\alpha u(a)=0,\text{ or }\ \Delta u'=\frac{2m\alpha}{\hbar^2}u(a).$$

Now $\quad u=rR,\quad$ so $u'=R+rR'$; $\quad \Delta u'=\Delta R+a\Delta R'=a\Delta R'=\frac{2m\alpha}{\hbar^2}aR(a)$, or $\Delta\psi'=\frac{2m\alpha}{\hbar^2}\psi(a)=\frac{\beta}{a}\psi(a).$

$$\frac{A}{ka}\left[k\cos(ka)+a_0ik^2e^{ika}\right]-\frac{A}{ka^2}\cancel{\left[\sin(ka)+a_0ke^{ika}\right]}-\frac{b}{ka}k\cos(ka)+\cancel{\frac{b}{ka^2}\sin ka}=\frac{\beta}{a}b\frac{\sin(ka)}{ka}.$$

The indicated terms cancel (by **(1)**), leaving $\quad A\left[\cos(ka)+ia_0ke^{ika}\right]=b\left[\cos(ka)+\frac{\beta}{ka}\sin(ka)\right].$

Using **(1)** to eliminate b: $\quad A\left[\cos(ka)+ia_0ke^{ika}\right]=\left[\cot(ka)+\frac{\beta}{ka}\right]\left[\sin(ka)+a_0ke^{ika}\right]A.$

$$\cancel{\cos(ka)}+ia_0ke^{ika}=\cancel{\cos(ka)}+\frac{\beta}{ka}\sin(ka)+a_0k\cot(ka)e^{ika}+\beta\frac{a_0}{a}e^{ika}.$$

$$ia_0ke^{ika}\left[1+i\cot(ka)+i\frac{\beta}{ka}\right]=\frac{\beta}{ka}\sin(ka).\quad\text{But } ka\ll1,\text{ so }\sin(ka)\approx ka,\text{ and }\cot(ka)=\frac{\cos(ka)}{\sin(ka)}\approx\frac{1}{ka}.$$

$$ia_0k(1+ika)\left[1+\frac{i}{ka}(1+\beta)\right]=\beta;\quad ia_0k\left[1+\frac{i}{ka}(1+\beta)+ika-1-\beta\right]\approx ia_0k\left[\frac{i}{ka}(1+\beta)\right]=\beta.$$

$\boxed{a_0=-\frac{a\beta}{1+\beta}.}$ Equation 10.25 $\Rightarrow f(\theta)\approx a_0=\boxed{-\frac{a\beta}{1+\beta}.}$ Equation 10.14 $\Rightarrow D=|f|^2=\boxed{\left(\frac{a\beta}{1+\beta}\right)^2.}$

Equation 10.27 $\quad\Rightarrow\ \sigma=4\pi D=\boxed{4\pi\left(\frac{a\beta}{1+\beta}\right)^2.}$

Problem 10.5

(a) In the region to the left

$$\psi(x)=Ae^{ikx}+Be^{-ikx}\quad(x\le -a).$$

In the region $-a<x<0$, the Schrödinger equation gives

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}-V_0\psi=E\psi\quad\Rightarrow\quad\frac{d^2\psi}{dx^2}=-(k')^2\psi$$

where $k'=\sqrt{2m(E+V_0)}/\hbar$. $\quad$ The general solution is

$$\psi=C\sin(k'x)+D\cos(k'x)$$

But $\psi(0)=0$ implies $D=0$, so

$$\psi(x)=C\sin(k'x)\quad(-a\le x\le 0).$$

The continuity of $\psi(x)$ and $\psi'(x)$ at $x = -a$ says

$$Ae^{-ika} + Be^{ika} = -C\sin(k'a), \quad ikAe^{-ika} - ikBe^{ika} = k'C\cos(k'a).$$

Divide and solve for B:

$$\frac{ikAe^{-ika} - ikBe^{ika}}{Ae^{-ika} + Be^{ika}} = -k'\cot(k'a),$$

$$ikAe^{-ika} - ikBe^{ika} = -Ae^{-ika}k'\cot(k'a) - Be^{ika}k'\cot(k'a),$$

$$Be^{ika}\left[-ik + k'\cot(k'a)\right] = Ae^{-ika}\left[-ik - k'\cot(k'a)\right].$$

$$\boxed{B = Ae^{-2ika}\left[\frac{k - ik'\cot(k'a)}{k + ik'\cot(k'a)}\right].}$$

(b)

$$|B|^2 = |A|^2\left[\frac{k - ik'\cot(k'a)}{k + ik'\cot(k'a)}\right]\cdot\left[\frac{k + ik'\cot(k'a)}{k - ik'\cot(k'a)}\right] = |A|^2. \quad \checkmark$$

(c) From part (a) the wave function for $x < -a$ is

$$\psi(x) = Ae^{ikx} + Ae^{-2ika}\left[\frac{k - ik'\cot(k'a)}{k + ik'\cot(k'a)}\right]e^{-ikx}.$$

But by definition of the phase shift (Eq. 10.40)

$$\psi(x) = A\left[e^{ikx} - e^{i(2\delta - kx)}\right].$$

so

$$e^{-2ika}\left[\frac{k - ik'\cot(k'a)}{k + ik'\cot(k'a)}\right] = -e^{2i\delta}.$$

This is *exact.* For a very deep well, $E \ll V_0$, $\quad k = \sqrt{2mE}/\hbar \ll \sqrt{2m(E+V_0)}/\hbar = k'$, so

$$e^{-2ika}\left[\frac{-ik'\cot(k'a)}{ik'\cot(k'a)}\right] = -e^{2i\delta}; \quad e^{-2ika} = e^{2i\delta}; \quad \boxed{\delta = -ka.}$$

Problem 10.6

From Eq. 10.46, $\quad a_\ell = \dfrac{1}{k}e^{i\delta_\ell}\sin\delta_\ell$, $\quad$ and Eq. 10.33, $\quad a_\ell = i\dfrac{j_\ell(ka)}{kh_\ell^{(1)}(ka)}$, $\quad$ it follows that $\quad e^{i\delta_\ell}\sin\delta_\ell = i\dfrac{j_\ell(ka)}{h_\ell^{(1)}(ka)}$.

But (Eq. 10.19) $\quad h_\ell^{(1)}(x) = j_\ell(x) + in_\ell(x)$, $\quad$ so

$$e^{i\delta_\ell}\sin\delta_\ell = i\frac{j_\ell(ka)}{j_\ell(ka) + in_\ell(ka)} = i\frac{1}{1 + i(n/j)} = i\frac{1 - i(n/j)}{1 + (n/j)^2} = \frac{(n/j) + i}{1 + (n/j)^2},$$

(writing (n/j) as shorthand for $n_\ell(ka)/j_\ell(ka)$). Equating the real and imaginary parts:

$$\cos\delta_\ell\sin\delta_\ell = \frac{(n/j)}{1 + (n/j)^2}; \quad \sin^2\delta_\ell = \frac{1}{1 + (n/j)^2}.$$

Dividing the second by the first, I conclude that

$$\tan\delta_\ell = \frac{1}{(n/j)}, \qquad \text{or} \qquad \boxed{\delta_\ell = \tan^{-1}\left[\frac{j_\ell(ka)}{n_\ell(ka)}\right].}$$

Problem 10.7

$r > a: \ u(r) = A\sin(kr+\delta);$

$r < a: \ u(r) = B\sin kr + D\cos kr = B\sin kr, \quad \text{because } \ u(0) = 0 \Longrightarrow D = 0.$

Continuity at $r = a \Longrightarrow B\sin(ka) = A\sin(ka+\delta) \Longrightarrow B = A\dfrac{\sin(ka+\delta)}{\sin(ka)}$. So $\quad u(r) = A\,\dfrac{\sin(ka+\delta)}{\sin(ka)}\sin kr.$

From Problem 10.4,

$$\Delta\left(\frac{du}{dr}\right)\bigg|_{r=a} = \frac{\beta}{a}u(a) \Rightarrow Ak\cos(ka+\delta) - A\frac{\sin(ka+\delta)}{\sin(ka)}k\cos(ka) = \frac{\beta}{a}A\sin(ka+\delta).$$

$$\cos(ka+\delta) - \frac{\sin(ka+\delta)}{\sin(ka)}\cos(ka) = \frac{\beta}{ka}\sin(ka+\delta),$$

$$\sin(ka)\cos(ka+\delta) - \sin(ka+\delta)\cos(ka) = \frac{\beta}{ka}\sin(ka+\delta)\sin(ka),$$

$$\sin(ka - ka - \delta) = \frac{\beta}{ka}\sin(ka)\left[\sin(ka)\cos\delta + \cos(ka)\sin\delta\right],$$

$$-\sin\delta = \beta\frac{\sin^2(ka)}{ka}\left[\cos\delta + \cot(ka)\sin\delta\right]; \quad -1 = \beta\frac{\sin^2(ka)}{ka}\left[\cot\delta + \cot(ka)\right].$$

$$\cot\delta = -\cot(ka) - \frac{ka}{\beta\sin^2(ka)}; \quad \boxed{\cot\delta = -\left[\cot(ka) + \frac{ka}{\beta\sin^2(ka)}\right].}$$

Problem 10.8

$$G = -\frac{e^{ikr}}{4\pi r} \Longrightarrow \nabla G = -\frac{1}{4\pi}\left(\frac{1}{r}\nabla e^{ikr} + e^{ikr}\nabla\frac{1}{r}\right) \Longrightarrow$$

$$\nabla^2 G = \nabla\cdot(\nabla G) = -\frac{1}{4\pi}\left[2\left(\nabla\frac{1}{r}\right)\cdot(\nabla e^{ikr}) + \frac{1}{r}\nabla^2(e^{ikr}) + e^{ikr}\nabla^2\left(\frac{1}{r}\right)\right].$$

But $\nabla\dfrac{1}{r} = -\dfrac{1}{r^2}\,\hat{r}; \quad \nabla(e^{ikr}) = ike^{ikr}\hat{r}; \quad \nabla^2 e^{ikr} = ik\nabla\cdot(e^{ikr}\hat{r}) = ik\dfrac{1}{r^2}\dfrac{d}{dr}(r^2e^{ikr}),$

$\nabla^2 e^{ikr} = \dfrac{ik}{r^2}(2re^{ikr} + ikr^2e^{ikr}) = ike^{ikr}\left(\dfrac{2}{r} + ik\right)$; and $\nabla^2\left(\dfrac{1}{r}\right) = -4\pi\delta^3(\mathbf{r})$

(see reference in footnote 13).

$$\text{So} \quad \nabla^2 G = -\frac{1}{4\pi}\left[2\left(-\frac{1}{r^2}\,\hat{r}\right)\cdot\left(ike^{ikr}\hat{r}\right) + \frac{1}{r}ike^{ikr}\left(\frac{2}{r} + ik\right) - 4\pi e^{ikr}\delta^3(\mathbf{r})\right].$$

But $\quad e^{ikr}\delta^3(\mathbf{r}) = \delta^3(\mathbf{r})$, so

$$\nabla^2 G = \delta^3(\mathbf{r}) - \frac{1}{4\pi}e^{ikr}\left[-\frac{2ik}{r^2} + \frac{2ik}{r^2} - \frac{k^2}{r}\right] = \delta^3(\mathbf{r}) + k^2\frac{e^{ikr}}{4\pi r} = \delta^3(\mathbf{r}) - k^2 G.$$

Therefore $\quad (\nabla^2 + k^2)G = \delta^3(\mathbf{r})$. QED

Problem 10.9

$$\psi = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}; \quad V = -\frac{e^2}{4\pi\epsilon_0 r} = -\frac{\hbar^2}{ma}\frac{1}{r} \quad \text{(Eq. 4.72)}; \quad k = i\frac{\sqrt{-2mE}}{\hbar} = \frac{i}{a}.$$

In this case there is no "incoming" wave, and $\psi_0(\mathbf{r}) = 0$. Our problem is to show that

$$-\frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|} V(\mathbf{r}_0)\psi(\mathbf{r}_0)\, d^3\mathbf{r}_0 = \psi(\mathbf{r}).$$

We proceed to evaluate the left side (call it I):

$$\begin{aligned} I &= \left(-\frac{m}{2\pi\hbar^2}\right)\left(-\frac{\hbar^2}{ma}\right)\frac{1}{\sqrt{\pi a^3}}\int \frac{e^{-|\mathbf{r}-\mathbf{r}_0|/a}}{|\mathbf{r}-\mathbf{r}_0|}\frac{1}{r_0}e^{-r_0/a}\, d^3\mathbf{r}_0 \\ &= \frac{1}{2\pi a}\frac{1}{\sqrt{\pi a^3}}\int \frac{e^{-\sqrt{r^2+r_0^2-2rr_0\cos\theta}/a}e^{-r_0/a}}{\sqrt{r^2+r_0^2-2rr_0\cos\theta}\, r_0} r_0^2 \sin\theta\, dr_0\, d\theta\, d\phi. \end{aligned}$$

(I have set the z_0 axis along the—fixed—direction $\mathbf{r}$, for convenience.) Doing the ϕ integral (2π):

$$I = \frac{1}{a\sqrt{\pi a^3}}\int_0^\infty r_0 e^{-r_0/a}\left[\int_0^\pi \frac{e^{-\sqrt{r^2+r_0^2-2rr_0\cos\theta}/a}}{\sqrt{r^2+r_0^2-2rr_0\cos\theta}}\sin\theta\, d\theta\right] dr_0. \quad \text{The } \theta \text{ integral is}$$

$$\int_0^\pi \frac{e^{-\sqrt{r^2+r_0^2-2rr_0\cos\theta}/a}}{\sqrt{r^2+r_0^2-2rr_0\cos\theta}}\sin\theta\, d\theta = -\frac{a}{rr_0}\, e^{-\sqrt{r^2+r_0^2-2rr_0\cos\theta}/a}\Big|_0^\pi = -\frac{a}{rr_0}\left[e^{-(r+r_0)/a} - e^{-|r-r_0|/a}\right].$$

$$\begin{aligned} I &= -\frac{1}{r\sqrt{\pi a^3}}\int_0^\infty e^{-r_0/a}\left[e^{-(r_0+r)/a} - e^{-|r_0-r|/a}\right] dr_0 \\ &= -\frac{1}{r\sqrt{\pi a^3}}\left[e^{-r/a}\int_0^\infty e^{-2r_0/a}\, dr_0 - e^{-r/a}\int_0^r dr_0 - e^{r/a}\int_r^\infty e^{-2r_0/a}\, dr_0\right] \\ &= -\frac{1}{r\sqrt{\pi a^3}}\left[e^{-r/a}\left(\frac{a}{2}\right) - e^{-r/a}(r) - e^{r/a}\left(-\frac{a}{2}e^{-2r_0/a}\right)\Big|_r^\infty\right] \\ &= -\frac{1}{r\sqrt{\pi a^3}}\left[\frac{a}{2}e^{-r/a} - re^{-r/a} - \frac{a}{2}e^{r/a}e^{-2r/a}\right] = \frac{1}{\sqrt{\pi a^3}}e^{-r/a} = \psi(r). \quad \text{QED} \end{aligned}$$

Problem 10.10

For the potential in Eq. 10.81, Eq. 10.88 $\Longrightarrow$

$$f(\theta) = -\frac{2m}{\hbar^2\kappa}V_0\int_0^a r\sin(\kappa r)\, dr = -\frac{2mV_0}{\hbar^2\kappa}\left[\frac{1}{\kappa^2}\sin(\kappa r) - \frac{r}{\kappa}\cos(\kappa r)\right]\Big|_0^a = \boxed{-\frac{2mV_0}{\hbar^2\kappa^3}\left[\sin(\kappa a) - \kappa a\cos(\kappa a)\right],}$$

where (Eq. 10.89) $\kappa = 2k\sin(\theta/2)$. For low-energy scattering ($ka \ll 1$):

$$\sin(\kappa a) \approx \kappa a - \frac{1}{3!}(\kappa a)^3; \quad \cos(\kappa a) \approx 1 - \frac{1}{2}(\kappa a)^2; \quad \text{so}$$

$$f(\theta) \approx -\frac{2mV_0}{\hbar^2\kappa^3}\left[\kappa a - \frac{1}{6}(\kappa a)^3 - \kappa a + \frac{1}{2}(\kappa a)^3\right] = \boxed{-\frac{2}{3}\frac{mV_0 a^3}{\hbar^2},} \quad \text{in agreement with Eq. 10.82.}$$

Problem 10.11

$$\sin(\kappa r) = \frac{1}{2i}\left(e^{i\kappa r} - e^{-i\kappa r}\right), \quad \text{so} \quad \int_0^\infty e^{-\mu r}\sin(\kappa r)\,dr = \frac{1}{2i}\int_0^\infty \left[e^{-(\mu-i\kappa)r} - e^{-(\mu+i\kappa)r}\right] dr$$

$$= \frac{1}{2i}\left[\frac{e^{-(\mu-i\kappa)r}}{-(\mu-i\kappa)} - \frac{e^{-(\mu+i\kappa)r}}{-(\mu+i\kappa)}\right]\Bigg|_0^\infty = \frac{1}{2i}\left[\frac{1}{\mu-i\kappa} - \frac{1}{\mu+i\kappa}\right] = \frac{1}{2i}\left(\frac{\mu+i\kappa-\mu+i\kappa}{\mu^2+\kappa^2}\right) = \frac{\kappa}{\mu^2+\kappa^2}.$$

So $f(\theta) = -\dfrac{2m\beta}{\hbar^2\kappa}\dfrac{\kappa}{\mu^2+\kappa^2} = -\dfrac{2m\beta}{\hbar^2(\mu^2+\kappa^2)}$. QED

Problem 10.12

Equation 10.91 $\Longrightarrow D(\theta) = |f(\theta)|^2 = \left(\dfrac{2m\beta}{\hbar^2}\right)^2 \dfrac{1}{(\mu^2+\kappa^2)^2}$, where Eq. 10.89 $\Rightarrow \kappa = 2k\sin(\theta/2)$.

$$\sigma = \int D(\theta)\sin\theta\,d\theta\,d\phi = 2\pi\left(\frac{2m\beta}{\hbar^2}\right)^2\frac{1}{\mu^4}\int_0^\pi \frac{1}{\left[1+(2k/\mu)^2\sin^2(\theta/2)\right]^2}2\sin(\theta/2)\cos(\theta/2)\,d\theta.$$

Let $\dfrac{2k}{\mu}\sin(\theta/2) \equiv x$, so $2\sin(\theta/2) = \dfrac{\mu}{k}x$, and $\cos(\theta/2)\,d\theta = \dfrac{\mu}{k}\,dx$. Then

$$\sigma = 2\pi\left(\frac{2m\beta}{\hbar^2}\right)^2\frac{1}{\mu^4}\left(\frac{\mu}{k}\right)^2\int_{x_0}^{x_1}\frac{x}{(1+x^2)^2}\,dx. \quad \text{The limits are} \quad \left\{\begin{array}{l}\theta = 0 \Longrightarrow x = x_0 = 0,\\ \theta = \pi \Longrightarrow x = x_1 = 2k/\mu.\end{array}\right\} \quad \text{So}$$

$$\sigma = 2\pi\left(\frac{2m\beta}{\hbar^2}\right)^2\frac{1}{(\mu k)^2}\left[-\frac{1}{2}\frac{1}{(1+x^2)}\right]\Bigg|_0^{2k/\mu} = \pi\left(\frac{2m\beta}{\hbar^2}\right)^2\frac{1}{(\mu k)^2}\left[1-\frac{1}{1+(2k/\mu)^2}\right]$$

$$= \pi\left(\frac{2m\beta}{\hbar^2}\right)^2\frac{1}{(\mu k)^2}\left[\frac{4(k/\mu)^2}{1+4k^2/\mu^2}\right] = \pi\left(\frac{4m\beta}{\hbar^2}\right)^2\frac{1}{\mu^2}\frac{1}{\mu^2+4k^2}. \quad \text{But} \quad k^2 = \frac{2mE}{\hbar^2}, \text{ so}$$

$$\boxed{\sigma = \pi\left(\frac{4m\beta}{\mu\hbar}\right)^2\frac{1}{(\mu\hbar)^2+8mE}.}$$

Problem 10.13

(a)

$$V(\mathbf{r}) = \alpha\delta(r-a). \quad \text{Eq. 10.80} \Longrightarrow f = -\frac{m}{2\pi\hbar^2}\int V(\mathbf{r})\,d^3\mathbf{r} = -\frac{m}{2\pi\hbar^2}\alpha 4\pi\int_0^\infty \delta(r-a)r^2dr.$$

$$\boxed{f = -\frac{2m\alpha}{\hbar^2}a^2;} \quad D = |f|^2 = \boxed{\left(\frac{2m\alpha}{\hbar^2}a^2\right)^2;} \quad \sigma = 4\pi D = \boxed{\pi\left(\frac{4m\alpha}{\hbar^2}a^2\right)^2.}$$

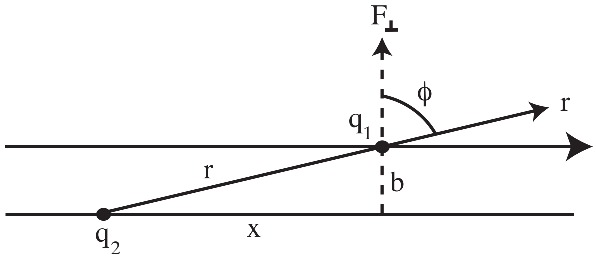
(b)

$$\text{Eq. 10.88} \Longrightarrow f = -\frac{2m}{\hbar^2\kappa}\alpha\int_0^\infty r\delta(r-a)\sin(\kappa r)\,dr = \boxed{-\frac{2m\alpha}{\hbar^2\kappa}a\sin(\kappa a)} \quad (\kappa = 2k\sin(\theta/2)).$$

(c) Note first that **(b)** reduces to **(a)** in the low-energy regime ($ka \ll 1 \Longrightarrow \kappa a \ll 1$). Since Problem 10.4 was also for low energy, what we must confirm is that Problem 10.4 reproduces **(a)** in the regime for which the Born approximation holds. Inspection shows that the answer to Problem 10.4 does reduce to $f = -2m\alpha a^2/\hbar^2$ when $\beta \ll 1$, which is to say when $f/a \ll 1$. This is the appropriate condition, since (Eq. 10.12) f/a is a measure of the relative size of the scattered wave, in the interaction region.

Problem 10.14

$$\mathbf{F} = \frac{1}{4\pi\epsilon_0}\frac{q_1q_2}{r^2}\,\hat{r}; \quad F_\perp = \frac{1}{4\pi\epsilon_0}\frac{q_1q_2}{r^2}\cos\phi; \quad \cos\phi = \frac{b}{r}, \quad \text{so} \quad F_\perp = \frac{1}{4\pi\epsilon_0}\frac{q_1q_2 b}{r^3}; \quad dt = \frac{dx}{v}.$$



$$I_\perp = \int F_\perp dt = \frac{1}{4\pi\epsilon_0}\frac{q_1q_2 b}{v}\int_{-\infty}^{\infty}\frac{dx}{(x^2+b^2)^{3/2}}. \quad \text{But}$$

$$\int_{-\infty}^{\infty}\frac{dx}{(x^2+b^2)^{3/2}} = 2\int_0^{\infty}\frac{dx}{(x^2+b^2)^{3/2}} = \left.\frac{2x}{b^2\sqrt{x^2+b^2}}\right|_0^{\infty} = \frac{2}{b^2}, \quad \text{so} \quad I_\perp = \frac{1}{4\pi\epsilon_0}\frac{2q_1q_2}{bv}.$$

$$\tan\theta = \frac{I_\perp}{mv} = \frac{q_1q_2}{4\pi\epsilon_0}\frac{1}{b(\frac{1}{2}mv^2)} = \frac{q_1q_2}{4\pi\epsilon_0}\frac{1}{bE}. \quad \boxed{\theta = \tan^{-1}\left[\frac{q_1q_2}{4\pi\epsilon_0 bE}\right].}$$

$$b = \frac{q_1q_2}{4\pi\epsilon_0}\frac{1}{E\tan\theta} = \left(\frac{q_1q_2}{8\pi\epsilon_0 E}\right)(2\cot\theta).$$

The exact answer is the same, only with $\cot(\theta/2)$ in place of $2\cot\theta$. So I must show that $\cot(\theta/2) \approx 2\cot\theta$, for small θ (that's the regime in which the impulse approximation should work). Well:

$$\cot(\theta/2) = \frac{\cos(\theta/2)}{\sin(\theta/2)} \approx \frac{1}{\theta/2} = \frac{2}{\theta}, \quad \text{for small } \theta, \quad \text{while } 2\cot\theta = 2\frac{\cos\theta}{\sin\theta} \approx 2\frac{1}{\theta}. \quad \text{So it works.}$$

Problem 10.15

First let's set up the general formalism. From Eq. 10.101:

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \int g(\mathbf{r}-\mathbf{r}_0)V(\mathbf{r}_0)\psi_0(\mathbf{r}_0)\,d^3\mathbf{r}_0 + \int g(\mathbf{r}-\mathbf{r}_0)V(\mathbf{r}_0)\left[\int g(\mathbf{r}_0-\mathbf{r}_1)V(\mathbf{r}_1)\psi_0(\mathbf{r}_1)\,d^3\mathbf{r}_1\right]d^3\mathbf{r}_0 + \cdots$$

$$\text{Put in } \psi_0(\mathbf{r}) = Ae^{ikz}, \quad g(\mathbf{r}) = -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}:$$

$$\psi(\mathbf{r}) = Ae^{ikz} - \frac{mA}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|}V(\mathbf{r}_0)e^{ikz_0}\,d^3\mathbf{r}_0$$
$$+\left(\frac{m}{2\pi\hbar^2}\right)^2 A\int \frac{e^{ik|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|}V(\mathbf{r}_0)\left[\int \frac{e^{ik|\mathbf{r}_0-\mathbf{r}_1|}}{|\mathbf{r}_0-\mathbf{r}_1|}V(\mathbf{r}_1)e^{ikz_1}\,d^3\mathbf{r}_1\right]d^3\mathbf{r}_0.$$

In the scattering region $r \gg r_0$, Eq. 10.73 $\Longrightarrow \dfrac{e^{ik|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|} \approx \dfrac{e^{ikr}}{r}e^{-i\mathbf{k}\cdot\mathbf{r}_0}$, with $\mathbf{k} \equiv k\hat{r}$, so

$$\psi(\mathbf{r}) = A\left\{e^{ikz} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int e^{-i\mathbf{k}\cdot\mathbf{r}_0}V(\mathbf{r}_0)e^{ikz_0}d^3\mathbf{r}_0\right.$$
$$\left.+\left(\frac{m}{2\pi\hbar^2}\right)^2\frac{e^{ikr}}{r}\int e^{-i\mathbf{k}\cdot\mathbf{r}_0}V(\mathbf{r}_0)\left[\int\frac{e^{ik|\mathbf{r}_0-\mathbf{r}_1|}}{|\mathbf{r}_0-\mathbf{r}_1|}V(\mathbf{r}_1)e^{ikz_1}d^3\mathbf{r}_1\right]d^3\mathbf{r}_0\right\}$$

$$\boxed{f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}V(\mathbf{r})\,d^3\mathbf{r} + \left(\frac{m}{2\pi\hbar^2}\right)^2\int e^{-i\mathbf{k}\cdot\mathbf{r}}V(\mathbf{r})\left[\int\frac{e^{ik|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|}V(\mathbf{r}_0)e^{ikz_0}d^3\mathbf{r}_0\right]d^3\mathbf{r}.}$$

I simplified the subscripts, since there is no longer any possible ambiguity. For *low-energy* scattering we drop the exponentials (see p. 393):

$$\boxed{f(\theta,\phi) \approx -\frac{m}{2\pi\hbar^2}\int V(\mathbf{r})\,d^3\mathbf{r} + \left(\frac{m}{2\pi\hbar^2}\right)^2\int V(\mathbf{r})\left[\int\frac{1}{|\mathbf{r}-\mathbf{r}_0|}V(\mathbf{r}_0)\,d^3\mathbf{r}_0\right]d^3\mathbf{r}.}$$

Now apply this to the potential in Eq. 10.81:

$$\int\frac{1}{|\mathbf{r}-\mathbf{r}_0|}V(\mathbf{r}_0)\,d^3\mathbf{r}_0 = V_0\int_0^a\frac{1}{|\mathbf{r}-\mathbf{r}_0|}r_0^2\sin\theta_0\,dr_0\,d\theta_0\,d\phi_0.$$

Orient the z_0 axis along $\mathbf{r}$, so $|\mathbf{r}-\mathbf{r}_0| = r^2 + r_0^2 - 2rr_0\cos\theta_0$.

$$\int\frac{1}{|\mathbf{r}-\mathbf{r}_0|}V(\mathbf{r}_0)\,d^3\mathbf{r}_0 = V_0 2\pi\int_0^a r_0^2\left[\int_0^\pi\frac{1}{\sqrt{r^2+r_0^2-2rr_0\cos\theta_0}}\sin\theta_0\,d\theta_0\right]dr_0.\quad\text{But}$$

$$\int_0^\pi\frac{1}{\sqrt{r^2+r_0^2-2rr_0\cos\theta_0}}\sin\theta_0\,d\theta_0 = \frac{1}{rr_0}\sqrt{r^2+r_0^2-2rr_0\cos\theta_0}\Big|_0^\pi = \frac{1}{rr_0}\left[(r_0+r)-|r_0-r|\right] = \begin{cases}2/r, & r_0<r;\\ 2/r_0, & r_0>r.\end{cases}$$

Here $r < a$ (from the "outer" integral), so

$$\int\frac{1}{|\mathbf{r}-\mathbf{r}_0|}V(\mathbf{r}_0)\,d^3\mathbf{r}_0 = 4\pi V_0\left[\frac{1}{r}\int_0^r r_0^2\,dr_0 + \int_r^a r_0\,dr_0\right] = 4\pi V_0\left[\frac{1}{r}\frac{r^3}{3}+\frac{1}{2}(a^2-r^2)\right] = 2\pi V_0\left(a^2-\frac{1}{3}r^2\right).$$

$$\int V(\mathbf{r})\left[\int\frac{1}{|\mathbf{r}-\mathbf{r}_0|}V(\mathbf{r}_0)\,d^3\mathbf{r}_0\right]d^3\mathbf{r} = V_0(2\pi V_0)4\pi\int_0^a\left(a^2-\frac{1}{3}r^2\right)r^2dr = 8\pi^2V_0^2\left[a^2\frac{a^3}{3}-\frac{1}{3}\frac{a^5}{5}\right] = \frac{32}{15}\pi^2V_0^2a^5.$$

$$f(\theta) = -\frac{m}{2\pi\hbar^2}V_0\frac{4}{3}\pi a^3 + \left(\frac{m}{2\pi\hbar^2}\right)^2\frac{32}{15}\pi^2V_0^2a^5 = \boxed{-\left(\frac{2mV_0a^3}{3\hbar^2}\right)\left[1-\frac{4}{5}\left(\frac{mV_0a^2}{\hbar^2}\right)\right].}$$

Problem 10.16

$$\left(\frac{d^2}{dx^2}+k^2\right)G(x)=\delta(x)\quad \text{(analog to Eq. 10.52).}\quad G(x)=\frac{1}{\sqrt{2\pi}}\int e^{isx}g(s)\,ds\quad \text{(analog to Eq. 10.54).}$$

$$\left(\frac{d^2}{dx^2}+k^2\right)G=\frac{1}{\sqrt{2\pi}}\int(-s^2+k^2)g(s)e^{isx}ds=\delta(x)=\frac{1}{2\pi}\int e^{isx}ds\Longrightarrow g(s)=\frac{1}{\sqrt{2\pi}(k^2-s^2)}.$$

$$G(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{isx}}{k^2-s^2}\,ds.\quad \text{Skirt the poles as in Fig. 10.10.}\quad \text{For } x>0\text{, close above:}$$

$$G(x)=-\frac{1}{2\pi}\oint\left(\frac{e^{isx}}{s+k}\right)\frac{1}{s-k}\,ds=-\frac{1}{2\pi}2\pi i\left(\frac{e^{isx}}{s+k}\right)\bigg|_{s=k}=-i\frac{e^{ikx}}{2k}.\quad \text{For}\quad x<0,\text{close below:}$$

$$G(x)=+\frac{1}{2\pi}\oint\left(\frac{e^{isx}}{s-k}\right)\frac{1}{s+k}\,ds=\frac{1}{2\pi}2\pi i\left(\frac{e^{isx}}{s-k}\right)\bigg|_{s=-k}=-i\frac{e^{-ikx}}{2k}.$$

In either case, then, $\boxed{G(x)=-\frac{i}{2k}e^{ik|x|}.}$ (Analog to Eq. 10.65.)

$$\psi(x)=\int G(x-x_0)\frac{2m}{\hbar^2}V(x_0)\psi(x_0)\,dx_0=-\frac{i}{2k}\frac{2m}{\hbar^2}\int e^{ik|x-x_0|}V(x_0)\psi(x_0)\,dx_0,$$

plus any solution $\psi_0(x)$ to the homogeneous Schrödinger equation:

$$\left(\frac{d^2}{dx^2}+k^2\right)\psi_0(x)=0.\quad \text{So:}$$

$$\boxed{\psi(x)=\psi_0(x)-\frac{im}{\hbar^2k}\int_{-\infty}^{\infty}e^{ik|x-x_0|}V(x_0)\psi(x_0)\,dx_0.}$$

Problem 10.17

For the Born approximation let $\psi_0(x)=Ae^{ikx}$, and $\psi(x)\approx Ae^{ikx}$.

$$\begin{aligned}\psi(x)&\approx A\left[e^{ikx}-\frac{im}{\hbar^2k}\int_{-\infty}^{\infty}e^{ik|x-x_0|}V(x_0)e^{ikx_0}dx_0\right]\\&=A\left[e^{ikx}-\frac{im}{\hbar^2k}\int_{-\infty}^{x}e^{ik(x-x_0)}V(x_0)e^{ikx_0}dx_0-\frac{im}{\hbar^2k}\int_{x}^{\infty}e^{ik(x_0-x)}V(x_0)e^{ikx_0}dx_0\right].\end{aligned}$$

$$\boxed{\psi(x)=A\left[e^{ikx}-\frac{im}{\hbar^2k}e^{ikx}\int_{-\infty}^{x}V(x_0)\,dx_0-\frac{im}{\hbar^2k}e^{-ikx}\int_{x}^{\infty}e^{2ikx_0}V(x_0)\,dx_0\right].}$$

Now assume $V(x)$ is localized; for large positive x, the third term is zero, and

$$\psi(x)=Ae^{ikx}\left[1-\frac{im}{\hbar^2k}\int_{-\infty}^{\infty}V(x_0)\,dx_0\right].\quad \text{This is the transmitted wave.}$$

For large negative x the middle term is zero:

$$\psi(x)=A\left[e^{ikx}-\frac{im}{\hbar^2k}e^{-ikx}\int_{-\infty}^{\infty}e^{2ikx_0}V(x_0)dx_0\right].$$

Evidently the first term is the incident wave and the second the reflected wave:

$$\boxed{R = \left(\frac{m}{\hbar^2 k}\right)^2 \left|\int_{-\infty}^{\infty} e^{2ikx} V(x)\,dx\right|^2.}$$

If you try in the same spirit to calculate the transmission coefficient, you get

$$T = \left|1 - \frac{im}{\hbar^2 k}\int_{-\infty}^{\infty} V(x)dx\right|^2 = 1 + \left(\frac{m}{\hbar^2 k}\right)^2 \left[\int_{-\infty}^{\infty} V(x)dx\right]^2,$$

which is nonsense (greater than 1). The first Born approximation gets R right, but all you can say to this order is $T \approx 1$ (you would do better using $T = 1 - R$).

Problem 10.18

Delta function: $V(x) = -\alpha\delta(x)$. $\displaystyle\int_{-\infty}^{\infty} e^{2ikx} V(x)\,dx = -\alpha$, so $R = \left(\dfrac{m\alpha}{\hbar^2 k}\right)^2,$

or, in terms of energy ($k^2 = 2mE/\hbar^2$):

$$R = \frac{m^2\alpha^2}{2mE\hbar^2} = \frac{m\alpha^2}{2\hbar^2 E}; \quad T = 1 - R = \boxed{1 - \frac{m\alpha^2}{2\hbar^2 E}.}$$

The exact answer (Eq. 2.144) is $\dfrac{1}{1 + \frac{m\alpha^2}{2\hbar^2 E}} \approx 1 - \dfrac{m\alpha^2}{2\hbar^2 E}$, so they agree provided $E \gg \dfrac{m\alpha^2}{2\hbar^2}$.

Finite square well: $V(x) = \left\{\begin{matrix} -V_0 & (-a < x < a) \\ 0 & (\text{otherwise}) \end{matrix}\right\}.$

$$\int_{-\infty}^{\infty} e^{2ikx} V(x)\,dx = -V_0 \int_{-a}^{a} e^{2ikx} dx = -V_0 \left.\frac{e^{2ikx}}{2ik}\right|_{-a}^{a} = -\frac{V_0}{k}\left(\frac{e^{2ika} - e^{-2ika}}{2i}\right) = -\frac{V_0}{k}\sin(2ka).$$

So $R = \left[\left(\dfrac{m}{\hbar^2 k}\right)^2 \left(\dfrac{V_0}{k}\sin(2ka)\right)\right]^2.$ $\boxed{T = 1 - \left[\dfrac{V_0}{2E}\sin\left(\dfrac{2a}{\hbar}\sqrt{2mE}\right)\right]^2.}$

If $E \gg V_0$, the exact answer (Eq. 2.172) becomes

$$T^{-1} \approx 1 + \left[\frac{V_0}{2E}\sin\left(\frac{2a}{\hbar}\sqrt{2mE}\right)\right]^2 \Longrightarrow T \approx 1 - \left(\frac{V_0}{2E}\sin\left[\frac{2a}{\hbar}\sqrt{2mE}\right)\right]^2,$$

so they agree provided $E \gg V_0$.

Problem 10.19

The Legendre polynomials satisfy $P_l(1) = 1$ (see footnote 39, p. 124), so Eq. 10.47 $\Rightarrow$

$$f(0) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l. \quad \text{Therefore} \quad \text{Im}[f(0)] = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l,$$

and hence (Eq. 10.48):

$$\sigma = \frac{4\pi}{k}\text{Im}[f(0)]. \quad \text{QED}$$

Problem 10.20

Using Eq. 10.88 and integration by parts:

$$\begin{aligned}
f(\theta) &= -\frac{2m}{\hbar^2\kappa}\int_0^\infty rAe^{-\mu r^2}\sin(\kappa r)\,dr = -\frac{2mA}{\hbar^2\kappa}\int_0^\infty \frac{d}{dr}\left(-\frac{1}{2\mu}e^{-\mu r^2}\right)\sin(\kappa r)\,dr \\
&= \frac{2mA}{2\mu\hbar^2\kappa}\left\{e^{-\mu r^2}\sin(\kappa r)\Big|_0^\infty - \int_0^\infty e^{-\mu r^2}\frac{d}{dr}\left[\sin(\kappa r)\right]\,dr\right\} \\
&= \frac{mA}{\mu\hbar^2\kappa}\left\{0-\kappa\int_0^\infty e^{-\mu r^2}\cos(\kappa r)\,dr\right\} = -\frac{mA}{\mu\hbar^2}\left(\frac{\sqrt{\pi}}{2\sqrt{\mu}}e^{-\kappa^2/4\mu}\right) \\
&= -\frac{mA\sqrt{\pi}}{2\hbar^2\mu^{3/2}}e^{-\kappa^2/4\mu}, \quad \text{where} \quad \kappa = 2k\sin(\theta/2) \quad \text{(Eq. 10.89).}
\end{aligned}$$

From Eq. 10.14, then,

$$\frac{d\sigma}{d\Omega} = \frac{\pi m^2A^2}{4\hbar^4\mu^3}e^{-\kappa^2/2\mu},$$

and hence

$$\begin{aligned}
\sigma &= \int\frac{d\sigma}{d\Omega}\,d\Omega = \frac{\pi m^2A^2}{4\hbar^4\mu^3}\int e^{-4k^2\sin^2(\theta/2)/2\mu}\sin\theta\,d\theta\,d\phi \\
&= \frac{\pi^2m^2A^2}{2\hbar^4\mu^3}\int_0^\pi e^{-2k^2\sin^2(\theta/2)/\mu}\sin\theta\,d\theta; \quad \text{write } \sin\theta = 2\sin(\theta/2)\cos(\theta/2) \quad \text{and let } x\equiv\sin(\theta/2) \\
&= \frac{\pi^2m^2A^2}{2\hbar^4\mu^3}\int_0^1 e^{-2k^2x^2/\mu}2x\,2\,dx = \frac{2\pi^2m^2A^2}{\hbar^4\mu^3}\int_0^1 xe^{-2k^2x^2/\mu}\,dx \\
&= \frac{2\pi^2m^2A^2}{\hbar^4\mu^3}\left[-\frac{\mu}{4k^2}e^{-2k^2x^2/\mu}\right]\Bigg|_0^1 = -\frac{\pi^2m^2A^2}{2\hbar^4\mu^2k^2}\left(e^{-2k^2/\mu}-1\right) \\
&= \boxed{\frac{\pi^2m^2A^2}{2\hbar^4\mu^2k^2}\left(1-e^{-2k^2/\mu}\right).}
\end{aligned}$$

Problem 10.21

(a) In the first Born approximation (Equation 10.79):

$$\begin{aligned}
f(\theta,\phi) &\approx -\frac{m}{2\pi\hbar^2}\int e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_0}V(\mathbf{r}_0)\,d^3\mathbf{r}_0 = -\frac{m}{2\pi\hbar^2}\frac{2\pi\hbar^2b}{m}\sum_i\int e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_0}\delta^3(\mathbf{r}_0-\mathbf{r}_i)\,d^3\mathbf{r}_0 \\
&= -b\sum_i e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_i} = -b\sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i}; \\
\frac{d\sigma}{d\Omega} &= |f|^2 = b^2\left|\sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i}\right|^2. \quad \checkmark
\end{aligned}$$

(b)

$$\sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i} = \sum_{l,m,n}e^{-i(q_xla+q_yma+q_zna)} = \sum_{l=0}^{N-1}e^{-iq_xla}\sum_{m=0}^{N-1}e^{-iq_yma}\sum_{n=0}^{N-1}e^{-iq_zna}.$$

Now, letting $u \equiv \exp(-iq_x a)$,

$$\sum_{l=0}^{N-1} e^{-iq_x la} = \sum_{l=0}^{N-1} u^l = \frac{1-u^N}{1-u} = \frac{1-e^{-iq_x aN}}{1-e^{-iq_x a}} = \frac{e^{-iq_x aN/2}\left(e^{iq_x aN/2} - e^{-iq_x aN/2}\right)}{e^{-iq_x a/2}\left(e^{iq_x a/2} - e^{-iq_x a/2}\right)}$$

$$= e^{-iq_x a(N-1)/2}\,\frac{\sin(q_x aN/2)}{\sin(q_x a/2)},$$

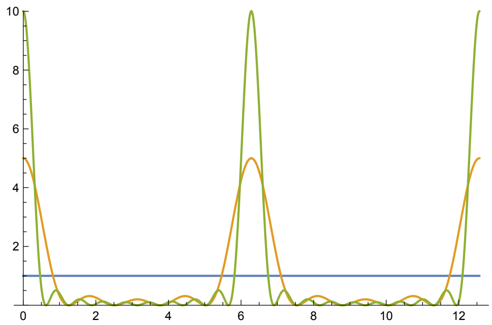
so

$$\frac{d\sigma}{d\Omega} = b^2 \frac{\sin^2(q_x aN/2)}{\sin^2(q_x a/2)}\frac{\sin^2(q_y aN/2)}{\sin^2(q_y a/2)}\frac{\sin^2(q_z aN/2)}{\sin^2(q_z a/2)}. \quad \checkmark$$

(c) Here's the graph:

```
f[N_, x_] := (1/N) (Sin[N x / 2] / Sin[x / 2])^2

Plot[{f[1, x], f[5, x], f[10, x]}, {x, 0, 4 π}, PlotRange → {0, 10}]
```



(d) The vectors $\mathbf{k}$, $\mathbf{k}'$ and $\mathbf{G}$ form an isosceles triangle (Figure 10.11), and

$$\sin(\theta/2) = \frac{G/2}{k} = \frac{\pi}{ka}\sqrt{l^2+m^2+n^2},$$

so, in terms of the wavelength $\lambda = 2\pi/k$,

$$\theta = 2\arcsin\left(\frac{\lambda}{2a}\sqrt{l^2+m^2+n^2}\right).$$

The smallest (nonzero) angles occur when $(l^2+m^2+n^2) = 1,\ 2,$ or 3, corresponding to angles

$$\boxed{\pi/3, \pi/2, \text{and } 2\pi/3.}$$

Problem 10.22

(a) $-\dfrac{\hbar^2}{2m}\left(\dfrac{\partial^2}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial}{\partial r} + \dfrac{1}{r^2}\dfrac{\partial^2}{\partial\theta^2}\right)\psi(r,\theta) + V(r)\psi(r,\theta) = E\psi(r,\theta)$. Let $\psi(r,\theta) = R(r)\,\Theta(\theta)$:

$-\dfrac{\hbar^2}{2m}\left\{\Theta\left[\dfrac{d^2R}{dr^2} + \dfrac{1}{r}\dfrac{dR}{dr}\right] + \dfrac{R}{r^2}\dfrac{d^2\Theta}{d\theta^2}\right\} + V(r)\,R\Theta = E\,R\Theta.$ Multiply by r^2 and divide by $R\Theta$:

$$-\frac{\hbar^2}{2m}\left[\frac{r^2}{R}\frac{d^2R}{dr^2}+\frac{r}{R}\frac{dR}{dr}\right]-\frac{\hbar^2}{2m}\frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2}+r^2V(r)=r^2E.$$ The Θ term must be constant:

$$\frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2}=-j^2 \quad\Rightarrow\quad \frac{d^2\Theta}{d\theta^2}=-j^2\,\Theta \quad\Rightarrow\quad \Theta(\theta)=Ae^{ij\theta},$$

where A is a constant (which we might as well absorb into R), and j could be positive or negative (it has to be an integer, since $\Theta(\theta+2\pi)=\Theta(\theta)$). This leaves the radial equation,

$$-\frac{\hbar^2}{2m}\left[r^2\frac{d^2R}{dr^2}+r\frac{dR}{dr}\right]+\frac{\hbar^2}{2m}j^2\,R+r^2V(r)R=r^2E\,R.$$

Let $u(r)\equiv\sqrt{r}\,R(r)$, so $R=\dfrac{u}{\sqrt{r}}$, $\dfrac{dR}{dr}=\dfrac{1}{\sqrt{r}}\dfrac{du}{dr}-\dfrac{1}{2}\dfrac{u}{r^{3/2}}$, $\dfrac{d^2R}{dr^2}=\dfrac{1}{\sqrt{r}}\dfrac{d^2u}{dr^2}-\dfrac{1}{r^{3/2}}\dfrac{du}{dr}+\dfrac{3}{4}\dfrac{u}{r^{5/2}}$. Then

$$-\frac{\hbar^2}{2m}\left[\left(\frac{1}{\sqrt{r}}\frac{d^2u}{dr^2}-\frac{1}{r^{3/2}}\frac{du}{dr}+\frac{3}{4}\frac{u}{r^{5/2}}\right)+\frac{1}{r}\left(\frac{1}{\sqrt{r}}\frac{du}{dr}-\frac{1}{2}\frac{u}{r^{3/2}}\right)\right]+\frac{\hbar^2}{2m}j^2\frac{1}{r^2}\frac{u}{\sqrt{r}}+V(r)\frac{u}{\sqrt{r}}=E\frac{u}{\sqrt{r}};$$

$$\boxed{\psi(r,\theta)=\frac{u}{\sqrt{r}}e^{ij\theta},\qquad -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[V(r)+\frac{\hbar^2}{2m}\frac{(j^2-1/4)}{r^2}\right]u=Eu.}$$

(b) $-\dfrac{\hbar^2}{2m}\dfrac{d^2u}{dr^2}=E\,u \;\Rightarrow\; \dfrac{d^2u}{dr^2}=-k^2u$ where $k\equiv\frac{\sqrt{2mE}}{\hbar}$. The general solution is $u(r)=Ae^{ikr}+Be^{-ikr}$, but for an *outgoing* wave we want only the first term: $R(r)=A\dfrac{e^{ikr}}{\sqrt{r}}$. Notice that this asymptotic form is the same for all j, so when we form the general linear combination of separable solutions (from Part (a)), at large r the radial term will factor out, leaving some function of θ: $\psi\approx Af(\theta)\dfrac{e^{ikr}}{\sqrt{r}}$. ✓

$$-\frac{\hbar^2}{2m}\nabla^2\psi=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)Ae^{ikx}=-\frac{\hbar^2}{2m}(-k^2)Ae^{ikx}=E\,\psi.\quad ✓$$

(c) $-\dfrac{\hbar^2}{2m}\dfrac{d^2u}{dr^2}+\dfrac{\hbar^2}{2m}\dfrac{(j^2-1/4)}{r^2}u=Eu \quad\Rightarrow\quad \dfrac{d^2u}{dr^2}-\dfrac{j^2-1/4)}{r^2}u=-k^2u.$

This is a form of Bessel's equation; in Boas' notation (her Equation 16.1), $a=1/2,\ b=k,\ c=1,\ p=j$, and the solution is $u(r)=\sqrt{r}\,Z_j(kr)$, where Z is a Bessel/Neumann/Hankel function of order j. The outgoing one is $H^{(1)}$, so $u(r)=\sqrt{r}H_j^{(1)}(kr)$, the separable solution is $\psi(r,\theta)=H_j^{(1)}(kr)e^{ij\theta}$, and the general solution is the linear combination

$$\psi_{\text{out}}(r,\theta)=A\sum_{-\infty}^{\infty}c_j\,H_j^{(1)}(kr)\,e^{ij\theta}.$$

Combining this with the incident wave (Ae^{ikx}) we have

$$\boxed{\psi(r,\theta)=A\left(e^{ikx}+\sum_{-\infty}^{\infty}c_j\,H_j^{(1)}(kr)\,e^{ij\theta}\right).}$$

(d) At large r:

$$\psi(r,\theta)\sim A\left\{e^{ikx}+\sqrt{\frac{2}{\pi}}\,e^{-i\pi/4}\left(\sum_{-\infty}^{\infty}c_j(-i)^je^{ij\theta}\right)\frac{e^{ikr}}{\sqrt{kr}}\right\}.$$

Comparing Equation (10.109), we read off

$$f(\theta)=\sqrt{\frac{2}{\pi k}}\,e^{-i\pi/4}\sum_{-\infty}^{\infty}c_j(-i)^j e^{ij\theta}.\quad\checkmark$$

(e) Following the argument leading to Equation (10.14), the probability that an incident particle (traveling at speed v) passes through an infinitesimal length (differential impact parameter) db is

$$dP=|\psi_{\text{incident}}|^2\,da=|A|^2(v\,dt)db=|\psi_{\text{scattered}}|^2\,da=\frac{|A|^2|f|^2}{r}(v\,dt)r\,d\theta\Rightarrow db=|f|^2\,d\theta\Rightarrow D(\theta)=|f(\theta)|^2.\quad\checkmark$$

$$B=\int_0^{2\pi}D(\theta)\,d\theta=\int_0^{2\pi}|f(\theta)|^2\,d\theta=\int_0^{2\pi}\frac{2}{\pi k}\left(\sum_j(-i)^jc_je^{ij\theta}\right)\left(\sum_{j'}(i)^{j'}c^*_{j'}e^{-ij'\theta}\right)d\theta$$
$$=\frac{2}{\pi k}\sum_{j,j'}(i)^{j'-j}c_jc^*_{j'}\int_0^{2\pi}e^{i(j-j')\theta}\,d\theta=\frac{2}{\pi k}\sum_{j,j'}(i)^{j'-j}c_jc^*_{j'}(2\pi\delta_{j,j'})=\frac{4}{k}\sum_{j=-\infty}^{\infty}|c_j|^2.\quad\checkmark$$

(f)

$$\psi(a,\theta)=A\left\{\sum_{j=-\infty}^{\infty}(i)^j\,J_j(ka)e^{ij\theta}+\sum_{j=-\infty}^{\infty}c_j\,H_j^{(1)}(ka)e^{ij\theta}\right\}=A\sum_{j=-\infty}^{\infty}\left(i^jJ_j+c_jH_j^{(1)}\right)e^{ij\theta}=0.$$

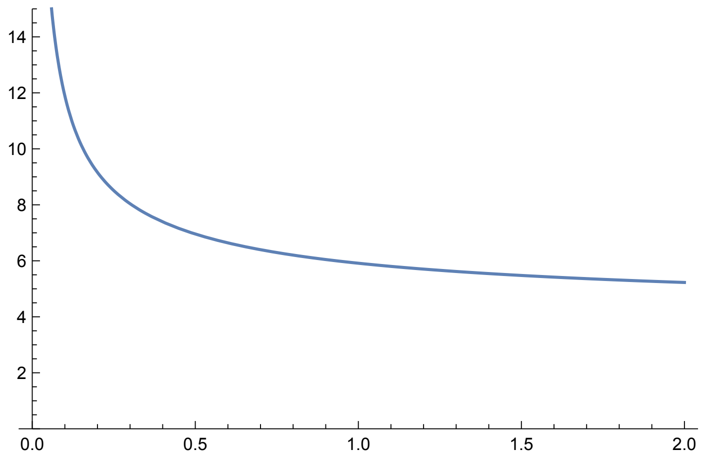
Each coefficient must vanish (prove it, if you like, by multiplying by $e^{-ij'\theta}$ and integrating over θ from 0 to 2π):

$$i^jJ_j(ka)+c_jH_j^{(1)}(ka)=0\quad\Rightarrow\quad c_j=-\frac{i^jJ_j(ka)}{H_j^{(1)}(ka)}\quad\Rightarrow\quad\boxed{B=\frac{4}{k}\sum_{j=-\infty}^{\infty}\left|\frac{J_j(ka)}{H_j^{(1)}(ka)}\right|^2.}$$

To create the plot, note that $H_j^{(1)}=J_j+iN_j$, while J_j and N_j (the Neumann function) are *real*, so $\left|\frac{J_j}{H_j^{(1)}}\right|^2=\left[1+(N_j/J_j)^2\right]^{-1}$. Then

```
b[x_] := 4/x Sum[(1 + (BesselY[j, x]/BesselJ[j, x])^2)^-1, {j, -100, 100}]

Plot[b[x], {x, 0, 2}, PlotRange → {0, 15}]
```



Problem 10.23

(a) The center of mass and relative coordinates are $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$. Therefore interchanging the two particles leaves $\mathbf{R}$ untouched, but switches the sign of $\mathbf{r}$. Since the wave function must be symmetric under interchange, this means $\psi_r(-\mathbf{r}) = \psi_r(\mathbf{r})$. ✓

(b) Because the potential is spherically symmetric, if $\psi_r(\mathbf{r})$ is a solution to Equation 10.118 with energy E_r, so too is $\psi_r(-\mathbf{r})$. We can therefore construct a symmetric solution from the sum: $\psi_r(\mathbf{r}) + \psi_r(-\mathbf{r})$. Applying this to Equation 10.12 gives

$$\psi(r,\theta) = A\left\{e^{ikz} + e^{-ikz} + [f(\theta) + f(\pi - \theta)]\,\frac{e^{ikr}}{r}\right\},$$

using the fact that in polar coordinates $\mathbf{r} \to -\mathbf{r}$ is achieved by $(r,\,\theta,\,\phi) \to (r,\,\pi - \theta,\,\phi + \pi)$. We can then read off the scattering amplitude: $\boxed{f_B(\theta) = f(\theta) + f(\pi - \theta).}$ ✓

(c) From Equation 10.25,

$$\begin{aligned} f_B(\theta) &= \sum_{\ell=0}^{\infty}(2\ell+1)a_\ell[P_\ell(\cos\theta) + P_\ell(\cos(\pi-\theta))] \\ &= \sum_{\ell=0}^{\infty}(2\ell+1)a_\ell[P_\ell(\cos\theta) + P_\ell(-\cos\theta)] = \sum_{\ell\,\text{even}} 2(2\ell+1)a_\ell\,P_\ell(\cos\theta), \end{aligned}$$

since $P_\ell(-x) = (-1)^\ell P_\ell(x)$ (Equation 4.28).

(d) In this case the wave function must be *odd*: $\psi_r(-\mathbf{r}) = -\psi_r(\mathbf{r})$. We construct *anti*symmetric solutions, $\psi_r(\mathbf{r}) - \psi_r(-\mathbf{r})$, and by the same reasoning we get $\boxed{f_F(\theta) = f(\theta) - f(\pi - \theta).}$ This time the partial waves include only *odd* values of ℓ.

(e) $f_F(\pi/2) = f(\pi/2) - f(\pi - \pi/2) = f(\pi/2) - f(\pi/2) = 0.$ ✓

(f) $f(\theta) = \dfrac{A}{\sin^2(\theta/2)}$; $f_{B/F} = A\left[\dfrac{1}{\sin^2(\theta/2)} \pm \dfrac{1}{\sin^2((\theta-\pi/2)/2)}\right]$. But $\sin^2(\theta/2) = \dfrac{1}{2}[1 - \cos\theta]$, and hence $\sin^2((\theta-\pi/2)/2) = \dfrac{1}{2}[1 - \cos(\theta - \pi/2)] = \dfrac{1}{2}[1 + \cos\theta]$, so $f_{B/F} = 2A\left(\dfrac{1}{1-\cos\theta} \pm \dfrac{1}{1+\cos\theta}\right) = 2A\dfrac{(1+\cos\theta)\pm(1-\cos\theta)}{1-\cos^2\theta}$. $f_B = 4A\left(\dfrac{1}{\sin^2\theta}\right)$, $f_F = 4A\left(\dfrac{\cos\theta}{\sin^2\theta}\right)$.

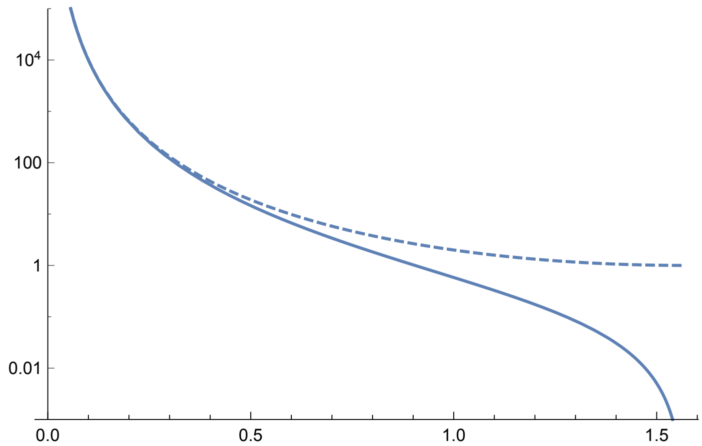
$$\boxed{\left(\frac{d\sigma}{d\Omega}\right)_B = (4A)^2\left(\frac{1}{\sin^4\theta}\right); \quad \left(\frac{d\sigma}{d\Omega}\right)_F = (4A)^2\left(\frac{\cos^2\theta}{\sin^4\theta}\right).}$$

In the plot below the dashed line is $(d\sigma/d\Omega)_B$, and the solid line is $(d\sigma/d\Omega)_F$.

```
LogPlot[(Sin[x])^-4, {x, 0, π/2},
 PlotRange → {.001, 10^5}, PlotStyle -> Dashing[{0.01, 0.01}]]

LogPlot[(Cos[x])^2 (Sin[x])^-4, {x, 0, π/2}, PlotRange → {.001, 10^5}]

Show[%9, %5]
```



Chapter 11

Quantum Dynamics

Problem 11.1

(a) This equation can be solved by separation of variables:

$$\begin{aligned}\frac{df}{dt} &= k\,f \\ \frac{df}{f} &= k\,dt \\ \int \frac{df}{f} &= \int k\,dt \\ \ln f &= k\,t + C \\ f(t) &= f_0\,e^{k\,t}\,,\end{aligned}$$

where we've defined the new constant $f_0 = e^C$ in the last line.

(b) If k is a function of time, the same procedure holds. Skipping to the third line in the derivation of part (a):

$$\begin{aligned}\int_{f_0}^{f} \frac{df'}{f'} &= \int_0^t k(t')\;dt' \\ \ln f - \ln f_0 &= \int_0^t k(t')\;dt' \\ f(t) &= f_0\,\exp\left[\int_0^t k(t')\;dt'\right]\,,\end{aligned}$$

where this time I've done the integrals as definite integrals rather than specify the integration constant at the end.

(d) These two are not the same because $\hat{H}$ is an operator and for operators $\hat{A}$ and $\hat{B}$

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}+\hat{B}}$$

only if $\hat{A}$ and $\hat{B}$ commute.

Problem 11.2

$\psi_{nlm} = R_{nl}Y_l^m$. From Tables 4.3 and 4.7:

$$\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}; \quad \psi_{200} = \frac{1}{\sqrt{8\pi a^3}}\left(1 - \frac{r}{2a}\right) e^{-r/2a};$$

$$\psi_{210} = \frac{1}{\sqrt{32\pi a^3}} \frac{r}{a} e^{-r/2a}\cos\theta; \quad \psi_{21\pm1} = \mp\frac{1}{\sqrt{64\pi a^3}} \frac{r}{a} e^{-r/2a}\sin\theta\, e^{\pm i\phi}.$$

But $r\cos\theta = z$ and $r\sin\theta e^{\pm i\phi} = r\sin\theta(\cos\phi \pm i\sin\phi) = r\sin\theta\cos\phi \pm ir\sin\theta\sin\phi = x \pm iy$. So $|\psi|^2$ is an *even* function of z in all cases, and hence $\int z|\psi|^2 dx\, dy\, dz = 0$, so $\boxed{H'_{ii} = 0.}$ Moreover, ψ_{100} is even in z, and so are ψ_{200}, ψ_{211}, and ψ_{21-1}, so $\boxed{H'_{ij} = 0}$ for all *except*

$$H'_{100,210} = eE\frac{1}{\sqrt{\pi a^3}}\frac{1}{\sqrt{32\pi a^3}}\frac{1}{a}\int e^{-r/a}e^{-r/2a}z^2\, d^3\mathbf{r} = \frac{eE}{4\sqrt{2}\pi a^4}\int e^{-3r/2a}r^2\cos^2\theta\, r^2\sin\theta\, dr\, d\theta\, d\phi$$

$$= \frac{eE}{4\sqrt{2}\pi a^4}\int_0^\infty r^4 e^{-3r/2a}dr\int_0^\pi \cos^2\theta\sin\theta\, d\theta\int_0^{2\pi} d\phi = \frac{eE}{4\sqrt{2}\pi a^4}4!\left(\frac{2a}{3}\right)^5\frac{2}{3}2\pi = \boxed{\left(\frac{2^8}{3^5\sqrt{2}}\right)eEa,}$$

or $\boxed{0.7449\, eEa.}$

Problem 11.3

$\dot{c}_a = -\frac{i}{\hbar}H'_{ab}e^{-i\omega_0 t}c_b; \quad \dot{c}_b = -\frac{i}{\hbar}H'_{ba}e^{i\omega_0 t}c_a$. Differentiating with respect to t:

$$\ddot{c}_b = -\frac{i}{\hbar}H'_{ba}\left[i\omega_0 e^{i\omega_0 t}c_a + e^{i\omega_0 t}\dot{c}_a\right] = i\omega_0\left[-\frac{i}{\hbar}H'_{ba}e^{i\omega_0 t}c_a\right] - \frac{i}{\hbar}H'_{ba}e^{i\omega_o t}\left[-\frac{i}{\hbar}H'_{ab}e^{-i\omega_0 t}c_b\right], \text{ or}$$

$\ddot{c}_b = i\omega_0\dot{c}_b - \frac{1}{\hbar^2}|H'_{ab}|^2 c_b$. Let $\alpha^2 \equiv \frac{1}{\hbar^2}|H'_{ab}|^2$. Then $\ddot{c}_b - i\omega_0\dot{c}_b + \alpha^2 c_b = 0$.

This is a linear differential equation with constant coefficients, so it can be solved by a function of the form $c_b = e^{\lambda t}$:

$$\lambda^2 - i\omega_0\lambda + \alpha^2 = 0 \Longrightarrow \lambda = \frac{1}{2}\left[i\omega_0 \pm \sqrt{-\omega_0^2 - 4\alpha^2}\right] = \frac{i}{2}(\omega_0 \pm \omega), \text{ where } \omega \equiv \sqrt{\omega_0^2 + 4\alpha^2}.$$

The general solution is therefore

$$c_b(t) = Ae^{i(\omega_0+\omega)t/2} + Be^{i(\omega_0-\omega)t/2} = e^{i\omega_0 t/2}\left(Ae^{i\omega t/2} + Be^{-i\omega t/2}\right), \text{ or}$$

$c_b(t) = e^{i\omega_0 t/2}\left[C\cos(\omega t/2) + D\sin(\omega t/2)\right]$. But $c_b(0) = 0$, so $C = 0$, and hence

$c_b(t) = De^{i\omega_0 t/2}\sin(\omega t/2)$. Then

$$\dot{c}_b = D\left[\frac{i\omega_0}{2}e^{i\omega_0 t/2}\sin(\omega t/2) + \frac{\omega}{2}e^{i\omega_0 t/2}\cos(\omega t/2)\right] = \frac{\omega}{2}De^{i\omega_0 t/2}\left[\cos(\omega t/2) + i\frac{\omega_0}{\omega}\sin(\omega t/2)\right] = -\frac{i}{\hbar}H'_{ba}e^{i\omega_0 t}c_a.$$

$c_a = \frac{i\hbar}{H'_{ba}}\frac{\omega}{2}e^{-i\omega_0 t/2}D\left[\cos(\omega t/2) + i\frac{\omega_0}{\omega}\sin(\omega t/2)\right]$. But $c_a(0) = 1$, so $\frac{i\hbar}{H'_{ba}}\frac{\omega}{2}D = 1$. *Conclusion:*

$$\boxed{\begin{aligned} c_a(t) &= e^{-i\omega_0 t/2}\left[\cos(\omega t/2) + i\frac{\omega_0}{\omega}\sin(\omega t/2)\right], \\ c_b(t) &= \frac{2H'_{ba}}{i\hbar\omega}e^{i\omega_0 t/2}\sin(\omega t/2), \end{aligned}} \quad \text{where } \boxed{\omega \equiv \sqrt{\omega_0^2 + 4\frac{|H'_{ab}|^2}{\hbar^2}}.}$$

$$\begin{aligned} |c_a|^2 + |c_b|^2 &= \cos^2(\omega t/2) + \frac{\omega_0^2}{\omega^2}\sin^2(\omega t/2) + \frac{4|H'_{ab}|^2}{\hbar^2\omega^2}\sin^2(\omega t/2) \\ &= \cos^2(\omega t/2) + \frac{1}{\omega^2}\left(\omega_0^2 + 4\frac{|H'_{ab}|^2}{\hbar^2}\right)\sin^2(\omega t/2) = \cos^2(\omega t/2) + \sin^2(\omega t/2) = 1. \quad \checkmark \end{aligned}$$

[In light of the **Comment** you might question the initial conditions. If the perturbation includes a factor $\theta(t)$, are we sure this doesn't alter $c_a(0)$ and $c_b(0)$? That is, are we sure $c_a(t)$ and $c_b(t)$ are *continuous* at a step function potential? The answer is "yes", for if we integrate Eq. 11.17 from $-\epsilon$ to ϵ,

$$c_a(\epsilon) - c_a(-\epsilon) = -\frac{i}{\hbar}H'_{ab}\int_0^\epsilon e^{-i\omega_0 t}c_b(t)\,dt.$$

But $|c_b(t)| \leq 1$, so the integral goes to zero as $\epsilon \to 0$, and hence $c_a(-\epsilon) = c_a(\epsilon)$. The same goes for c_b, of course.]

Problem 11.4

This is a tricky problem, and I thank Prof. Onuttom Narayan for showing me the correct solution. The safest approach is to represent the delta function as a sequence of rectangles:

$$\delta_\epsilon(t) = \left\{\begin{array}{ll} (1/2\epsilon), & -\epsilon < t < \epsilon, \\ 0, & \text{otherwise.} \end{array}\right\}$$

Then Eq. 11.17 $\Rightarrow$

$$\begin{cases} t < -\epsilon: & c_a(t) = 1,\; c_b(t) = 0, \\ t > \epsilon: & c_a(t) = a,\; c_b(t) = b, \\ -\epsilon < t < \epsilon: & \begin{cases} \dot{c}_a &= -\frac{i\alpha}{2\epsilon\hbar}e^{-i\omega_0 t}c_b, \\ \dot{c}_b &= -\frac{i\alpha^*}{2\epsilon\hbar}e^{i\omega_0 t}c_a. \end{cases} \end{cases}$$

In the interval $-\epsilon < t < \epsilon$,

$$\frac{d^2c_b}{dt^2} = -\frac{i\alpha^*}{2\epsilon\hbar}\left[i\omega_0 e^{i\omega_0 t}c_a + e^{i\omega_0 t}\left(\frac{-i\alpha}{2\epsilon\hbar}e^{-i\omega_0 t}c_b\right)\right] = -\frac{i\alpha^*}{2\epsilon\hbar}\left[i\omega_0\frac{i2\epsilon\hbar}{\alpha^*}\frac{dc_b}{dt} - \frac{i\alpha}{2\epsilon\hbar}c_b\right] = i\omega_0\frac{dc_b}{dt} - \frac{|\alpha|^2}{(2\epsilon\hbar)^2}c_b.$$

Thus c_b satisfies a homogeneous linear differential equation with constant coefficients:

$$\frac{d^2c_b}{dt^2} - i\omega_0\frac{dc_b}{dt} + \frac{|\alpha|^2}{(2\epsilon\hbar)^2}c_b = 0.$$

Try a solution of the form $c_b(t) = e^{\lambda t}$:

$$\lambda^2 - i\omega_0\lambda + \frac{|\alpha|^2}{(2\epsilon\hbar)^2} = 0 \Rightarrow \lambda = \frac{i\omega_0 \pm \sqrt{-\omega_0^2 - |\alpha|^2/(\epsilon\hbar)^2}}{2},$$

or

$$\lambda = \frac{i\omega_0}{2} \pm \frac{i\omega}{2}, \text{ where } \omega \equiv \sqrt{\omega_0^2 + |\alpha|^2/(\epsilon\hbar)^2}.$$

The general solution is

$$c_b(t) = e^{i\omega_0 t/2}\left(Ae^{i\omega t/2} + Be^{-i\omega t/2}\right).$$

But

$$c_b(-\epsilon) = 0 \Rightarrow Ae^{-i\omega\epsilon/2} + Be^{i\omega\epsilon/2} = 0 \Rightarrow B = -Ae^{-i\omega\epsilon},$$

so

$$c_b(t) = Ae^{i\omega_0 t/2}\left(e^{i\omega t/2} - e^{-i\omega(\epsilon+t/2)}\right).$$

Meanwhile

$$\begin{aligned} c_a(t) &= \frac{2i\epsilon\hbar}{\alpha^*}e^{-i\omega_0 t}\dot{c}_b = \frac{2i\epsilon\hbar}{\alpha^*}e^{-i\omega_0 t/2}A\left[\frac{i\omega_0}{2}\left(e^{i\omega t/2} - e^{-i\omega(\epsilon+t/2)}\right) + \frac{i\omega}{2}\left(e^{i\omega t/2} + e^{-i\omega(\epsilon+t/2)}\right)\right] \\ &= -\frac{\epsilon\hbar}{\alpha^*}e^{-i\omega_0 t/2}A\left[(\omega+\omega_0)e^{i\omega t/2} + (\omega-\omega_0)e^{-i\omega(\epsilon+t/2)}\right]. \end{aligned}$$

But $\quad c_a(-\epsilon) = 1 = -\dfrac{\epsilon\hbar}{\alpha^*}e^{i(\omega_0-\omega)\epsilon/2}A\left[(\omega+\omega_0)+(\omega-\omega_0)\right] = -\dfrac{2\epsilon\hbar\omega}{\alpha^*}e^{i(\omega_0-\omega)\epsilon/2}A, \quad$ so $\quad A = -\dfrac{\alpha^*}{2\epsilon\hbar\omega}e^{i(\omega-\omega_0)\epsilon/2}.$

$$\begin{aligned} c_a(t) &= \frac{1}{2\omega}e^{-i\omega_0(t+\epsilon)/2}\left[(\omega+\omega_0)e^{i\omega(t+\epsilon)/2} + (\omega-\omega_0)e^{-i\omega(t+\epsilon)/2}\right] \\ &= e^{-i\omega_0(t+\epsilon)/2}\left\{\cos\left[\frac{\omega(t+\epsilon)}{2}\right] + i\frac{\omega_0}{\omega}\sin\left[\frac{\omega(t+\epsilon)}{2}\right]\right\}; \\ c_b(t) &= -\frac{\alpha^*}{2\epsilon\hbar\omega}e^{i\omega_0(t-\epsilon)/2}\left[e^{i\omega(t+\epsilon)/2} - e^{-i\omega(t+\epsilon)/2}\right] = -\frac{i\alpha^*}{\epsilon\hbar\omega}e^{i\omega_0(t-\epsilon)/2}\sin\left[\frac{\omega(t+\epsilon)}{2}\right]. \end{aligned}$$

Thus

$$a = c_a(\epsilon) = e^{-i\omega_0\epsilon}\left[\cos(\omega\epsilon) + i\frac{\omega_0}{\omega}\sin(\omega\epsilon)\right], \quad b = c_b(\epsilon) = -\frac{i\alpha^*}{\epsilon\hbar\omega}\sin(\omega\epsilon).$$

This is for the rectangular pulse; it remains to take the limit $\epsilon \to 0$: $\omega \to |\alpha|/\epsilon\hbar$, so

$$a \to \cos\left(\frac{|\alpha|}{\hbar}\right) + i\frac{\omega_0\epsilon\hbar}{|\alpha|}\sin\left(\frac{|\alpha|}{\hbar}\right) \to \cos\left(\frac{|\alpha|}{\hbar}\right), \quad b \to -\frac{i\alpha^*}{|\alpha|}\sin\left(\frac{|\alpha|}{\hbar}\right),$$

and we conclude that for the delta function

$$\boxed{\begin{aligned} c_a(t) &= \begin{cases} 1, & t<0, \\ \cos(|\alpha|/\hbar), & t>0; \end{cases} \\ c_b(t) &= \begin{cases} 0, & t<0, \\ -i\sqrt{\dfrac{\alpha^*}{\alpha}}\sin(|\alpha|/\hbar), & t>0. \end{cases} \end{aligned}}$$

Obviously, $|c_a(t)|^2 + |c_b(t)|^2 = 1$ in both time periods. Finally,

$$\boxed{P_{a\to b} = |b|^2 = \sin^2(|\alpha|/\hbar).}$$

Problem 11.5

(a)

$$\left.\begin{array}{l}\text{Eq. 11.14} \implies \dot{c}_a = -\dfrac{i}{\hbar}\left[c_a H'_{aa} + c_b H'_{ab} e^{-i\omega_0 t}\right] \\ \text{Eq. 11.17} \implies \dot{c}_b = -\dfrac{i}{\hbar}\left[c_b H'_{bb} + c_a H'_{ba} e^{i\omega_0 t}\right]\end{array}\right\} \text{(these are \textit{exact}, and replace Eq. 11.15).}$$

<u>Initial conditions</u>: $c_a(0) = 1, \quad c_b(0) = 0.$

<u>Zeroth order</u>: $c_a(t) = 1, \quad c_b(t) = 0.$

<u>First order</u>:
$$\begin{cases}\dot{c}_a = -\dfrac{i}{\hbar}H'_{aa} \implies \\ \dot{c}_b = -\dfrac{i}{\hbar}H'_{ba}e^{i\omega_0 t} \implies\end{cases} \boxed{\begin{array}{l} c_a(t) = 1 - \dfrac{i}{\hbar}\displaystyle\int_0^t H'_{aa}(t')\,dt' \\ c_b(t) = -\dfrac{i}{\hbar}\displaystyle\int_0^t H'_{ba}(t')e^{i\omega_0 t'}\,dt'\end{array}}$$

$$|c_a|^2 = \left[1 - \frac{i}{\hbar}\int_0^t H'_{aa}(t')\,dt'\right]\left[1 + \frac{i}{\hbar}\int_0^t H'_{aa}(t')\,dt'\right] = 1 + \left[\frac{1}{\hbar}\int_0^t H'_{aa}(t')\,dt'\right]^2 = 1 \text{ (to first order in } H').$$

$$|c_b|^2 = \left[-\frac{i}{\hbar}\int_0^t H'_{ba}(t')e^{i\omega_0 t'}\,dt'\right]\left[\frac{i}{\hbar}\int_0^t H'_{ab}(t')e^{-i\omega_0 t'}\,dt'\right] = 0 \text{ (to first order in } H').$$

So $|c_a|^2 + |c_b|^2 = 1$ (to first order).

(b)

$$\dot{d}_a = e^{\frac{i}{\hbar}\int_0^t H'_{aa}(t')\,dt'}\left(\frac{i}{\hbar}H'_{aa}\right)c_a + e^{\frac{i}{\hbar}\int_0^t H'_{aa}(t')\,dt'}\dot{c}_a. \quad \text{But } \dot{c}_a = -\frac{i}{\hbar}\left[c_a H'_{aa} + c_b H'_{ab}e^{-i\omega_0 t}\right]$$

Two terms cancel, leaving

$$\begin{aligned}\dot{d}_a &= -\frac{i}{\hbar}e^{\frac{i}{\hbar}\int_0^t H'_{aa}(t')\,dt'}c_b H'_{ab}e^{-i\omega_0 t}. \quad \text{But } c_b = e^{-\frac{i}{\hbar}\int_0^t H'_{bb}(t')\,dt'}d_b. \\ &= -\frac{i}{\hbar}e^{\frac{i}{\hbar}\int_0^t [H'_{aa}(t') - H'_{bb}(t')]dt'}H'_{ab}e^{-i\omega_0 t}d_b, \quad \text{or} \quad \dot{d}_a = -\frac{i}{\hbar}e^{i\phi}H'_{ab}e^{-i\omega_0 t}d_b.\end{aligned}$$

Similarly,

$$\begin{aligned}\dot{d}_b &= e^{\frac{i}{\hbar}\int_0^t H'_{bb}(t')\,dt'}\left(\frac{i}{\hbar}H'_{bb}\right)c_b + e^{\frac{i}{\hbar}\int_0^t H'_{bb}(t')\,dt'}\dot{c}_b. \quad \text{But } \dot{c}_b = -\frac{i}{\hbar}\left[c_b H'_{bb} + c_a H'_{ba}e^{i\omega_0 t}\right]. \\ &= -\frac{i}{\hbar}e^{\frac{i}{\hbar}\int_0^t H'_{bb}(t')\,dt'}c_a H'_{ba}e^{i\omega_0 t}. \quad \text{But } c_a = e^{-\frac{i}{\hbar}\int_0^t H'_{aa}(t')\,dt'}d_a. \\ &= -\frac{i}{\hbar}e^{\frac{i}{\hbar}\int_0^t [H'_{bb}(t') - H'_{aa}(t')]dt'}H'_{ba}e^{i\omega_0 t}d_a = -\frac{i}{\hbar}e^{-i\phi}H'_{ba}e^{i\omega_0 t}d_a. \quad \text{QED}\end{aligned}$$

(c)

<u>Initial conditions</u>: $c_a(0) = 1 \implies d_a(0) = 1; \quad c_b(0) = 0 \implies d_b(0) = 0.$

<u>Zeroth order</u>: $d_a(t) = 1, \quad d_b(t) = 0.$

<u>First order</u>: $\dot{d}_a = 0 \implies d_a(t) = 1 \implies \boxed{c_a(t) = e^{-\frac{i}{\hbar}\int_0^t H'_{aa}(t')\,dt'}.}$

$$\dot{d}_b = -\frac{i}{\hbar}e^{-i\phi}H'_{ba}e^{i\omega_0 t} \Longrightarrow d_b = -\frac{i}{\hbar}\int_0^t e^{-i\phi(t')}H'_{ba}(t')e^{i\omega_0 t'}\,dt' \Longrightarrow$$

$$\boxed{c_b(t) = -\frac{i}{\hbar}e^{-\frac{i}{\hbar}\int_0^t H'_{bb}(t')dt'}\int_0^t e^{-i\phi(t')}H'_{ba}(t')e^{i\omega_0 t'}\,dt'.}$$

These don't *look* much like the results in (a), but remember, we're only working to *first order* in H', so $c_a(t) \approx 1 - \frac{i}{\hbar}\int_0^t H'_{aa}(t')\,dt'$ (to this order), while for c_b, the factor H'_{ba} in the integral means it is *already* first order and hence both the exponential factor in front and $e^{-i\phi}$ should be replaced by 1. Then $c_b(t) \approx -\frac{i}{\hbar}\int_0^t H'_{ba}(t')e^{i\omega_0 t'}\,dt'$, and we recover the results in (a).

Problem 11.6

Zeroth order: $c_a^{(0)}(t) = a, \quad c_b^{(0)}(t) = b.$

First order:
$$\begin{cases} \dot{c}_a = -\frac{i}{\hbar}H'_{ab}e^{-i\omega_0 t}b \Longrightarrow c_a^{(1)}(t) = a - \frac{ib}{\hbar}\int_0^t H'_{ab}(t')e^{-i\omega_0 t'}\,dt'. \\ \dot{c}_b = -\frac{i}{\hbar}H'_{ba}e^{i\omega_0 t}a \Longrightarrow c_b^{(1)}(t) = b - \frac{ia}{\hbar}\int_0^t H'_{ba}(t')e^{i\omega_0 t'}\,dt'. \end{cases}$$

Second order: $\dot{c}_a = -\frac{i}{\hbar}H'_{ab}e^{-i\omega_0 t}\left[b - \frac{ia}{\hbar}\int_0^t H'_{ba}(t')e^{i\omega_0 t'}\,dt'\right] \Longrightarrow$

$$\boxed{c_a^{(2)}(t) = a - \frac{ib}{\hbar}\int_0^t H'_{ab}(t')e^{-i\omega_0 t'}\,dt' - \frac{a}{\hbar^2}\int_0^t H'_{ab}(t')e^{-i\omega_0 t'}\left[\int_0^{t'} H'_{ba}(t'')e^{i\omega_0 t''}\,dt''\right]dt'.}$$

To get c_b, just switch $a \leftrightarrow b$ (which entails also changing the sign of ω_0):

$$\boxed{c_b^{(2)}(t) = b - \frac{ia}{\hbar}\int_0^t H'_{ba}(t')e^{i\omega_0 t'}\,dt' - \frac{b}{\hbar^2}\int_0^t H'_{ba}(t')e^{i\omega_0 t'}\left[\int_0^{t'} H'_{ab}(t'')e^{-i\omega_0 t''}\,dt''\right]dt'.}$$

Problem 11.7

For H' independent of t, Eq. 11.21 $\Longrightarrow c_b^{(2)}(t) = c_b^{(1)}(t) = -\frac{i}{\hbar}H'_{ba}\int_0^t e^{i\omega_0 t'}\,dt' \Longrightarrow$

$$c_b^{(2)}(t) = -\frac{i}{\hbar}H'_{ba}\left.\frac{e^{i\omega_0 t'}}{i\omega_0}\right|_0^t = \boxed{-\frac{H'_{ba}}{\hbar\omega_0}\left(e^{i\omega_0 t} - 1\right).}$$ Meanwhile Eq. 11.22 $\Longrightarrow$

$$c_a^{(2)}(t) = 1 - \frac{1}{\hbar^2}|H'_{ab}|^2\int_0^t e^{-i\omega_0 t'}\left[\int_0^{t'} e^{i\omega_0 t''}\,dt''\right]dt' = 1 - \frac{1}{\hbar^2}|H'_{ab}|^2\frac{1}{i\omega_0}\int_0^t\left(1 - e^{-i\omega_0 t'}\right)dt'$$

$$= 1 + \frac{i}{\omega_0\hbar^2}|H'_{ab}|^2\left.\left(t' + \frac{e^{-i\omega_0 t'}}{i\omega_0}\right)\right|_0^t = \boxed{1 + \frac{i}{\omega_0\hbar^2}|H'_{ab}|^2\left[t + \frac{1}{i\omega_0}\left(e^{-i\omega_0 t} - 1\right)\right].}$$

For comparison with the exact answers (Problem 11.3), note first that $c_b(t)$ is already first order (because of the H'_{ba} in front), whereas ω differs from ω_0 only in second order, so it suffices to replace $\omega \to \omega_0$ in the exact formula to get the second-order result:

$$c_b(t) \approx \frac{2H'_{ba}}{i\hbar\omega_0}e^{i\omega_0 t/2}\sin(\omega_0 t/2) = \frac{2H'_{ba}}{i\hbar\omega_0}e^{i\omega_0 t/2}\frac{1}{2i}\left(e^{i\omega_0 t/2} - e^{-i\omega_0 t/2}\right) = -\frac{H'_{ba}}{\hbar\omega_0}\left(e^{i\omega_0 t} - 1\right),$$

in agreement with the result above. Checking c_a is more difficult. Note that

$$\omega = \omega_0\sqrt{1 + \frac{4|H'_{ab}|^2}{\omega_0^2\hbar^2}} \approx \omega_0\left(1 + 2\frac{|H'_{ab}|^2}{\omega_0^2\hbar^2}\right) = \omega_0 + 2\frac{|H'_{ab}|^2}{\omega_0\hbar^2}; \quad \frac{\omega_0}{\omega} \approx 1 - 2\frac{|H'_{ab}|^2}{\omega_0^2\hbar^2}.$$

Taylor expansion:

$$\begin{cases} \cos(x+\epsilon) = \cos x - \epsilon\sin x \implies \cos(\omega t/2) = \cos\left(\dfrac{\omega_0 t}{2} + \dfrac{|H'_{ab}|^2 t}{\omega_0\hbar^2}\right) \approx \cos(\omega_0 t/2) - \dfrac{|H'_{ab}|^2 t}{\omega_0\hbar^2}\sin(\omega_0 t/2) \\ \sin(x+\epsilon) = \sin x + \epsilon\cos x \implies \sin(\omega t/2) = \sin\left(\dfrac{\omega_0 t}{2} + \dfrac{|H'_{ab}|^2 t}{\omega_0\hbar^2}\right) \approx \sin(\omega_0 t/2) + \dfrac{|H'_{ab}|^2 t}{\omega_0\hbar^2}\cos(\omega_0 t/2) \end{cases}$$

$$\begin{aligned} c_a(t) &\approx e^{-i\omega_0 t/2}\left\{\cos\left(\frac{\omega_0 t}{2}\right) - \frac{|H'_{ab}|^2 t}{\omega_0\hbar^2}\sin\left(\frac{\omega_0 t}{2}\right) + i\left(1 - 2\frac{|H'_{ab}|^2}{\omega_0^2\hbar^2}\right)\left[\sin\left(\frac{\omega_0 t}{2}\right) + \frac{|H'_{ab}|^2 t}{\omega_0\hbar^2}\cos\left(\frac{\omega_0 t}{2}\right)\right]\right\} \\ &= e^{-i\omega_0 t/2}\left\{\left[\cos\left(\frac{\omega_0 t}{2}\right) + i\sin\left(\frac{\omega_0 t}{2}\right)\right] - \frac{|H'_{ab}|^2}{\omega_0\hbar^2}\left[t\left(\sin\left(\frac{\omega_0 t}{2}\right) - i\cos\left(\frac{\omega_0 t}{2}\right)\right) + \frac{2i}{\omega_0}\sin\left(\frac{\omega_0 t}{2}\right)\right]\right\} \\ &= e^{-i\omega_0 t/2}\left\{e^{i\omega_0 t/2} - \frac{|H'_{ab}|^2}{\omega_0\hbar^2}\left[-ite^{i\omega_0 t/2} + \frac{2i}{\omega_0}\frac{1}{2i}\left(e^{i\omega_0 t/2} - e^{-i\omega_0 t/2}\right)\right]\right\} \\ &= 1 - \frac{|H'_{ab}|^2}{\omega_0\hbar^2}\left[-it + \frac{1}{\omega_0}\left(1 - e^{-i\omega_0 t}\right)\right] = 1 + \frac{i}{\omega_0\hbar^2}|H'_{ab}|^2\left[t + \frac{1}{i\omega_0}\left(e^{-i\omega_0 t} - 1\right)\right], \text{ as above.} \quad \checkmark \end{aligned}$$

Problem 11.8

(a) Using Equation (11.21),

$$c_b^{(1)}(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} H'_{ba}(t')e^{i\omega_0 t'}\,dt' = -\frac{i\alpha}{\hbar\tau\sqrt{\pi}}\int_{-\infty}^{t} e^{-(t'/\tau)^2}e^{i\omega_0 t'}\,dt'.$$

Complete the square: $-\left(\dfrac{t'}{\tau}\right)^2 + i\omega_0 t' = -\left(\dfrac{t'}{\tau} - i\dfrac{\omega_0\tau}{2}\right)^2 - \left(\dfrac{\omega_0\tau}{2}\right)^2$. Let $t \to \infty$ and $t'/\tau \equiv u$:

$$c_b^{(1)}(\infty) = -\frac{i\alpha}{\hbar\tau\sqrt{\pi}}e^{-(\omega_0\tau/2)^2}\tau\int_{-\infty}^{\infty} e^{-u^2}\,du = -\frac{i\alpha}{\hbar\sqrt{\pi}}e^{-(\omega_0\tau/2)^2}\sqrt{\pi} = -\frac{i\alpha}{\hbar}e^{-(\omega_0\tau)^2/4}.$$

The probability of a transition, then, is

$$P_{a\to b} \approx |c_b^{(1)}(\infty)|^2 = \boxed{\left(\frac{\alpha}{\hbar}\right)^2\exp\left[-\frac{1}{2}(\omega_0\tau)^2\right].}$$

(b) In the limit $\tau \to 0$,

$$P_{a\to b} \approx \left(\frac{\alpha}{\hbar}\right)^2.$$

The *exact* result (from Problem 11.4) is $\sin^2(\alpha/\hbar)$, and expanding this as a power series we get $P_{a\to b} = (\alpha/\hbar)^2 + \cdots$. First-order perturbation theory is precisely the lowest-order term.

(c) In this limit $\boxed{P_{a\to b} = 0}$ (no transition occurs). [Interestingly, it is *not* zero for *all* times—only as $t \to \infty$ (where the perturbation turns off). In fact, if you compute the probability of a transition at a finite time you get:

$$P_{a\to b}(t) = \left(\frac{\alpha}{\hbar}\right)^2 e^{-(\omega_0\tau)^2/2}\left|1 - \frac{1}{2}\mathrm{erfc}\left(\frac{t}{\tau} - i\frac{\omega_0\tau}{2}\right)\right|^2.$$

For large $\omega_0\tau$, the rise and fall of the transition probability can also be computed from the overlap of the *instantaneous* energy eigenstate with the unperturbed state ψ_b.]

Problem 11.9

(a)

$$\dot{c}_a = -\frac{i}{2\hbar}V_{ab}e^{i\omega t}e^{-i\omega_0 t}c_b; \quad \dot{c}_b = -\frac{i}{2\hbar}V_{ba}e^{-i\omega t}e^{i\omega_0 t}c_a.$$

Differentiate the latter, and substitute in the former:

$$\begin{aligned}\ddot{c}_b &= -i\frac{V_{ba}}{2\hbar}\left[i(\omega_0-\omega)e^{i(\omega_0-\omega)t}c_a + e^{i(\omega_0-\omega)t}\dot{c}_a\right]\\ &= i(\omega_0-\omega)\left[-i\frac{V_{ba}}{2\hbar}e^{i(\omega_0-\omega)t}c_a\right] - i\frac{V_{ba}}{2\hbar}e^{i(\omega_0-\omega)t}\left[-i\frac{V_{ab}}{2\hbar}e^{-i(\omega_0-\omega)t}c_b\right] = i(\omega_0-\omega)\dot{c}_b - \frac{|V_{ab}|^2}{(2\hbar)^2}c_b.\end{aligned}$$

$$\frac{d^2c_b}{dt^2} + i(\omega-\omega_0)\frac{dc_b}{dt} + \frac{|V_{ab}|^2}{4\hbar^2}c_b = 0. \quad \text{Solution is of the form } c_b = e^{\lambda t}: \quad \lambda^2 + i(\omega-\omega_0)\lambda + \frac{|V_{ab}|^2}{4\hbar^2} = 0.$$

$$\lambda = \frac{1}{2}\left[-i(\omega-\omega_0) \pm \sqrt{-(\omega-\omega_0)^2 - \frac{|V_{ab}|^2}{\hbar^2}}\right] = i\left[-\frac{(\omega-\omega_0)}{2} \pm \omega_r\right], \text{ with } \omega_r \text{ defined in Eq. 11.37.}$$

General solution: $c_b(t) = Ae^{i\left[-\frac{(\omega-\omega_0)}{2}+\omega_r\right]t} + Be^{i\left[-\frac{(\omega-\omega_0)}{2}-\omega_r\right]t} = e^{-i(\omega-\omega_0)t/2}\left[Ae^{i\omega_r t} + Be^{-i\omega_r t}\right]$,

or, more conveniently: $c_b(t) = e^{-i(\omega-\omega_0)t/2}\left[C\cos(\omega_r t) + D\sin(\omega_r t)\right]$. But $c_b(0) = 0$, so $C = 0$:

$$\begin{aligned}c_b(t) &= De^{i(\omega_0-\omega)t/2}\sin(\omega_r t). \quad \dot{c}_b = D\left[i\left(\frac{\omega_0-\omega}{2}\right)e^{i(\omega_0-\omega)t/2}\sin(\omega_r t) + \omega_r e^{i(\omega_0-\omega)t/2}\cos(\omega_r t)\right];\\ c_a(t) &= i\frac{2\hbar}{V_{ba}}e^{i(\omega-\omega_0)t}\dot{c}_b = i\frac{2\hbar}{V_{ba}}e^{i(\omega-\omega_0)t/2}D\left[i\left(\frac{\omega_0-\omega}{2}\right)\sin(\omega_r t) + \omega_r\cos(\omega_r t)\right]. \quad \text{But } c_a(0) = 1:\\ 1 &= i\frac{2\hbar}{V_{ba}}D\omega_r, \quad \text{or} \quad D = \frac{-iV_{ba}}{2\hbar\omega_r}.\end{aligned}$$

$$\boxed{c_b(t) = -\frac{i}{2\hbar\omega_r}V_{ba}e^{i(\omega_0-\omega)t/2}\sin(\omega_r t), \quad c_a(t) = e^{i(\omega-\omega_0)t/2}\left[\cos(\omega_r t) + i\left(\frac{\omega_0-\omega}{2\omega_r}\right)\sin(\omega_r t)\right].}$$

(b)

$$P_{a\to b}(t) = |c_b(t)|^2 = \boxed{\left(\frac{|V_{ab}|}{2\hbar\omega_r}\right)^2\sin^2(\omega_r t).} \quad \text{The largest this gets (when } \sin^2 = 1) \text{ is } \quad \frac{|V_{ab}|^2/\hbar^2}{4\omega_r^2},$$

and the denominator, $4\omega_r^2 = (\omega-\omega_0)^2+|V_{ab}|^2/\hbar^2$, exceeds the numerator, so $P \leq 1$ (and 1 only if $\omega = \omega_0$).

$$\begin{aligned} |c_a|^2 + |c_b|^2 &= \cos^2(\omega_r t) + \left(\frac{\omega_0-\omega}{2\omega_r}\right)^2 \sin^2(\omega_r t) + \left(\frac{|V_{ab}|}{2\hbar\omega_r}\right)^2 \sin^2(\omega_r t) \\ &= \cos^2(\omega_r t) + \frac{(\omega-\omega_0)^2 + (|V_{ab}|/\hbar)^2}{4\omega_r^2} \sin^2(\omega_r t) = \cos^2(\omega_r t) + \sin^2(\omega_r t) = 1. \quad \checkmark \end{aligned}$$

(c) If $\boxed{|V_{ab}|^2 \ll \hbar^2(\omega-\omega_0)^2,}$ then $\omega_r \approx \frac{1}{2}|\omega-\omega_0|$, and $P_{a\to b} \approx \dfrac{|V_{ab}|^2}{\hbar^2} \dfrac{\sin^2\left(\frac{\omega-\omega_0}{2}t\right)}{(\omega-\omega_0)^2}$, confirming Eq. 11.35.

(d) $\omega_r t = \pi \Longrightarrow \boxed{t = \pi/\omega_r.}$

Problem 11.10

Spontaneous emission rate (Eq. 11.63): $A = \dfrac{\omega^3|\wp|^2}{3\pi\epsilon_0\hbar c^3}$. Thermally stimulated emission rate (Eq. 11.54):

$$R = \frac{\pi}{3\epsilon_0\hbar^2}|\wp|^2\rho(\omega), \quad \text{with} \quad \rho(\omega) = \frac{\hbar}{\pi^2c^3}\frac{\omega^3}{(e^{\hbar\omega/k_BT}-1)} \quad \text{(Eq. 11.59).}$$

So the ratio is

$$\frac{A}{R} = \frac{\omega^3|\wp|^2}{3\pi\epsilon_0\hbar c^3} \cdot \frac{3\epsilon_0\hbar^2}{\pi|\wp|^2} \cdot \frac{\pi^2c^3\left(e^{\hbar\omega/k_BT}-1\right)}{\hbar\omega^3} = e^{\hbar\omega/k_BT} - 1.$$

The ratio is a monotonically increasing function of ω, and is 1 when

$$e^{\hbar\omega/k_bT} = 2, \quad \text{or} \quad \frac{\hbar\omega}{k_BT} = \ln 2, \quad \omega = \frac{k_BT}{\hbar}\ln 2, \quad \text{or} \quad \nu = \frac{\omega}{2\pi} = \frac{k_BT}{h}\ln 2.$$ For $T = 300$ K,

$$\nu = \frac{(1.38\times10^{-23}\ \text{J/K})(300\ \text{K})}{(6.63\times10^{-34}\ \text{J}\cdot\text{s})}\ln 2 = 4.35\times10^{12}\ \text{Hz}.$$

For higher frequencies, (including light, at 10^{14} Hz), spontaneous emission dominates.

Problem 11.11

(a) Look for solutions of the form $f(x,y,z,t) = X(x)Y(y)Z(z)T(t)$. Plug this into the wave equation,

$$\frac{1}{c^2}XYZ\frac{d^2T}{dt^2} - \left(YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2}\right)T = 0.$$

Divide by $XYZT$:

$$\frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2} - \frac{1}{X}\frac{d^2X}{dx^2} - \frac{1}{Y}\frac{d^2Y}{dy^2} - \frac{1}{Z}\frac{d^2Z}{dz^2} = 0.$$

Since they are functions of independent variables, each term must be a constant:

$$\frac{d^2T}{dt^2} = -\omega^2T, \quad \frac{d^2X}{dx^2} = -k_x^2X, \quad \frac{d^2Y}{dy^2} = -k_y^2Y, \quad \frac{d^2Z}{dz^2} = -k_z^2Z,$$

with
$$-\frac{\omega^2}{c^2}+k_x^2+k_y^2+k_z^2=0.$$
The general solution for $T(t)$ is $A\sin(\omega t)+B\cos(\omega t)$, but we may as well start the clock so that $T(t)=B\cos(\omega t)$. The general solution for $X(x)$ is $A_x\sin(k_x x)+B_x\cos(k_x x)$, but the boundary condition at $x=0$ means $B_x=0$, and the boundary condition at $x=l$ then says $\sin(k_x l)=0$, so $k_x=n_x\pi/l$, for some integer n_x. Negative n_x doesn't give us a new solution (it just switches the sign, and we can absorb that into A_x), and $n_x=0$ gives us no solution at all, so in fact $n_x=1,2,3,\ldots$. The same applies to $Y(y)$ and $Z(z)$, so (combining the overall constants):
$$f(x,y,z,t)=A\cos(\omega t)\sin\left(\frac{n_x\pi}{l}x\right)\sin\left(\frac{n_y\pi}{l}y\right)\sin\left(\frac{n_z\pi}{l}z\right)$$
with
$$\omega=\frac{\pi c}{l}\sqrt{n_x^2+n_y^2+n_z^2},\quad \text{where}\quad n_x,\,n_y,\,n_z\quad \text{are positive integers.}$$

(b) As in Figure 5.3, one octant of a spherical shell of radius $n=\sqrt{n_x^2+n_y^2+n_z^2}$ and thickness dn contains $2(1/8)4\pi n^2\,dn=\pi n^2\,dn$ modes, and hence energy
$$dE=(\hbar\omega)\pi n^2\,dn=\pi\hbar\omega\left(\frac{l}{\pi c}\right)^3\omega^2\,d\omega\quad\Rightarrow\quad\frac{dE}{l^3}=\left(\frac{\hbar\omega^3}{pi^2c^3}\right)d\omega.$$
So $\boxed{\rho_0(\omega)=\frac{\hbar\omega^3}{\pi^2c^3}.}$

(c) Plug this into Eq. 11.54:
$$R_{b\to a}=\frac{\pi}{3\epsilon_0\hbar^2}|\wp|^2\frac{\hbar\omega^3}{\pi^2c^3}=\boxed{\frac{\omega^3|\wp|^2}{3\pi\epsilon_0\hbar c^3},}$$
reproducing Eq. 11.63.

Problem 11.12

$N(t)=e^{-t/\tau}N(0)$ (Eqs. 11.65 and 11.66). After one half-life, $N(t)=\frac{1}{2}N(0)$, so $\frac{1}{2}=e^{-t/\tau}$, or $2=e^{t/\tau}$, so $t/\tau=\ln 2$, or $\boxed{t_{1/2}=\tau\ln 2.}$

Problem 11.13

In Problem 11.2 we calculated the matrix elements of z; all of them are zero except $\langle 1\,0\,0|z|2\,1\,0\rangle=\frac{2^8}{3^5\sqrt{2}}a$. As for x and y, we noted that $|1\,0\,0\rangle$, $|2\,0\,0\rangle$, and $|2\,1\,0\rangle$ are *even* (in x, y), whereas $|2\,1\pm1\rangle$ is odd. So the only non-zero matrix elements are $\langle 1\,0\,0|x|2\,1\pm1\rangle$ and $\langle 1\,0\,0|y|2\,1\pm1\rangle$. Using the wave functions in Problem 11.2:
$$\begin{aligned}\langle 1\,0\,0|x|2\,1\pm1\rangle &= \frac{1}{\sqrt{\pi a^3}}\left(\frac{\mp1}{8\sqrt{\pi a^3}}\right)\frac{1}{a}\int e^{-r/a}re^{-r/2a}\sin\theta\,e^{\pm i\phi}(r\sin\theta\cos\phi)r^2\sin\theta\,dr\,d\theta\,d\phi\\ &=\mp\frac{1}{8\pi a^4}\int_0^\infty r^4e^{-3r/2a}dr\int_0^\pi\sin^3\theta\,d\theta\int_0^{2\pi}(\cos\phi\pm i\sin\phi)\cos\phi\,d\phi\\ &=\frac{\mp1}{8\pi a^4}\left[4!\left(\frac{2a}{3}\right)^5\right]\left(\frac{4}{3}\right)(\pi)=\mp\frac{2^7}{3^5}a.\end{aligned}$$

$$\begin{aligned}
\langle 1\,0\,0|y|2\,1\pm 1\rangle &= \frac{\mp 1}{8\pi a^4}\left[4!\left(\frac{2a}{3}\right)^5\right]\left(\frac{4}{3}\right)\int_0^{2\pi}(\cos\phi \pm i\sin\phi)\sin\phi\,d\phi \\
&= \frac{\mp 1}{8\pi a^4}\left[4!\left(\frac{2a}{3}\right)^5\right]\left(\frac{4}{3}\right)(\pm i\pi) = -i\frac{2^7}{3^5}a.
\end{aligned}$$

$\langle 1\,0\,0|\mathbf{r}|2\,0\,0\rangle = 0;\quad \langle 1\,0\,0|\mathbf{r}|2\,1\,0\rangle = \dfrac{2^7\sqrt{2}}{3^5}a\,\hat{k};\quad \langle 1\,0\,0|\mathbf{r}|2\,1\pm 1\rangle = \dfrac{2^7}{3^5}a\left(\mp\hat{\imath} - i\,\hat{\jmath}\right)$, and hence

$\wp^2 = 0$ (for $|2\,0\,0\rangle \to |1\,0\,0\rangle$), and $|\wp|^2 = (qa)^2\dfrac{2^{15}}{3^{10}}$ (for $|2\,1\,0\rangle \to |1\,0\,0\rangle$ and $|2\,1\pm 1\rangle \to |1\,0\,0\rangle$).

Meanwhile, $\omega = \dfrac{E_2 - E_1}{\hbar} = \dfrac{1}{\hbar}\left(\dfrac{E_1}{4} - E_1\right) = -\dfrac{3E_1}{4\hbar}$, so for the three $l = 1$ states:

$$\begin{aligned}
A &= -\frac{3^3E_1^3}{2^6\hbar^3}\frac{(ea)^2 2^{15}}{3^{10}}\frac{1}{3\pi\epsilon_0\hbar c^3} = -\frac{2^9}{3^8\pi}\frac{E_1^3e^2a^2}{\epsilon_0\hbar^4c^3} = \frac{2^{10}}{3^8}\left(\frac{E_1}{mc^2}\right)^2\frac{c}{a} \\
&= \frac{2^{10}}{3^8}\left(\frac{13.6}{0.511\times 10^6}\right)^2\frac{(3.00\times 10^8\ \text{m/s})}{(0.529\times 10^{-10}\ \text{m})} = 6.27\times 10^8/\text{s};\quad \tau = \frac{1}{A} = \boxed{1.60\times 10^{-9}\ \text{s}}
\end{aligned}$$

for the three $l = 1$ states (all have the *same* lifetime); $\boxed{\tau = \infty}$ for the $l = 0$ state.

Problem 11.14

$$\begin{aligned}
&\langle n'\ell'm'|(L_zx - xL_z)|n\ell m\rangle = \hbar(m'-m)\langle n'\ell'm'|x|n\ell m\rangle = i\hbar\langle n'\ell'm'|y|n\ell m\rangle, \\
&\langle n'\ell'm'|(L_zy - yL_z)|n\ell m\rangle = \hbar(m'-m)\langle n'\ell'm'|y|n\ell m\rangle = -i\hbar\langle n'\ell'm'|x|n\ell m\rangle, \\
&\langle n'\ell'm'|(L_zz - zL_z)|n\ell m\rangle = \hbar(m'-m)\langle n'\ell'm'|z|n\ell m\rangle = 0.
\end{aligned}$$

It follows that

$$\begin{cases}
\text{if } m' = m, & \text{then } \langle n'\ell'm'|x|n\ell m\rangle = \langle n'\ell'm'|y|n\ell m\rangle = 0, \\
\text{if } m' = m\pm 1, & \text{then } \langle n'\ell'm'|x|n\ell m\rangle = \pm i\langle n'\ell'm'|y|n\ell m\rangle = 0,\ \langle n'\ell'm'|z|n\ell m\rangle = 0, \\
\text{otherwise,} & \langle n'\ell'm'|x|n\ell m\rangle = \langle n'\ell'm'|y|n\ell m\rangle = \langle n'\ell'm'|z|n\ell m\rangle = 0.
\end{cases}$$

To establish the last line, note that

$$(m'-m)^2\langle n'\ell'm'|x|n\ell m\rangle = (m'-m)i\langle n'\ell'm'|y|n\ell m\rangle = i(-i)\langle n'\ell'm'|x|n\ell m\rangle = \langle n'\ell'm'|x|n\ell m\rangle,$$

so unless $(m'-m)^2 = 1, \langle n'\ell'm'|x|n\ell m\rangle = 0$ (and the same goes for y).

Problem 11.15

(a)

$$[L^2, z] = [L_x^2, z] + [L_y^2, z] + [L_z^2, z] = L_x[L_x, z] + [L_x, z]L_x + L_y[L_y, z] + [L_y, z]L_y + L_z[L_z, z] + [L_z, z]L_z$$

$$\text{But}\ \begin{cases}
[L_x, z] = [yp_z - zp_y, z] = [yp_z, z] - [zp_y, z] = y[p_z, z] = -i\hbar y, \\
[L_y, z] = [zp_x - xp_z, z] = [zp_x, z] - [xp_z, z] = -x[p_z, z] = i\hbar x, \\
[L_z, z] = [xp_y - yp_x, z] = [xp_y, z] - [yp_x, z] = 0.
\end{cases}$$

So: $[L^2, z] = L_x(-i\hbar y) + (-i\hbar y)L_x + L_y(i\hbar x) + (i\hbar x)L_y = i\hbar(-L_x y - yL_x + L_y x + xL_y)$.

But $\begin{cases} L_x y = L_x y - yL_x + yL_x = [L_x, y] + yL_x = i\hbar z + yL_x, \\ L_y x = L_y x - xL_y + xL_y = [L_y, x] + xL_y = -i\hbar z + xL_y. \end{cases}$

So: $[L^2, z] = i\hbar(2xL_y - i\hbar z - 2yL_x - i\hbar z) \Longrightarrow [L^2, z] = 2i\hbar(xL_y - yL_x - i\hbar z)$. ✓

$$\begin{aligned}\left[L^2,[L^2,z]\right] &= 2i\hbar\left\{[L^2, xL_y] - [L^2, yL_x] - i\hbar[L^2, z]\right\} \\ &= 2i\hbar\left\{[L^2, x]L_y + x[L^2, L_y] - [L^2, y]L_x - y[L^2, L_x] - i\hbar(L^2 z - zL^2)\right\}.\end{aligned}$$

But $[L^2, L_y] = [L^2, L_x] = 0$ (Eq. 4.102), so

$$\left[L^2,[L^2,z]\right] = 2i\hbar\left\{2i\hbar\,(yL_z - zL_y - i\hbar x)\,L_y - 2i\hbar\,(zL_x - xL_z - i\hbar y)\,L_x - i\hbar\left(L^2 z - zL^2\right)\right\}, \text{ or}$$

$$\begin{aligned}\left[L^2,[L^2,z]\right] &= -2\hbar^2\left(2yL_zL_y \underbrace{-2zL_y^2 - 2zL_x^2}_{-2z(L_x^2+L_y^2+L_z^2)+2zL_z^2} -2i\hbar xL_y + 2xL_zL_x + 2i\hbar yL_x - L^2 z + zL^2\right) \\ &= -2\hbar^2\left(2yL_zL_y - 2i\hbar xL_y + 2xL_zL_x + 2i\hbar yL_x + 2zL_z^2 - 2zL^2 - L^2 z + zL^2\right) \\ &= 2\hbar^2\left(zL^2 + L^2 z\right) - 4\hbar^2\left[\underbrace{(yL_z - i\hbar x)}_{L_z y}L_y + \underbrace{(xL_z + i\hbar y)}_{L_z x}L_x + zL_zL_z\right] \\ &= 2\hbar^2\left(zL^2 + L^2 z\right) - 4\hbar^2\underbrace{(L_z yL_y + L_z xL_x + L_z zL_z)}_{L_z(\mathbf{r}\cdot\mathbf{L})=0} = 2\hbar^2(zL^2 + L^2 z). \quad \text{QED}\end{aligned}$$

(b) Making the obvious generalization of part (a):

$$\left[L^2,[L^2,\mathbf{r}]\right] = 2\hbar^2(\mathbf{r}L^2 + L^2\mathbf{r}).$$

As before, we sandwich this commutator between $\langle n'\ell'm'|$ and $|n\ell m\rangle$ to derive the selection rule:

$$\begin{aligned}&\langle n'\ell'm'|\left[L^2,[L^2,\mathbf{r}]\right]|n\ell m\rangle = 2\hbar^2\langle n'\ell'm'|(\mathbf{r}L^2 + L^2\mathbf{r})|n\ell m\rangle \\ &= 2\hbar^4[\ell(\ell+1) + \ell'(\ell'+1)]\langle n'\ell'm'|\mathbf{r}|n\ell m\rangle = \langle n'\ell'm'|(L^2[L^2,\mathbf{r}] - [L^2,\mathbf{r}]L^2)|n\ell m\rangle \\ &= \hbar^2[\ell'(\ell'+1) - \ell(\ell+1)]\langle n'\ell'm'|[L^2,\mathbf{r}]|n\ell m\rangle = \hbar^2[\ell'(\ell'+1) - \ell(\ell+1)]\langle n'\ell'm'|(L^2\mathbf{r} - \mathbf{r}L^2)|n\ell m\rangle \\ &= \hbar^4[\ell'(\ell'+1) - \ell(\ell+1)]^2\langle n'\ell'm'|\mathbf{r}|n\ell m\rangle.\end{aligned}$$

Conclusion: Either

$$2[\ell(\ell+1) + \ell'(\ell'+1)] = [\ell'(\ell'+1) - \ell(\ell+1)]^2, \quad \text{or else} \quad \langle n'\ell'm'|\mathbf{r}|n\ell m\rangle = 0.$$

But

$$[\ell'(\ell'+1) - \ell(\ell+1)] = (\ell' + \ell + 1)(\ell' - \ell)$$

and

$$2[\ell(\ell+1) + \ell'(\ell'+1)] = (\ell' + \ell + 1)^2 + (\ell' - \ell)^2 - 1,$$

so the first possibility can be written in the form

$$[(\ell' + \ell + 1)^2 - 1][(\ell' - \ell)^2 - 1] = 0.$$

The first factor *cannot* be zero (unless $\ell' = \ell = 0$, but $\langle n'00|\mathbf{r}|n00\rangle$ is trivially zero, since the integrand is odd), so the condition simplifies to $\ell' = \ell \pm 1$. Thus we obtain the selection rule for ℓ:

$$\boxed{\text{No transitions occur unless } \Delta\ell = \pm 1.}$$

Problem 11.16

(a)

$$\boxed{|3\,0\,0\rangle \to \left\{\begin{array}{c} |2\,1\,0\rangle \\ |2\,1\,1\rangle \\ |2\,1{-}1\rangle \end{array}\right\} \to |1\,0\,0\rangle.} \quad (|3\,0\,0\rangle \to |2\,0\,0\rangle \text{ and } |3\;0\;0\rangle \to |1\;0\;0\rangle \text{ violate } \Delta l = \pm 1 \text{ rule.})$$

(b)

From Eq. 11.76: $\langle 2\,1\,0|\mathbf{r}|3\,0\,0\rangle = \langle 2\,1\,0|z|3\,0\,0\rangle\,\hat{k}$.

$\langle 2\,1\pm 1|\mathbf{r}|3\,0\,0\rangle = \langle 2\,1\pm 1|x|3\,0\,0\rangle\,\hat{\imath} + \langle 2\,1\pm 1|y|3\,0\,0\rangle\,\hat{\jmath}$.

$\pm\langle 2\,1\pm 1|x|3\,0\,0\rangle = i\langle 2\,1\pm 1|y|3\,0\,0\rangle$.

Thus $|\langle 2\,1\,0|\mathbf{r}|3\,0\,0\rangle|^2 = |\langle 2\,1\,0|z|3\,0\,0\rangle|^2$ and $|\langle 2\,1\pm 1|\mathbf{r}|3\,0\,0\rangle|^2 = 2|\langle 2\,1\pm 1|x|3\,0\,0\rangle|^2$,

so there are really just two matrix elements to calculate.

$\psi_{21m} = R_{21}Y_1^m$, $\quad \psi_{300} = R_{30}Y_0^0$. From Table 4.3:

$$\int Y_1^0 Y_0^0 \cos\theta \sin\theta\, d\theta\, d\phi = \sqrt{\frac{3}{4\pi}}\sqrt{\frac{1}{4\pi}}\int_0^\pi \cos^2\theta\sin\theta\, d\theta \int_0^{2\pi} d\phi = \frac{\sqrt{3}}{4\pi}\left(-\frac{\cos^3\theta}{3}\right)\Big|_0^\pi (2\pi) = \frac{\sqrt{3}}{2}\left(\frac{2}{3}\right) = \frac{1}{\sqrt{3}}.$$

$$\int \left(Y_1^{\pm 1}\right)^* Y_0^0 \sin^2\theta\cos\phi\, d\theta\, d\phi = \mp\sqrt{\frac{3}{8\pi}}\sqrt{\frac{1}{4\pi}}\int_0^\pi \sin^3\theta\, d\theta\int_0^{2\pi}\cos\phi\, e^{\mp i\phi}\, d\phi$$

$$= \mp\frac{1}{4\pi}\sqrt{\frac{3}{2}}\left(\frac{4}{3}\right)\left[\int_0^{2\pi}\cos^2\phi\, d\phi \mp i\int_0^{2\pi}\cos\phi\sin\phi\, d\phi\right] = \mp\frac{1}{\pi\sqrt{6}}(\pi \mp 0) = \mp\frac{1}{\sqrt{6}}.$$

From Table 4.7:

$$K \equiv \int_0^\infty R_{21}R_{30}\, r^3\, dr = \frac{1}{\sqrt{24}a^{3/2}}\frac{2}{\sqrt{27}a^{3/2}}\int_0^\infty \frac{r}{a}e^{-r/2a}\left[1 - \frac{2}{3}\frac{r}{a} + \frac{2}{27}\left(\frac{r}{a}\right)^2\right]e^{-r/3a}r^3\, dr$$

$$= \frac{1}{9\sqrt{2}a^3}a^4\int_0^\infty\left(1 - \frac{2}{3}u + \frac{2}{27}u^2\right)u^4 e^{-5u/6}\, du = \frac{a}{9\sqrt{2}}\left[4!\left(\frac{6}{5}\right)^5 - \frac{2}{3}5!\left(\frac{6}{5}\right)^6 + \frac{2}{27}6!\left(\frac{6}{5}\right)^7\right]$$

$$= \frac{a}{9\sqrt{2}}\frac{4!\,6^5}{5^6}\left(5 - \frac{2}{3}6\cdot 5 + \frac{2}{27}6^3\right) = \frac{a}{9\sqrt{2}}\frac{4!\,6^5}{5^6} = \frac{2^7 3^4}{5^6}\sqrt{2}\, a.$$

So:

$$\langle 2\,1\pm 1|x|3\,0\,0\rangle = \int R_{21}(Y_1^{\pm 1})^*(r\sin\theta\cos\phi)R_{30}Y_0^0\, r^2\sin\theta\, dr\, d\theta\, d\phi = K\left(\mp\frac{1}{\sqrt{6}}\right).$$

$$\langle 2\,1\,0|z|3\,0\,0\rangle = \int R_{21}Y_1^0(r\cos\theta)R_{30}Y_0^0\, r^2\sin\theta\, dr\, d\theta\, d\phi = K\left(\frac{1}{\sqrt{3}}\right).$$

$|\langle 2\,1\,0|\mathbf{r}|3\,0\,0\rangle|^2 = |\langle 2\,1\,0|z|3\,0\,0\rangle|^2 = K^2/3$;

$|\langle 2\,1\pm 1|\mathbf{r}|3\,0\,0\,\rangle|^2 = 2|\langle 2\,1\pm 1|x|3\,0\,0\,\rangle|^2 = K^2/3$.

Evidently the three transition rates are *equal*, and hence $\boxed{1/3}$ go by each route.

(c) For each mode, $A = \dfrac{\omega^3 e^2 |\langle \mathbf{r} \rangle|^2}{3\pi\epsilon_0 \hbar c^3}$; here $\omega = \dfrac{E_3 - E_2}{\hbar} = \dfrac{1}{\hbar}\left(\dfrac{E_1}{9} - \dfrac{E_1}{4}\right) = -\dfrac{5}{36}\dfrac{E_1}{\hbar}$, so the *total* decay rate is

$$R = 3\left(-\frac{5}{36}\frac{E_1}{\hbar}\right)^3 \frac{e^2}{3\pi\epsilon_0\hbar c^3}\frac{1}{3}\left(\frac{2^7 3^4}{5^6}\sqrt{2}a\right)^2 = 6\left(\frac{2}{5}\right)^9 \left(\frac{E_1}{mc^2}\right)^2 \left(\frac{c}{a}\right)$$
$$= 6\left(\frac{2}{5}\right)^9 \left(\frac{13.6}{0.511 \times 10^6}\right)^2 \left(\frac{3 \times 10^8}{0.529 \times 10^{-10}}\right) /\text{s} = 6.32 \times 10^6/\text{s}. \quad \tau = \frac{1}{R} = \boxed{1.58 \times 10^{-7}\ \text{s.}}$$

Problem 11.17

(a) $R = \dfrac{2\pi}{\hbar}\left|\dfrac{V_{if}}{2}\right|^2 \rho(E_f)$. From Eqs. 11.31 and 11.39, $V_{if} = \langle \psi_i | V | \psi_f \rangle$, where $V = eE_0 z$, so

$$V_{if} = eE_0 \langle \psi_0 | z | \psi_f \rangle = eE_0 \frac{1}{\sqrt{\pi a^3}} \frac{1}{\sqrt{l^3}} \int e^{-r/a} z e^{i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{r} = \frac{eE_0}{\sqrt{\pi a^3 l^3}}\left(-i\frac{\partial}{\partial k_z}\right)\int e^{-r/a} e^{i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{r}.$$

To evaluate the integral, set the z axis along $\mathbf{k}$, so

$$\int e^{-r/a} e^{i\mathbf{k}\cdot\mathbf{r}}\, d^4\mathbf{r} = \int e^{-r/a} e^{ikr\cos\theta}\, r^2 \sin\theta\, dr\, d\theta\, d\phi = 2\pi \int_0^\infty r^2 e^{-r/a}\left\{\int_0^\pi e^{ikr\cos\theta}\sin\theta\, d\theta\right\} dr$$
$$= 2\pi \int_0^\infty r^2 e^{-r/a}\left\{-\frac{e^{ikr\cos\theta}}{ikr}\Bigg|_0^\pi\right\} dr = \frac{2\pi i}{k}\int_0^\infty r e^{-r/a}\left(e^{-ikr} - e^{ikr}\right) dr$$
$$= \frac{2\pi i}{k}\left\{\int_0^\infty r e^{-r(1/a+ik)}\, dr - \int_0^\infty r e^{-r(1/a-ik)}\, dr\right\} =$$
$$= \frac{2\pi i}{k}\left[\frac{1}{(1/a+ik)^2} - \frac{1}{(1/a-ik)^2}\right] = \left(\frac{2\pi a^2 i}{k}\right)\frac{(1-ika)^2 - (1+ika)^2}{[1+(ka)^2]^2}$$
$$= \left(\frac{2\pi a^2 i}{k}\right)\frac{(-4ika}{[1+(ka)^2]^2} = \frac{8\pi a^3}{[1+(ka)^2]^2}.$$

$$V_{if} = -\frac{ieE_0}{\sqrt{\pi a^3 l^3}}\frac{\partial}{\partial k_z}\left(\frac{8\pi a^3}{\left[1+k^2a^2\right]^2}\right) = -8ieE_0\sqrt{\frac{\pi a^3}{l^3}}\frac{-4a^2 k_z}{\left[1+k^2a^2\right]^3} = \frac{32 ieE_0 a^2 k\cos\theta}{\left[1+k^2a^2\right]^3}\sqrt{\frac{\pi a^3}{l^3}}.$$

Finally, quoting Eq. 11.85,

$$\rho(E_f) = \left(\frac{l}{2\pi}\right)^3 \frac{\sqrt{2m^3 E_f}}{\hbar^3}\, d\Omega, \quad \text{where} \quad E_f = \frac{\hbar^2 k^2}{2m}, \quad \text{so} \quad \rho(E_f) = \left(\frac{l}{2\pi}\right)^3 \frac{mk}{\hbar^2}\, d\Omega.$$

Putting it all together,

$$R = \frac{\pi}{2\hbar}\left(\frac{32eE_0 a^2 k\cos\theta}{\left[1+k^2a^2\right]^3}\sqrt{\frac{\pi a^3}{l^3}}\right)^2 \left(\frac{l}{2\pi}\right)^3 \frac{mk}{\hbar^2}\, d\Omega, \quad \text{or, using} \quad me^2 = \frac{4\pi\epsilon_0\hbar^2}{a},$$
$$= \boxed{\frac{256}{\hbar}\epsilon_0 E_0^2 \frac{k^3 a^6}{\left[1+k^2a^2\right]^6}\cos^2\theta\, d\Omega.}$$

(b) Integrating over all angles, using $d\Omega = \sin\theta\, d\theta\, d\phi$,

$$R_{i\to\text{all}} = \frac{256}{\hbar}\,\epsilon_0 E_0^2\,\frac{k^3a^6}{[1+k^2a^2]^6}\int \cos^2\theta\,\sin\theta\,d\theta\,d\phi = \frac{256}{\hbar}\,\epsilon_0 E_0^2\,\frac{k^3a^6}{[1+k^2a^2]^6}\left(\frac{4\pi}{3}\right),$$

and noting that

$$\hbar\omega = \frac{\hbar^2k^2}{2m} + \frac{\hbar^2}{2ma^2} = \frac{\hbar^2}{2ma^2}(1+k^2a^2),$$

the cross-section is

$$\sigma(k) = \frac{1}{\frac{1}{2}\epsilon_0 E_0^2 c}\,\frac{256}{\hbar}\,\epsilon_0 E_0^2\,\frac{k^3a^6}{[1+k^2a^2]^6}\left(\frac{4\pi}{3}\right)\frac{\hbar^2}{2ma^2}(1+k^2a^2) = \boxed{\frac{1024\,\pi\hbar}{3mc}\,\frac{k^3a^4}{[1+k^2a^2]^5}.}$$

(c)

$$\lambda = \frac{2\pi c}{\omega} \quad\Rightarrow\quad \hbar\omega = \hbar\frac{2\pi c}{\lambda} = \frac{\hbar^2}{2ma^2}(1+k^2a^2) \quad\Rightarrow\quad (1+k^2a^2) = \frac{2ma^2}{\hbar^2}\frac{\hbar 2\pi c}{\lambda} = \frac{4\pi m a^2 c}{\hbar\lambda}.$$

But $\quad ma^2 = \dfrac{\hbar^2}{2|E_1|}, \quad$ so

$$(1+k^2a^2) = \frac{4\pi c}{\hbar\lambda}\,\frac{\hbar^2}{2|E_1|} = \frac{2\pi\hbar c}{\lambda|E_1|} = \frac{2\pi(1.055\times10^{-34})(3\times10^8)}{(220\times10^{-10})(13.6)(1.6\times10^{-19})} = 4.15.$$

$$(ka)^2 = 3.15 \quad\Rightarrow\quad ka = 1.77.$$

$$\sigma = \frac{1024\,\pi(1.055\times10^{-34})(1.77)^3(5.29\times10^{-11})}{3(9.11\times10^{-31})(3\times10^8)(4.15)^5} = 0.986\times10^{-22}\,\text{m}^2 = \boxed{1\ \text{Mb.}}$$

Problem 11.18

(a) New allowed energies: $E_n = \dfrac{n^2\pi^2\hbar^2}{2m(2a)^2}$; $\quad \Psi(x,0) = \sqrt{\dfrac{2}{a}}\sin\left(\dfrac{\pi}{a}x\right),\ \psi_n(x) = \sqrt{\dfrac{2}{2a}}\sin\left(\dfrac{n\pi}{2a}x\right).$

$$\begin{aligned}
c_n &= \frac{\sqrt{2}}{a}\int_0^a \sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{n\pi}{2a}x\right)dx = \frac{\sqrt{2}}{2a}\int_0^a\left\{\cos\left[\left(\frac{n}{2}-1\right)\frac{\pi x}{a}\right] - \cos\left[\left(\frac{n}{2}+1\right)\frac{\pi x}{a}\right]\right\}dx \\
&= \frac{1}{\sqrt{2}a}\left\{\frac{\sin\left[\left(\frac{n}{2}-1\right)\frac{\pi x}{a}\right]}{\left(\frac{n}{2}-1\right)\frac{\pi}{a}} - \frac{\sin\left[\left(\frac{n}{2}+1\right)\frac{\pi x}{a}\right]}{\left(\frac{n}{2}+1\right)\frac{\pi}{a}}\right\}\Bigg|_0^a \qquad (\text{for } n\neq 2) \\
&= \frac{1}{\sqrt{2}\pi}\left\{\frac{\sin\left[\left(\frac{n}{2}-1\right)\pi\right]}{\left(\frac{n}{2}-1\right)} - \frac{\sin\left[\left(\frac{n}{2}+1\right)\pi\right]}{\left(\frac{n}{2}+1\right)}\right\} = \frac{\sin\left[\left(\frac{n}{2}+1\right)\pi\right]}{\sqrt{2}\pi}\left[\frac{1}{\left(\frac{n}{2}-1\right)} - \frac{1}{\left(\frac{n}{2}+1\right)}\right] \\
&= \frac{4\sqrt{2}}{\pi}\frac{\sin\left[\left(\frac{n}{2}+1\right)\pi\right]}{(n^2-4)} = \left\{\begin{array}{ll} 0, & \text{if } n \text{ is even} \\ \pm\frac{4\sqrt{2}}{\pi(n^2-4)}, & \text{if } n \text{ is odd}\end{array}\right\}.
\end{aligned}$$

$c_2 = \dfrac{\sqrt{2}}{a}\displaystyle\int_0^a \sin^2\left(\frac{\pi}{a}x\right)dx = \frac{\sqrt{2}}{a}\int_0^a \frac{1}{2}dx = \frac{1}{\sqrt{2}}.$ So the probability of getting E_n is

$$P_n = |c_n|^2 = \left\{ \begin{array}{ll} \frac{1}{2}, & \text{if } n = 2 \\ \frac{32}{\pi^2(n^2-4)^2}, & \text{if } n \text{ is odd} \\ 0, & \text{otherwise} \end{array} \right\}.$$

Most probable: $E_2 = \boxed{\dfrac{\pi^2\hbar^2}{2ma^2}}$ (same as before). Probability: $P_2 = \boxed{1/2.}$

(b) Next most probable: $E_1 = \boxed{\dfrac{\pi^2\hbar^2}{8ma^2},}$ with probability $P_1 = \boxed{\dfrac{32}{9\pi^2} = 0.36025.}$

(c) $\langle H \rangle = \int \Psi^* H \Psi \, dx = \frac{2}{a}\int_0^a \sin\left(\frac{\pi}{a}x\right)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\sin\left(\frac{\pi}{a}x\right) dx$, but this is exactly the same as before the wall moved – for which we know the answer: $\boxed{\dfrac{\pi^2\hbar^2}{2ma^2}.}$

Problem 11.19

The new allowed energies are $E_n' = (n+\frac{1}{2})\hbar\omega' = 2(n+\frac{1}{2})\hbar\omega = \hbar\omega, 3\hbar\omega, 5\hbar\omega, \ldots$. So the probability of getting $\frac{1}{2}\hbar\omega$ is $\boxed{\text{zero.}}$ The probability of getting $\hbar\omega$ (the new ground state energy) is $P_0 = |c_0|^2$, where $c_0 = \int \Psi(x,0)\psi_0' \, dx$, with

$$\Psi(x,0) = \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}, \quad \psi_0(x)' = \left(\frac{m2\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m2\omega}{2\hbar}x^2}.$$

So

$$c_0 = 2^{1/4}\sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty} e^{-\frac{3m\omega}{2\hbar}x^2}\, dx = 2^{1/4}\sqrt{\frac{m\omega}{\pi\hbar}}2\sqrt{\pi}\left(\frac{1}{2}\sqrt{\frac{2\hbar}{3m\omega}}\right) = 2^{1/4}\sqrt{\frac{2}{3}}.$$

Therefore

$$P_0 = \boxed{\frac{2}{3}\sqrt{2} = 0.9428.}$$

Problem 11.20

To show: $\quad i\hbar\dfrac{\partial\chi}{\partial t} = H\chi,\quad$ where χ is given by Eq. 11.103 and H is given by Eq. 11.97.

$$\frac{\partial\chi}{\partial t} =$$

$$\begin{pmatrix} \frac{\lambda}{2}\left[-\sin\left(\frac{\lambda t}{2}\right) - i\frac{(\omega_1-\omega)}{\lambda}\cos\left(\frac{\lambda t}{2}\right)\right]\cos\left(\frac{\alpha}{2}\right)e^{-i\omega t/2} - \frac{i\omega}{2}\left[\cos\left(\frac{\lambda t}{2}\right) - \frac{i(\omega_1-\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\cos\left(\frac{\alpha}{2}\right)e^{-i\omega t/2} \\ \frac{\lambda}{2}\left[-\sin\left(\frac{\lambda t}{2}\right) - i\frac{(\omega_1+\omega)}{\lambda}\cos\left(\frac{\lambda t}{2}\right)\right]\sin\left(\frac{\alpha}{2}\right)e^{i\omega t/2} + \frac{i\omega}{2}\left[\cos\left(\frac{\lambda t}{2}\right) - \frac{i(\omega_1+\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\sin\left(\frac{\alpha}{2}\right)e^{i\omega t/2} \end{pmatrix}$$

$$H\chi =$$

$$\frac{\hbar\omega_1}{2}\begin{pmatrix} \cos\alpha\left[\cos(\frac{\lambda t}{2}) - i\frac{(\omega_1-\omega)}{\lambda}\sin(\frac{\lambda t}{2})\right]\cos\frac{\alpha}{2}e^{-i\omega t/2} + e^{-i\omega t}\sin\alpha\left[\cos(\frac{\lambda t}{2}) - \frac{i(\omega_1+\omega)}{\lambda}\sin(\frac{\lambda t}{2})\right]\sin\frac{\alpha}{2}e^{i\omega t/2} \\ e^{i\omega t}\sin\alpha\left[\cos(\frac{\lambda t}{2}) - i\frac{(\omega_1-\omega)}{\lambda}\sin(\frac{\lambda t}{2})\right]\cos\frac{\alpha}{2}e^{-i\omega t/2} - \cos\alpha\left[\cos(\frac{\lambda t}{2}) - \frac{i(\omega_1+\omega)}{\lambda}\sin(\frac{\lambda t}{2})\right]\sin\frac{\alpha}{2}e^{i\omega t/2} \end{pmatrix}$$

(1) Upper elements:

$$i\cancel{\hbar}\left\{\frac{\lambda}{\cancel{2}}\left[-\sin\left(\frac{\lambda t}{2}\right)-i\frac{(\omega_1-\omega)}{\lambda}\cos\left(\frac{\lambda t}{2}\right)\right]\cancel{\cos\frac{\alpha}{2}}-\frac{i\omega}{\cancel{2}}\left[\cos\left(\frac{\lambda t}{2}\right)-\frac{i(\omega_1-\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\cancel{\cos\frac{\alpha}{2}}\right\}$$

$$\overset{?}{=}\frac{\cancel{\hbar}\omega_1}{\cancel{2}}\left\{\left[\cos\left(\frac{\lambda t}{2}\right)-i\frac{(\omega_1-\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\cos\alpha\cancel{\cos\frac{\alpha}{2}}+\left[\cos\left(\frac{\lambda t}{2}\right)-i\frac{(\omega_1+\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\underbrace{\sin\alpha}_{\bigstar}\sin\frac{\alpha}{2}\right\},$$

where $\bigstar = 2\sin\frac{\alpha}{2}\cancel{\cos\frac{\alpha}{2}}$

The sine terms:

$$\sin\left(\frac{\lambda t}{2}\right)\left[-i\lambda-\frac{i\omega(\omega_1-\omega)}{\lambda}+\frac{i\omega_1(\omega_1-\omega)}{\lambda}\cos\alpha+\frac{i\omega_1(\omega_1+\omega)}{\lambda}\,2\,\sin^2\frac{\alpha}{2}\right]\overset{?}{=}0.$$

$$\frac{i}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\left[\cancel{-\omega^2}-\omega_1^2+2\omega\omega_1\cos\alpha-\omega\omega_1+\cancel{\omega^2}+(\omega_1^2-\omega\omega_1)\cos\alpha+(\omega_1^2+\omega\omega_1)(1-\cos\alpha)\right]$$

$$=-\frac{i}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\left[\cancel{-\omega_1^2}+2\omega\omega_1\cos\alpha-\cancel{\omega\omega_1}+\cancel{\omega_1^2\cos\alpha}-\omega\omega_1\cos\alpha+\cancel{\omega_1^2}+\cancel{\omega\omega_1}-\cancel{\omega_1^2\cos\alpha}-\omega\omega_1\cos\alpha\right]=0.\quad\checkmark$$

The cosine terms:

$$\cos\left(\frac{\lambda t}{2}\right)\left[(\omega_1-\cancel{\omega})+\cancel{\omega}-\omega_1\cos\alpha-\omega_1\,2\,\sin^2\frac{\alpha}{2}\right]=-\omega_1\cos\left(\frac{\lambda t}{2}\right)[-1+\cos\alpha+(1-\cos\alpha)]=0.\quad\checkmark$$

(2) Lower elements:

$$i\cancel{\hbar}\left\{\frac{\lambda}{\cancel{2}}\left[-\sin\left(\frac{\lambda t}{2}\right)-i\frac{(\omega_1+\omega)}{\lambda}\cos\left(\frac{\lambda t}{2}\right)\right]\cancel{\sin\left(\frac{\alpha}{2}\right)}+\frac{i\omega}{\cancel{2}}\left[\cos\left(\frac{\lambda t}{2}\right)-\frac{i(\omega_1+\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\cancel{\sin\left(\frac{\alpha}{2}\right)}\right\}$$

$$\overset{?}{=}\frac{\cancel{\hbar}\omega_1}{\cancel{2}}\left\{\left[\cos\left(\frac{\lambda t}{2}\right)-i\frac{(\omega_1-\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]2\cancel{\sin\frac{\alpha}{2}}\cos^2\frac{\alpha}{2}-\left[\cos\left(\frac{\lambda t}{2}\right)-\frac{i(\omega_1+\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\cos\alpha\cancel{\sin\frac{\alpha}{2}}\right\}.$$

The sine terms:

$$\sin\left(\frac{\lambda t}{2}\right)\left[-i\lambda+\frac{i\omega(\omega_1+\omega)}{\lambda}+\frac{i\omega_1(\omega_1-\omega)}{\lambda}\,2\cos^2\left(\frac{\alpha}{2}\right)-\frac{i\omega_1(\omega_1+\omega)}{\lambda}\cos\alpha\right]\overset{?}{=}0.$$

$$\frac{i}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\left[-\cancel{\omega^2}-\omega_1^2+2\omega\omega_1\cos\alpha+\omega\omega_1+\cancel{\omega^2}+(\omega_1^2-\omega\omega_1)(1+\cos\alpha)-(\omega_1^2+\omega\omega_1)\cos\alpha\right]$$

$$=\frac{i}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\left[-\cancel{\omega_1^2}+2\omega\omega_1\cos\alpha+\cancel{\omega\omega_1}+\cancel{\omega_1^2}-\cancel{\omega\omega_1}+\cancel{\omega_1^2\cos\alpha}-\omega\omega_1\cos\alpha-\cancel{\omega_1^2\cos\alpha}-\omega\omega_1\cos\alpha\right]=0.\quad\checkmark$$

The cosine terms:

$$\cos\left(\frac{\lambda t}{2}\right)\left[(\omega_1+\cancel{\omega})-\cancel{\omega}-\omega_1\,2\cos^2\frac{\alpha}{2}+\omega_1\cos\alpha\right]=\cos\left(\frac{\lambda t}{2}\right)[\omega_1-\omega_1(1+\cos\alpha)+\omega_1\cos\alpha]=0.\quad\checkmark$$

As for Eq. 11.105:

$$\left[\cos\left(\frac{\lambda t}{2}\right)-i\frac{(\omega_1-\omega\cos\alpha)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]e^{-i\omega t/2}\begin{pmatrix}\cos\frac{\alpha}{2}\\ e^{i\omega t}\sin\frac{\alpha}{2}\end{pmatrix}+i\left[\frac{\omega}{\lambda}\sin\alpha\sin\left(\frac{\lambda t}{2}\right)\right]e^{-i\omega t/2}\begin{pmatrix}\sin\frac{\alpha}{2}\\ -e^{i\omega t}\cos\frac{\alpha}{2}\end{pmatrix}$$

$$=\begin{pmatrix}\alpha\\ \beta\end{pmatrix},\quad \text{with}$$

$$\alpha = \left\{ \left[\cos\left(\frac{\lambda t}{2}\right) - \frac{i\omega_1}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\cos\frac{\alpha}{2} + \frac{i\omega}{\lambda}\left[\underbrace{\cos\alpha\cos\frac{\alpha}{2} + \sin\alpha\sin\frac{\alpha}{2}}_{\cos(\alpha-\frac{\alpha}{2})=\cos\frac{\alpha}{2}}\right]\sin\left(\frac{\lambda t}{2}\right)\right\} e^{-i\omega t/2}$$

$$= \left[\cos\left(\frac{\lambda t}{2}\right) - \frac{i(\omega_1-\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\cos\frac{\alpha}{2}e^{-i\omega t/2} \quad \text{(confirming the top entry).}$$

$$\beta = \left\{ \left[\cos\left(\frac{\lambda t}{2}\right) - \frac{i\omega_1}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\sin\frac{\alpha}{2} + \frac{i\omega}{\lambda}\left[\underbrace{\cos\alpha\sin\frac{\alpha}{2} - \sin\alpha\cos\frac{\alpha}{2}}_{\sin(\frac{\alpha}{2}-\alpha)=-\sin\frac{\alpha}{2}}\right]\sin\left(\frac{\lambda t}{2}\right)\right\} e^{i\omega t/2}$$

$$= \left[\cos\left(\frac{\lambda t}{2}\right) - \frac{i(\omega_1+\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\sin\frac{\alpha}{2}e^{i\omega t/2} \quad \text{(confirming the bottom entry).}$$

$$\begin{aligned}
|c_+|^2 + |c_-|^2 &= \cos^2\left(\frac{\lambda t}{2}\right) + \frac{(\omega_1 - \omega\cos\alpha)^2}{\lambda^2}\sin^2\left(\frac{\lambda t}{2}\right) + \frac{\omega^2}{\lambda^2}\sin^2\alpha\sin^2\left(\frac{\lambda t}{2}\right) \\
&= \cos^2\left(\frac{\lambda t}{2}\right) + \frac{1}{\lambda^2}\Big(\underbrace{\omega_1^2 - 2\omega\omega_1\cos\alpha + \omega^2\cos^2\alpha + \omega^2\sin^2\alpha}_{\omega^2+\omega_1^2-2\omega\omega_1\cos\alpha=\lambda^2}\Big)\sin^2\left(\frac{\lambda t}{2}\right) \\
&= \cos^2\left(\frac{\lambda t}{2}\right) + \sin^2\left(\frac{\lambda t}{2}\right) = 1. \quad \checkmark
\end{aligned}$$

Problem 11.21

In the adiabatic regime, $\omega \ll \omega_1$, Eq. 11.104 becomes

$$\lambda = \omega_1\sqrt{1 - 2\frac{\omega}{\omega_1}\cos\alpha + \left(\frac{\omega}{\omega_1}\right)^2} \approx \omega_1\left(1 - \frac{\omega}{\omega_1}\cos\alpha\right) = \omega_1 - \omega\cos\alpha,$$

and Eq. 11.105 says

$$\begin{aligned}
\chi(t) &\approx \left[\cos\left(\frac{\lambda t}{2}\right) - i\sin\left(\frac{\lambda t}{2}\right)\right]e^{-i\omega t/2}\chi_+(t) + i\left[\frac{\omega}{\omega_1 - \omega\cos\alpha}\sin\alpha\sin\left(\frac{\lambda t}{2}\right)\right]e^{i\omega t/2}\chi_-(t) \\
&= e^{-i(\omega_1-\omega\cos\alpha)t/2}e^{-i\omega t/2}\chi_+(t) + i\left[\frac{\omega}{\omega_1}\sin\alpha\sin\left(\frac{\omega_1 t}{2}\right)\right]e^{+i\omega t/2}\chi_-(t).
\end{aligned}$$

As $\omega/\omega_1 \to 0$ the second term drops out completely; the electron remains in the state $\chi_+(t)$, acquiring a total phase

$$[\omega\cos\alpha - (\omega + \omega_1)]\,\frac{t}{2}.$$

The dynamic phase is

$$\theta_+(t) = -\frac{1}{\hbar}\int_0^t E_+(t')\,dt' = -\frac{\omega_1 t}{2},$$

(where $E_+ = \hbar\omega_1/2$, from Eq. 11.101), so the geometric phase is

$$\gamma_+(t) = [\omega\cos\alpha - (\omega+\omega_1)]\,\frac{t}{2} + \frac{\omega_1 t}{2} = (\cos\alpha - 1)\frac{\omega t}{2}.$$

For a complete cycle $T = 2\pi/\omega$, and therefore Berry's phase is $\boxed{\gamma_+(T) = \pi(\cos\alpha - 1).}$

Problem 11.22

According to the adiabatic theorem (Equation 11.93),

$$\Psi(x,t) = e^{i\,\theta(t)}\, e^{i\,\gamma(t)}\, \psi(x,t) \qquad [\bigstar]$$

where $\psi(x,t)$ is the instantaneous eigenstate, in this case (Equation 2.132)

$$\psi(x,t) = \frac{\sqrt{m\,\alpha(t)}}{\hbar}\ \exp\left[-\frac{m\,\alpha(t)\ |x|}{\hbar^2}\right], \qquad [\bigstar\bigstar]$$

and where θ is the dynamical phase:

$$\theta(t) = -\frac{1}{\hbar}\int_0^t E(t')\ dt' \qquad \dot{\theta} = -\frac{1}{\hbar}\,E(t) \qquad [\bigstar\bigstar\bigstar]$$

with, in this case (Equation 2.132),

$$E(t) = -\frac{m\,\alpha(t)^2}{2\,\hbar^2}\,. \qquad [\bigstar\bigstar\bigstar\bigstar]$$

We may plug [★] in the time-dependent Schrödinger equation to obtain

$$\begin{aligned}
\hat{H}(t)\ \Psi(x,t) &= i\,\hbar\,\frac{\partial\,\Psi}{\partial t} \\
e^{i\,\theta(t)}\,e^{i\,\gamma(t)}\,\hat{H}(t)\,\psi(x,t) &= i\,\hbar\,\left[i\,\dot{\theta}\,\psi(x,t) + i\,\dot{\gamma}\,\psi(x,t) + \dot{\psi}(x,t)\right]\,e^{i\,\theta(t)}\,e^{i\,\gamma(t)} \\
\hat{H}(t)\,\psi(x,t) &= i\,\hbar\,\left[i\,\dot{\theta}\,\psi(x,t) + i\,\dot{\gamma}\,\psi(x,t) + \dot{\psi}(x,t)\right] \\
E(t)\,\psi(x,t) &= E(t)\,\psi(x,t) - \hbar\,\dot{\gamma}\,\psi(x,t) + i\,\hbar\,\dot{\psi}(x,t) \\
\dot{\gamma}\,\psi(x,t) &= i\,\frac{\partial\psi}{\partial t} \qquad [\bigstar\bigstar\bigstar\bigstar\bigstar]
\end{aligned}$$

Taking the derivative of Equation [★★] gives

$$\begin{aligned}
\frac{\partial\psi}{\partial t} &= \frac{\partial\psi}{\partial\alpha}\,\frac{d\alpha}{dt} \\
&= \left[\frac{1}{2}\,\frac{\sqrt{m}}{\hbar\,\sqrt{\alpha}}\,e^{-m\,\alpha\,|x|/\hbar^2} - \frac{\sqrt{m\,\alpha}}{\hbar}\,\frac{m\ |x|}{\hbar^2}\,e^{-m\,\alpha\,|x|/\hbar^2}\right]\,\dot{\alpha} \\
&= \left[\frac{1}{2\,\alpha} - \frac{m\ |x|}{\hbar^2}\right]\,\dot{\alpha}\,\psi
\end{aligned}$$

and from Equation [★★★★★] we have

$$\dot{\gamma} = i\,\left[\frac{1}{2}\,\frac{\dot{\alpha}}{\alpha} - \frac{m\,\dot{\alpha}\ |x|}{\hbar^2}\right]\,.$$

But in the adiabatic limit $\dot{\alpha} \to 0$, so $\dot{\gamma} \to 0$, so γ is a constant, and at $t = 0$ $\gamma = 0$, so $\boxed{\gamma = 0}$. [Note, by contrast, that $\dot{\theta} = -E(t)\,/\hbar$ is *not* small, regardless of $\dot{\alpha}$.]

Meanwhile, from [★★★] and [★★★★]:

$$\begin{aligned}\theta(t) &= -\frac{1}{\hbar}\int_0^t E(t')\,dt' = -\frac{1}{\hbar}\int_{\alpha_1}^{\alpha_2} E(\alpha)\,\frac{d\alpha}{d\alpha/dt'}\\ &= \frac{m}{2\,\hbar^3}\int_{\alpha_1}^{\alpha_2}\alpha^2\,\frac{d\alpha}{c}\\ &= \boxed{\frac{m}{6\,c}\left[\left(\frac{\alpha_2}{\hbar}\right)^3 - \left(\frac{\alpha_1}{\hbar}\right)^3\right]}\end{aligned}$$

Problem 11.23

(a) Using Equation 11.108 we have

$$\begin{aligned} i\,\hbar\,\frac{\partial\Psi}{\partial t} &= i\,\hbar\,\frac{\partial}{\partial t}e^{\hat{G}(t)}\,\Psi(0)\\ &= i\,\hbar\,\frac{\partial}{\partial t}\left[1+\hat{G}(t)+\frac{1}{2}\,\hat{G}(t)\,\hat{G}(t)+\frac{1}{3!}\,\hat{G}(t)\,\hat{G}(t)\,\hat{G}(t)+\cdots\right]\Psi(0)\end{aligned}$$

and noting that $i\,\hbar\,\dot{G} = H$, this is

$$\begin{aligned} i\,\hbar\,\frac{\partial\Psi}{\partial t} &= i\,\hbar\,\Big[0+\dot{\hat{G}}(t)+\frac{1}{2}\,\dot{\hat{G}}(t)\,\hat{G}(t)+\frac{1}{2}\,\hat{G}(t)\,\dot{\hat{G}}(t)+\frac{1}{3!}\,\dot{\hat{G}}(t)\,\hat{G}(t)\,\hat{G}(t)\\ &\qquad +\frac{1}{3!}\,\hat{G}(t)\,\dot{\hat{G}}(t)\,\hat{G}(t)+\frac{1}{3!}\,\hat{G}(t)\,\hat{G}(t)\,\dot{\hat{G}}(t)+\cdots\Big]\,\Psi(0)\\ &= \Big[\hat{H}(t)+\frac{1}{2}\,\hat{H}(t)\,\hat{G}(t)+\frac{1}{2}\,\hat{G}(t)\,\hat{H}(t)+\frac{1}{3!}\,\hat{H}(t)\,\hat{G}(t)\,\hat{G}(t)\\ &\qquad +\frac{1}{3!}\,\hat{G}(t)\,\hat{H}(t)\,\hat{G}(t)+\frac{1}{3!}\,\hat{G}(t)\,\hat{G}(t)\,\hat{H}(t)+\cdots\Big]\,\Psi(0)\ .\end{aligned}$$

Now *if* $\left[\hat{G},\hat{H}\right]=0$ this becomes

$$\begin{aligned} i\,\hbar\,\frac{\partial\Psi}{\partial t} &= \hat{H}(t)\,\left[1+\hat{G}(t)+\frac{1}{2}\,\hat{G}(t)\,\hat{G}(t)+\cdots\right]\Psi(0)\\ &= \hat{H}(t)\,e^{\hat{G}(t)}\,\Psi(0)\\ &= \hat{H}(t)\,\Psi(t)\ .\end{aligned}$$

so Eq. 11.108 is a solution to the Schrödinger equation *if* G and H commute which is not typically the case for time-dependent Hamiltonians.

(b) Now we try Equation 11.109. Taking the derivative and recalling that

$$\frac{d}{dx}\int_a^x f(u)\,du = f(x)$$

we have

$$\begin{aligned} i\,\hbar\,\frac{\partial\Psi}{\partial t} &= \left\{0+\hat{H}(t)+\left(-\frac{i}{\hbar}\right)\hat{H}(t)\int_0^t \hat{H}(t_2)\,dt_2\right.\\ &\qquad \left.+\left(-\frac{i}{\hbar}\right)^2\hat{H}(t)\int_0^t \hat{H}(t_2)\left(\int_0^{t_2}\hat{H}(t_3)\,dt_3\right)dt_2\right\}\Psi(0)\ .\end{aligned}$$

In this case all the $\hat{H}(t)$'s are on the left so we don't have to worry about operators commuting. t_2 and t_3 are dummy variables so we can rename them to t_1 and t_2 and we have

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}(t)\left\{1+\left(-\frac{i}{\hbar}\right)\int_0^t \hat{H}(t_1)\, dt_1 + \left(-\frac{i}{\hbar}\right)^2\int_0^t \hat{H}(t_1)\left(\int_0^{t_1}\hat{H}(t_2)\, dt_1\right) dt_1\right\}\Psi(0)\ .$$

which looking back to Equation 11.109 is

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}(t)\ \Psi(t)\ ,$$

as required.

(c) We consider

$$\begin{aligned}\mathbf{T}\left[\hat{G}(t)\ \hat{G}(t)\right] &= \mathbf{T}\left[\left(-\frac{i}{\hbar}\right)^2\int_0^t \hat{H}(t')\, dt' \int_0^t \hat{H}(t'')\, dt''\right] \\ &= \left(-\frac{i}{\hbar}\right)^2\int_0^t\int_0^t \mathbf{T}\left[\hat{H}(t')\ \hat{H}(t'')\right] dt'\, dt'' \\ &= \left(-\frac{i}{\hbar}\right)^2\left[\int_0^t\int_0^{t''}\hat{H}(t'')\ \hat{H}(t')\, dt'\, dt'' + \int_0^t\int_0^{t'}\hat{H}(t')\ \hat{H}(t'')\, dt''\, dt'\right]\end{aligned}$$

Replacing the variables with $t' \to t_2$ and $t'' \to t_1$ in the first integral and $t' \to t_1$ and $t'' \to t_2$ in the second integral we have

$$\mathbf{T}\left[\hat{G}(t)\ \hat{G}(t)\right] = 2\left(-\frac{i}{\hbar}\right)^2\int_0^t \hat{H}(t_1)\left[\int_0^{t_1}\hat{H}(t_2)\, dt_2\right] dt_1\, ,$$

the desired result.

The generalization for G^n is

$$\mathbf{T}\left[\hat{G}^n\right] = n!\left(-\frac{i}{\hbar}\right)^n\int_0^t \hat{H}(t_1)\int_0^{t_1}\hat{H}(t_2)\cdots\int_0^{t_{n-1}}\hat{H}(t_n)\, dt_n\, dt_{n-1}\cdots dt_2\, dt_1\, .$$

Note that it is $n!$ (not say, n) because there are $n!$ ways to order the n times t_1, t_2, ..., t_n.

Problem 11.24

(a)

$$\Psi(t) = \sum c_n(t)e^{-iE_nt/\hbar}\psi_n. \quad H\Psi = i\hbar\frac{\partial\Psi}{\partial t}; \quad H = H_0 + H'(t); \quad H_0\psi_n = E_n\psi_n. \quad \text{So}$$

$$\sum c_ne^{-iE_nt/\hbar}E_n\psi_n + \sum c_ne^{-iE_nt/\hbar}H'\psi_n = i\hbar\sum \dot{c}_ne^{-iE_nt/\hbar}\psi_n + i\hbar\left(-\frac{i}{\hbar}\right)\sum c_nE_ne^{-iE_nt/\hbar}\psi_n.$$

The first and last terms cancel, so

$$\sum c_n e^{-iE_nt/\hbar}H'\psi_n = i\hbar\sum \dot{c}_n e^{-iE_nt/\hbar}\psi_n. \quad \text{Take the inner product with } \psi_m:$$

$$\sum c_n e^{-iE_nt/\hbar}\langle\psi_m|H'|\psi_n\rangle = i\hbar\sum \dot{c}_n e^{-iE_nt/\hbar}\langle\psi_m|\psi_n\rangle.$$

Assume orthonormality of the unperturbed states, $\langle\psi_m|\psi_n\rangle = \delta_{mn}$, and define $H'_{mn} \equiv \langle\psi_m|H'|\psi_n\rangle$.

$$\sum c_n e^{-iE_nt/\hbar}H'_{mn} = i\hbar\,\dot{c}_m e^{-iE_mt/\hbar}, \quad \text{or} \quad \boxed{\dot{c}_m = -\frac{i}{\hbar}\sum_n c_n H'_{mn}e^{i(E_m-E_n)t/\hbar}.}$$

(b) Zeroth order: $c_N(t) = 1$, $c_m(t) = 0$ for $m \neq N$. Then in first order:

$$\dot{c}_N = -\frac{i}{\hbar}H'_{NN}, \quad \text{or} \quad \boxed{c_N(t) = 1 - \frac{i}{\hbar}\int_0^t H'_{NN}(t')\,dt',} \text{ whereas for } m \neq N:$$

$$\dot{c}_m = -\frac{i}{\hbar}H'_{mN}e^{i(E_m-E_N)t/\hbar}, \quad \text{or} \quad \boxed{c_m(t) = -\frac{i}{\hbar}\int_0^t H'_{mN}(t')e^{i(E_m-E_N)t'/\hbar}\,dt'.}$$

(c)

$$\begin{aligned} c_M(t) &= -\frac{i}{\hbar}H'_{MN}\int_0^t e^{i(E_M-E_N)t'/\hbar}\,dt' = -\frac{i}{\hbar}H'_{MN}\left[\frac{e^{i(E_M-E_N)t'/\hbar}}{i(E_M-E_N)/\hbar}\right]\Bigg|_0^t = -H'_{MN}\left[\frac{e^{i(E_M-E_N)t/\hbar}-1}{E_M-E_N}\right] \\ &= -\frac{H'_{MN}}{(E_M-E_N)}e^{i(E_M-E_N)t/2\hbar}\,2i\sin\left(\frac{E_M-E_N}{2\hbar}t\right). \end{aligned}$$

$$P_{N\to M} = |c_M|^2 = \boxed{\frac{4|H'_{MN}|^2}{(E_M-E_N)^2}\sin^2\left(\frac{E_M-E_N}{2\hbar}t\right).}$$

(d)

$$\begin{aligned} c_M(t) &= -\frac{i}{\hbar}V_{MN}\frac{1}{2}\int_0^t \left(e^{i\omega t'} + e^{-i\omega t'}\right)e^{i(E_M-E_N)t'/\hbar}\,dt' \\ &= -\frac{iV_{MN}}{2\hbar}\left[\frac{e^{i(\hbar\omega+E_M-E_N)t'/\hbar}}{i(\hbar\omega+E_M-E_N)/\hbar} + \frac{e^{i(-\hbar\omega+E_M-E_N)t'/\hbar}}{i(-\hbar\omega+E_M-E_N)/\hbar}\right]\Bigg|_0^t. \end{aligned}$$

If $E_M > E_N$, the second term dominates, and transitions occur only for $\omega \approx (E_M - E_N)/\hbar$:

$$c_M(t) \approx -\frac{iV_{MN}}{2\hbar}\frac{1}{(i/\hbar)(E_M-E_N-\hbar\omega)}e^{i(E_M-E_N-\hbar\omega)t/2\hbar}\,2i\sin\left(\frac{E_M-E_N-\hbar\omega}{2\hbar}t\right), \text{ so}$$

$$P_{N\to M} = |c_M|^2 = \frac{|V_{MN}|^2}{(E_M-E_N-\hbar\omega)^2}\sin^2\left(\frac{E_M-E_N-\hbar\omega}{2\hbar}t\right).$$

If $E_M < E_N$ the first term dominates, and transitions occur only for $\omega \approx (E_N - E_M)/\hbar$:

$$c_M(t) \approx -\frac{iV_{MN}}{2\hbar}\frac{1}{(i/\hbar)(E_M-E_N+\hbar\omega)}\,e^{i(E_M-E_N+\hbar\omega)t/2\hbar}\,2i\sin\left(\frac{E_M-E_N+\hbar\omega}{2\hbar}t\right), \text{ and hence}$$

$$P_{N\to M} = \frac{|V_{MN}|^2}{(E_M - E_N + \hbar\omega)^2}\sin^2\left(\frac{E_M - E_N + \hbar\omega}{2\hbar}t\right).$$

Combining the two results, we conclude that transitions occur to states with energy $E_M \approx E_N \pm \hbar\omega$, and

$$\boxed{P_{N\to M} = \frac{|V_{MN}|^2}{(E_M - E_N \pm \hbar\omega)^2}\sin^2\left(\frac{E_M - E_N \pm \hbar\omega}{2\hbar}t\right).}$$

(e) For light, $V_{ba} = -\wp E_0$ (Eq. 11.41). The rest is as before (Section 11.2.3), leading to Eq. 11.54:

$$\boxed{R_{N\to M} = \frac{\pi}{3\epsilon_0\hbar^2}|\wp|^2\rho(\omega), \text{ with } \omega = \pm(E_M - E_N)/\hbar} \quad (+ \text{ sign} \Rightarrow \text{absorption}, - \text{ sign} \Rightarrow \text{stimulated emission}).$$

Problem 11.25

For example (c):

$$\boxed{c_N(t) = 1 - \frac{i}{\hbar}H'_{NN}t; \quad c_m(t) = -2i\frac{H'_{mN}}{(E_m - E_N)}e^{i(E_m-E_N)t/2\hbar}\sin\left(\frac{E_m - E_N}{2\hbar}t\right) \quad (m \neq N).}$$

$$|c_N|^2 = 1 + \frac{1}{\hbar^2}|H'_{NN}|^2t^2, \quad |c_m|^2 = 4\frac{|H'_{mN}|^2}{(E_m - E_N)^2}\sin^2\left(\frac{E_m - E_N}{2\hbar}t\right), \text{ so}$$

$$\sum_m |c_m|^2 = 1 + \frac{t^2}{\hbar^2}|H'_{NN}|^2 + 4\sum_{m\neq N}\frac{|H'_{mN}|^2}{(E_m - E_N)^2}\sin^2\left(\frac{E_m - E_N}{2\hbar}t\right).$$

This is plainly *greater* than 1! But remember: The c's are accurate only to *first* order in H'; to this order the $|H'|^2$ terms do not belong. Only if terms of *first* order appeared in the sum would there be a genuine problem with normalization.

For example (d):

$$c_N = 1 - \frac{i}{\hbar}V_{NN}\int_0^t \cos(\omega t')\,dt' = 1 - \frac{i}{\hbar}V_{NN}\left.\frac{\sin(\omega t')}{\omega}\right|_0^t \Longrightarrow \boxed{c_N(t) = 1 - \frac{i}{\hbar\omega}V_{NN}\sin(\omega t).}$$

$$\boxed{c_m(t) = -\frac{V_{mN}}{2}\left[\frac{e^{i(E_m-E_N+\hbar\omega)t/\hbar} - 1}{(E_m - E_N + \hbar\omega)} + \frac{e^{i(E_m-E_N-\hbar\omega)t/\hbar} - 1}{(E_m - E_N - \hbar\omega)}\right] \quad (m \neq N).} \quad \text{So}$$

$$|c_N|^2 = 1 + \frac{|V_{NN}|^2}{(\hbar\omega)^2}\sin^2(\omega t); \quad \text{and in the rotating wave approximation}$$

$$|c_m|^2 = \frac{|V_{mN}|^2}{(E_m - E_N \pm \hbar\omega)^2}\sin^2\left(\frac{E_m - E_N \pm \hbar\omega}{2\hbar}t\right) \quad (m \neq N).$$

Again, ostensibly $\sum |c_m|^2 > 1$, but the "extra" terms are of *second* order in H', and hence do not belong (to first order).

You would do $\boxed{\text{better to use } 1 - \sum_{m\neq N}|c_m|^2.}$ Schematically: $c_m = a_1H + a_2H^2 + \cdots$, so $|c_m|^2 = a_1^2H^2 + 2a_1a_2H^3 + \cdots$, whereas $c_N = 1 + b_1H + b_2H^2 + \cdots$, so $|c_N|^2 = 1 + 2b_1H + (2b_2 + b_1^2)H^2 + \cdots$. Thus knowing c_m to *first* order (i.e., knowing a_1) gets you $|c_m|^2$ to *second* order, but knowing c_N to first order (i.e., b_1) does *not* get you $|c_N|^2$ to second order (you'd also need b_2). It is precisely this b_2 term that would cancel the "extra" (second-order) terms in the calculations of $\sum |c_m|^2$ above.

Problem 11.26

(a)

Equation 11.116 $\Rightarrow \dot{c}_m = -\frac{i}{\hbar}\sum_n c_n H'_{mn} e^{i(E_m-E_n)t/\hbar}$. Here $H'_{mn} = \langle\psi_m|V_0(t)|\psi_n\rangle = \delta_{mn}V_0(t)$.

$$\dot{c}_m = -\frac{i}{\hbar}c_m V_0(t); \quad \frac{dc_m}{c_m} = -\frac{i}{\hbar}V_0(t)\,dt \Rightarrow \ln c_m = -\frac{i}{\hbar}\int V_0(t')\,dt' + constant.$$

$c_m(t) = c_m(0)e^{-\frac{i}{\hbar}\int_0^t V_0(t')\,dt'}$. Let $\Phi(t) \equiv -\frac{1}{\hbar}\int_0^t V_0(t')\,dt'$; $c_m(t) = e^{i\Phi}c_m(0)$. Hence

$|c_m(t)|^2 = |c_m(0)|^2$, and there are *no* transitions. $\boxed{\Phi(T) = -\frac{1}{\hbar}\int_0^T V_0(t)\,dt.}$

(b)

$$\left.\begin{aligned}&\text{Eq. 11.118} \Rightarrow c_N(t) \approx 1 - \frac{i}{\hbar}\int_0^t V_0(t')\,dt = 1 + i\Phi.\\ &\text{Eq. 11.119} \Rightarrow c_m(t) = -\frac{i}{\hbar}\int_0^t \delta_{mN}V_0(t')e^{i(E_m-E_N)t'/\hbar}\,dt' = 0\ (m \neq N).\end{aligned}\right\} \boxed{\begin{aligned}c_N(t) &= 1 + i\Phi(t),\\ c_m(t) &= 0\ (m \neq N).\end{aligned}}$$

The *exact* answer is $c_N(t) = e^{i\Phi(t)}$, $c_m(t) = 0$, and they *are* consistent, since $e^{i\Phi} \approx 1 + i\Phi$, to first order.

Problem 11.27

Use result of Problem 11.24(c). Here $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$, so $E_2 - E_1 = \frac{3\pi^2\hbar^2}{2ma^2}$.

$$\begin{aligned}H'_{12} &= \frac{2}{a}\int_0^{a/2}\sin\left(\frac{\pi}{a}x\right)V_0\sin\left(\frac{2\pi}{a}x\right)dx\\ &= \frac{2V_0}{a}\left[\frac{\sin\left(\frac{\pi}{a}x\right)}{2(\pi/a)} - \frac{\sin\left(\frac{3\pi}{a}x\right)}{2(3\pi/a)}\right]\Bigg|_0^{a/2} = \frac{V_0}{\pi}\left[\sin\left(\frac{\pi}{2}\right) - \frac{1}{3}\sin\left(\frac{3\pi}{2}\right)\right] = \frac{4V_0}{3\pi}.\end{aligned}$$

$$\text{Eq. 11.120} \Longrightarrow P_{1\to2} = 4\left(\frac{4V_0}{3\pi}\right)^2\left(\frac{2ma^2}{3\pi^2\hbar^2}\right)^2\sin^2\left(\frac{3\pi^2\hbar}{4ma^2}t\right) = \boxed{\left[\frac{16ma^2V_0}{9\pi^3\hbar^2}\sin\left(\frac{3\pi^2\hbar T}{4ma^2}\right)\right]^2}.$$

Problem 11.28

Spontaneous absorption would involve taking energy (a photon) from the ground state of the electromagnetic field. But you can't *do* that, because the gound state already has the lowest allowed energy.

Problem 11.29

(a)

$$H = -\gamma\mathbf{B}\cdot\mathbf{S} = -\gamma\left(B_xS_x + B_yS_y + B_zS_z\right);$$

$$\begin{aligned}
\mathsf{H} &= -\gamma\frac{\hbar}{2}\left(B_x\sigma_x + B_y\sigma_y + B_z\sigma_z\right) = -\frac{\gamma\hbar}{2}\left[B_x\begin{pmatrix}0&1\\1&0\end{pmatrix} + B_y\begin{pmatrix}0&-i\\i&0\end{pmatrix} + B_z\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right]\\
&= -\frac{\gamma\hbar}{2}\begin{pmatrix}B_z & B_x - iB_y\\ B_x + iB_y & -B_z\end{pmatrix} = -\frac{\gamma\hbar}{2}\begin{pmatrix}B_0 & B_{\rm rf}(\cos\omega t + i\sin\omega t)\\ B_{\rm rf}(\cos\omega t - i\sin\omega t) & -B_0\end{pmatrix}\\
&= \boxed{-\frac{\gamma\hbar}{2}\begin{pmatrix}B_0 & B_{\rm rf}e^{i\omega t}\\ B_{\rm rf}e^{-i\omega t} & -B_0\end{pmatrix}.}
\end{aligned}$$

(b) $i\hbar\dot{\chi} = \mathsf{H}\chi \Rightarrow$

$$i\hbar\begin{pmatrix}\dot{a}\\ \dot{b}\end{pmatrix} = -\frac{\gamma\hbar}{2}\begin{pmatrix}B_0 & B_{\rm rf}e^{i\omega t}\\ B_{\rm rf}e^{-i\omega t} & -B_0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = -\frac{\gamma\hbar}{2}\begin{pmatrix}B_0a + B_{\rm rf}e^{i\omega t}b\\ B_{\rm rf}e^{-i\omega t}a - B_0b\end{pmatrix} \quad\Rightarrow$$

$$\begin{cases}\dot{a} = i\dfrac{\gamma}{2}\left(B_0a + B_{\rm rf}e^{i\omega t}b\right) = \dfrac{i}{2}\left(\Omega e^{i\omega t}b + \omega_0 a\right),\\[2mm] \dot{b} = -i\dfrac{\gamma}{2}\left(B_0b - B_{\rm rf}e^{-i\omega t}a\right) = \dfrac{i}{2}\left(\Omega e^{-i\omega t}a - \omega_0 b\right).\end{cases}$$

(c) You can decouple the equations by differentiating with respect to t, but it is simpler just to *check* the quoted results. First of all, they clearly satisfy the initial conditions: $a(0) = a_0$ and $b(0) = b_0$. Differentiating a:

$$\begin{aligned}
\dot{a} &= \frac{i\omega}{2}a + \left\{-a_0\frac{\omega'}{2}\sin(\omega' t/2) + \frac{i}{\omega'}\left[a_0(\omega_0-\omega) + b_0\Omega\right]\frac{\omega'}{2}\cos(\omega' t/2)\right\}e^{i\omega t/2}\\
&= \frac{i}{2}e^{i\omega t/2}\Big\{\omega a_0\cos(\omega' t/2) + i\frac{\omega}{\omega'}\left[a_0(\omega_0-\omega) + b_0\Omega\right]\sin(\omega' t/2)\\
&\qquad + i\omega' a_0\sin(\omega' t/2) + \left[a_0(\omega_0-\omega) + b_0\Omega\right]\cos(\omega' t/2)\Big\}
\end{aligned}$$

Equation 11.124 says this should be equal to

$$\begin{aligned}
\frac{i}{2}\left(\Omega e^{i\omega t}b + \omega_0 a\right) &= \frac{i}{2}e^{i\omega t/2}\Big\{\Omega b_0\cos(\omega' t/2) + i\frac{\Omega}{\omega'}\left[b_0(\omega-\omega_0) + a_0\Omega\right]\sin(\omega' t/2)\\
&\qquad + \omega_0 a_0\cos(\omega' t/2) + i\frac{\omega_0}{\omega'}\left[a_0(\omega_0-\omega) + b_0\Omega\right]\sin(\omega' t/2)\Big\}.
\end{aligned}$$

By inspection the $\cos(\omega' t/2)$ terms in the two expressions are equal; it remains to check that

$$i\frac{\omega}{\omega'}\left[a_0(\omega_0-\omega) + b_0\Omega\right] + i\omega' a_0 = i\frac{\Omega}{\omega'}\left[b_0(\omega-\omega_0) + a_0\Omega\right] + i\frac{\omega_0}{\omega'}\left[a_0(\omega_0-\omega) + b_0\Omega\right],$$

which is to say

$$a_0\omega(\omega_0-\omega) + b_0\omega\Omega + a_0(\omega')^2 = b_0\Omega(\omega-\omega_0) + a_0\Omega^2 + a_0\omega_0(\omega_0-\omega) + b_0\omega_0\Omega,$$

or

$$a_0\left[\omega\omega_0 - \omega^2 + (\omega')^2 - \Omega^2 - \omega_0^2 + \omega_0\omega\right] = b_0\left[\Omega\omega - \omega_0\Omega + \omega_0\Omega - \omega\Omega\right] = 0.$$

Substituting Eq. 11.125 for ω', the coefficient of a_0 on the left becomes

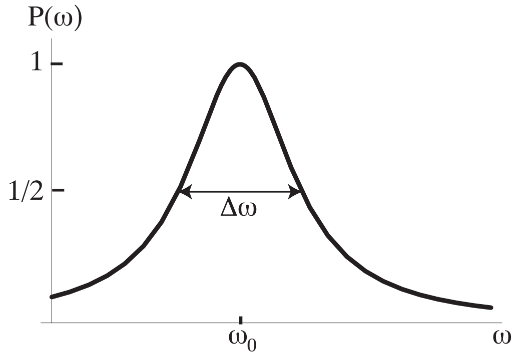
$$2\omega\omega_0 - \omega^2 + (\omega - \omega_0)^2 + \Omega^2 - \Omega^2 - \omega_0^2 = 0. \quad \checkmark$$

The check of $b(t)$ is identical, with $a \leftrightarrow b$, $\omega_0 \to -\omega_0$, and $\omega \to -\omega$.

(d)

$$b(t) = i\frac{\Omega}{\omega'}\sin(\omega' t/2)e^{-i\omega t/2}; \quad P(t) = |b(t)|^2 = \boxed{\left(\frac{\Omega}{\omega'}\right)^2 \sin^2(\omega' t/2).}$$

(e)



The maximum ($P_{\max} = 1$) occurs (obviously) at $\omega = \omega_0$.

$P = \frac{1}{2} \Rightarrow (\omega - \omega_0)^2 = \Omega^2 \Rightarrow \omega = \omega_0 \pm \Omega$, so $\Delta\omega = \omega_+ - \omega_- = \boxed{2\Omega.}$

(f) $B_0 = 10{,}000$ gauss $= 1$ T; $B_{\rm rf} = 0.01$ gauss $= 1 \times 10^{-6}$ T. $\omega_0 = \gamma B_0$. Comparing Eqs. 4.156 and 7.89, $\gamma = \dfrac{g_p e}{2m_p}$, where $g_p = 5.59$. So

$$\nu_{\rm res} = \frac{\omega_0}{2\pi} = \frac{g_p e}{4\pi m_p}B_0 = \frac{(5.59)(1.6 \times 10^{-19})}{4\pi(1.67 \times 10^{-27})}(1) = \boxed{4.26 \times 10^7 \text{ Hz.}}$$

$$\Delta\nu = \frac{\Delta\omega}{2\pi} = \frac{\Omega}{\pi} = \frac{\gamma}{2\pi}2B_{\rm rf} = \nu_{\rm res}\frac{2B_{\rm rf}}{B_0} = (4.26 \times 10^7)(2 \times 10^{-6}) = \boxed{85.2 \text{ Hz.}}$$

Problem 11.30

(a)

$$\mathbf{E} = -\boldsymbol{\nabla}\varphi - \frac{\partial \mathbf{A}}{\partial t} = -\frac{\mathbf{E}_0}{\omega}\cos(\mathbf{k}\cdot\mathbf{r} - \omega t)(-\omega) = \boxed{\mathbf{E}_0 \cos(\mathbf{k}\cdot\mathbf{r} - \omega t).}$$

$$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A} = \frac{1}{\omega}\sin(\mathbf{k}\cdot\mathbf{r} - \omega t)\boldsymbol{\nabla} \times \mathbf{E_0} - \frac{1}{\omega}\mathbf{E_0} \times \boldsymbol{\nabla}\left(\sin(\mathbf{k}\cdot\mathbf{r} - \omega t)\right)$$

$$= \mathbf{0} - \frac{1}{\omega}\mathbf{E_0} \times [\cos(\mathbf{k}\cdot\mathbf{r} - \omega t)\mathbf{k}] = \boxed{\frac{\mathbf{k} \times \mathbf{E_0}}{\omega}\cos(\mathbf{k}\cdot\mathbf{r} - \omega t) = \frac{1}{\omega}\mathbf{k} \times \mathbf{E}}$$

(note that $\mathbf{E}_0$ is a *constant*, so its derivatives are zero).

(b) From Eq. 4.188

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A}) \cdot (\mathbf{p} - q\mathbf{A}) + q\varphi + V = \frac{p^2}{2m} + V - \frac{q}{2m}(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + \frac{q^2}{2m}A^2$$
$$= H^0 - \frac{q}{2m}(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + \frac{q^2}{2m}A^2.$$

Now, acting on a test function $f(\mathbf{r})$,

$$(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p})f = -i\hbar\left[\boldsymbol{\nabla}(\mathbf{A}f) + \mathbf{A} \cdot (\boldsymbol{\nabla} f)\right] = -i\hbar\left[(\boldsymbol{\nabla} \cdot \mathbf{A})f + \mathbf{A} \cdot (\boldsymbol{\nabla} f) + \mathbf{A} \cdot (\boldsymbol{\nabla} f)\right].$$

But

$$\boldsymbol{\nabla} \cdot \mathbf{A} = \frac{1}{\omega}\boldsymbol{\nabla} \cdot [\mathbf{E_0} \sin(\mathbf{k} \cdot \mathbf{r} - \omega t)] = \frac{1}{\omega}\left[(\boldsymbol{\nabla} \cdot \mathbf{E})0) \sin(\mathbf{k} \cdot \mathbf{r} - \omega t) + \mathbf{E_0} \cdot (\boldsymbol{\nabla} \sin(\mathbf{k} \cdot \mathbf{r} - \omega t))\right]$$
$$= \frac{1}{\omega}\left[0 + \mathbf{E}_0 \cdot \cos(\mathbf{k} \cdot \mathbf{r} - \omega t)\mathbf{k}\right] = 0$$

(since $\mathbf{E}_0 \cdot \mathbf{k} = 0$.) So (dropping the test function)

$$(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) = 2\mathbf{A} \cdot \mathbf{p}.$$

Ignoring the $\mathbf{A}^2$ term, then,

$$H' = \frac{e}{m}\mathbf{A} \cdot \mathbf{p} = \frac{e}{m\omega}\sin(\mathbf{k} \cdot \mathbf{r} - \omega t)\mathbf{E_0} \cdot \mathbf{p} = \frac{e}{2im\omega}e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{E_0} \cdot \mathbf{p}e^{-i\omega t} - \frac{e}{2im\omega}e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{E_0} \cdot \mathbf{p}e^{i\omega t}. \quad \checkmark$$

(c) Referring to Eq. 11.36, we have

$$V_{ba} = \frac{e}{im\omega}E_0\langle b|p_z|a\rangle$$

But (using Eqs. 2.52 and 3.65)

$$[H^0, z] = \frac{1}{2m}[p^2, z] = \frac{1}{2m}[p_z^2, z] = \frac{1}{2m}\left(p_z[p_z, z] + [p_z, z]p_z\right) = \frac{-i\hbar}{m}p_z,$$

so (referring to Eqs. 11.18 and 11.40)

$$V_{ba} = \frac{e}{im\omega}E_0\frac{im}{\hbar}\langle b|[H^0, z]|a\rangle = \frac{eE_0}{\hbar\omega}\langle b|(H^0 z - zH^0)|a\rangle = \frac{eE_0}{\hbar\omega}(E_b - E_a)\langle b|z|a\rangle$$
$$= \frac{eE_0}{\hbar\omega}\hbar\omega_0\langle b|z|a\rangle = -\frac{\omega_0}{\omega}E_0\wp. \quad \checkmark$$

This differs from Eq. 11.41, which did not include the ratio of the ω's, but it does not affect our conclusions in Sections 11.2.3 or 11.3, because we only considered transitions *at resonance*, $\omega = \omega_0$ (the probability of a transition at other driving frequencies being negligible).

Problem 11.31

(a)

$$H' = -q\mathbf{E} \cdot \mathbf{r} = -q(\mathbf{E}_0 \cdot \mathbf{r})(\mathbf{k} \cdot \mathbf{r})\sin(\omega t). \quad \text{Write } \mathbf{E}_0 = E_0\hat{n},\ \mathbf{k} = \frac{\omega}{c}\hat{k}. \quad \text{Then}$$

$$H' = -q\frac{E_0\omega}{c}(\hat{n}\cdot\mathbf{r})(\hat{k}\cdot\mathbf{r})\sin(\omega t). \quad H'_{ba} = -\frac{qE_0\omega}{c}\langle b|(\hat{n}\cdot\mathbf{r})(\hat{k}\cdot\mathbf{r})|a\rangle\sin(\omega t).$$

This is the analog to Eq. 11.40: $H'_{ba} = -qE_0\langle b|\hat{n}\cdot\mathbf{r}|a\rangle\cos\omega t$. The rest of the analysis is identical to the dipole case (except that it is $\sin(\omega t)$ instead of $\cos(\omega t)$, but this amounts to resetting the clock, and clearly has no effect on the transition rate). We can skip therefore to Eq. 11.63, except for the factor of 1/3, which came from the averaging in Eq. 11.53:

$$A = \frac{\omega^3}{\pi\epsilon_0\hbar c^3}\frac{q^2\omega^2}{c^2}|\langle b|(\hat{n}\cdot\mathbf{r})(\hat{k}\cdot\mathbf{r})|a\rangle|^2 = \boxed{\frac{q^2\omega^5}{\pi\epsilon_0\hbar c^5}|\langle b|(\hat{n}\cdot\mathbf{r})(\hat{k}\cdot\mathbf{r})|a\rangle|^2.}$$

(b) Let the oscillator lie along the x direction, so $(\hat{n}\cdot\mathbf{r}) = \hat{n}_x x$ and $\hat{k}\cdot\mathbf{r} = \hat{k}_x x$. For a transition from n to n', we have

$$A = \frac{q^2\omega^5}{\pi\epsilon_0\hbar c^5}\left(\hat{k}_x\hat{n}_x\right)^2|\langle n'|x^2|n\rangle|^2. \quad \text{From Example 2.5,} \quad \langle n'|x^2|n\rangle = \frac{\hbar}{2m\bar{\omega}}\langle n'|(a_+^2+a_+a_-+a_-a_++a_-^2)|n\rangle,$$

where $\bar{\omega}$ is the frequency of the *oscillator*, not to be confused with ω, the frequency of the electromagnetic *wave*. Now, for spontaneous emission the final state must be *lower* in energy, so $n' < n$, and hence the only surviving term is a_-^2. Using Eq. 2.67:

$$\langle n'|x^2|n\rangle = \frac{\hbar}{2m\bar{\omega}}\langle n'|\sqrt{n(n-1)}|n-2\rangle = \frac{\hbar}{2m\bar{\omega}}\sqrt{n(n-1)}\,\delta_{n',n-2}.$$

Evidently transitions only go from $|n\rangle$ to $|n-2\rangle$, and hence

$$\omega = \frac{E_n - E_{n-2}}{\hbar} = \frac{1}{\hbar}\left[(n+\tfrac{1}{2})\hbar\bar{\omega} - (n-2+\tfrac{1}{2})\hbar\bar{\omega}\right] = 2\bar{\omega}.$$

$$\langle n'|x^2|n\rangle = \frac{\hbar}{m\omega}\sqrt{n(n-1)}\,\delta_{n',n-2}; \quad R_{n\to n-2} = \frac{q^2\omega^5}{\pi\epsilon_0\hbar c^5}(\hat{k}_x\hat{n}_x)^2\frac{\hbar^2}{m^2\omega^2}n(n-1).$$

It remains to calculate the average of $(\hat{k}_x\hat{n}_x)^2$. It's easiest to reorient the oscillator along a direction $\hat{r}$, making angle θ with the z axis, and let the radiation be incident from the z direction (so $\hat{k}_x \to \hat{k}_r = \cos\theta$). Averaging over the two polarizations ($\hat{\imath}$ and $\hat{\jmath}$): $\langle\hat{n}_r^2\rangle = \frac{1}{2}\left(\hat{\imath}_r^2 + \hat{\jmath}_r^2\right) = \frac{1}{2}\left(\sin^2\theta\cos^2\phi + \sin^2\theta\sin^2\phi\right) = \frac{1}{2}\sin^2\theta$. Now average overall directions:

$$\langle\hat{k}_r^2\hat{n}_r^2\rangle = \frac{1}{4\pi}\int\frac{1}{2}\sin^2\theta\cos^2\theta\sin\theta\,d\theta\,d\phi = \frac{1}{8\pi}2\pi\int_0^\pi(1-\cos^2\theta)\cos^2\theta\sin\theta\,d\theta$$
$$= \frac{1}{4}\left[-\frac{\cos^3\theta}{3} + \frac{\cos^5\theta}{5}\right]\Bigg|_0^\pi = \frac{1}{4}\left(\frac{2}{3} - \frac{2}{5}\right) = \frac{1}{15}.$$

$$\boxed{R = \frac{1}{15}\frac{q^2\hbar\omega^3}{\pi\epsilon_0 m^2c^5}n(n-1).} \quad \text{Comparing Eq. 11.70:} \quad \frac{R(\text{forbidden})}{R(\text{allowed})} = \boxed{\frac{2}{5}(n-1)\frac{\hbar\omega}{mc^2}.}$$

For a nonrelativistic system, $\hbar\omega \ll mc^2$; hence the term "forbidden".

(c) If both the initial state and the final state have $l = 0$, the wave function is independent of angle ($Y_0^0 = 1/\sqrt{4\pi}$), and the angular part of the integral is:

$$\langle a|(\hat{n}\cdot\mathbf{r})(\hat{k}\cdot\mathbf{r})|b\rangle = \cdots\int(\hat{n}\cdot\mathbf{r})(\hat{k}\cdot\mathbf{r})\sin\theta\,d\theta\,d\phi = \cdots\frac{4\pi}{3}(\hat{n}\cdot\hat{k}) \quad \text{(Eq. 6.95).}$$

But $\hat{n}\cdot\hat{k} = 0$, since electromagnetic waves are transverse. So $R = 0$ in this case, both for allowed and for forbidden transitions.

Problem 11.32

$\underline{\ell' = \ell + 1}$

From Eq. 11.76, $\langle n'\ell'm'|z|n\ell m\rangle = 0$ unless $m' = m$, so the only nonzero z term is

$$\begin{aligned}\langle n'\ell'm|z|n\ell m\rangle &= \int R_{n'\ell'}(Y_{\ell'}^m)^* r\cos\theta\, R_{n\ell}Y_\ell^m\, r^2\, dr\, \sin\theta\, d\theta\, d\phi \\ &= I\sqrt{\frac{(2\ell'+1)}{4\pi}\frac{(\ell'-|m|)!}{(\ell'+|m|)!}}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\, 2\pi\int_0^\pi P_{\ell'}^m P_\ell^m \cos\theta\sin\theta\, d\theta. \qquad [\bigstar 1]\end{aligned}$$

This is independent of the sign of m, so we might as well assume $m \geq 0$. The integral (changing variables to $x \equiv \cos\theta$) is (using Eq. 11.134)

$$\text{Int}_\theta = \int_{-1}^1 x\, P_{\ell+1}^m(x)P_\ell^m(x)\, dx = \frac{1}{(2\ell+1)}\left[(\ell+m)\int_{-1}^1 P_{\ell+1}^m P_{\ell-1}^m\, dx + (\ell-m+1)\int_{-1}^1 P_{\ell+1}^m P_{\ell+1}^m\, dx\right].$$

Now, it follows from Eq. 4.33 that the associated Legendre functions satisfy the orthogonality relation

$$\int_{-1}^1 P_{\ell'}^m(x)P_\ell^m(x)\, dx = \frac{2}{(2\ell+1)}\frac{(\ell+|m|)!}{(\ell-|m|)!}\,\delta_{\ell\ell'}, \qquad [\bigstar 2]$$

so

$$\text{Int}_\theta = \frac{(\ell-m+1)}{(2\ell+1)}\frac{2}{(2\ell+3)}\frac{(\ell+1+m)!}{(\ell+1-m)!} = \frac{2}{(2\ell+1)(2\ell+3)}\frac{(\ell+1+m)!}{(\ell-m)!}.$$

Putting this into Eq. [★1]:

$$\begin{aligned}\langle n'(\ell+1)m|z|n\ell m\rangle &= \frac{I}{2}\sqrt{(2\ell+3)\frac{(\ell+1-m)!}{(\ell+1+m)!}}\sqrt{(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}}\,\frac{2}{(2\ell+1)(2\ell+3)}\frac{(\ell+1+m)!}{(\ell-m)!} \\ &= I\sqrt{\frac{(\ell+1)^2-m^2}{(2\ell+1)(2\ell+3)}}. \qquad [\bigstar 3]\end{aligned}$$

From Eq. 11.76, $\langle n'\ell'm'|x|n\ell m\rangle = 0$ unless $m' = m \pm 1$; let's start with $m+1$:

$$\begin{aligned}\langle n'\ell'(m+1)|x|n\ell m\rangle &= \int R_{n'\ell'}(Y_{\ell'}^{m+1})^* r\sin\theta\cos\phi\, R_{n\ell}Y_\ell^m\, r^2\, dr\, \sin\theta\, d\theta\, d\phi \\ = I\sqrt{\frac{(2\ell'+1)}{4\pi}\frac{(\ell'-m-1)!}{(\ell'+m+1)!}}&\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\int_0^\pi P_{\ell'}^{m+1}P_\ell^m \sin^2\theta\, d\theta\int_0^{2\pi}\cos\phi e^{-i(m+1)\phi}e^{im\phi}\, d\phi. [\bigstar 4]\end{aligned}$$

$$\text{Int}_\phi = \frac{1}{2}\int_0^{2\pi}(e^{i\phi}+e^{-i\phi})e^{-i\phi}\, d\phi = \frac{1}{2}\int_0^{2\pi}(1+e^{-2i\phi})\, d\phi = \pi. \qquad [\bigstar 5]$$

Changing variables ($x \equiv \cos\theta$), and using Eqs. 11.135 and [★2]:

$$\begin{aligned}\text{Int}_\theta &= \int_{-1}^1 \sqrt{1-x^2}\, P_{\ell+1}^{m+1}(x)P_\ell^m(x)\, dx = \frac{1}{(2\ell+1)}\left[\int_{-1}^1 P_{\ell+1}^{m+1}P_{\ell+1}^{m+1}\, dx - \int_{-1}^1 P_{\ell+1}^{m+1}P_{\ell-1}^{m+1}\, dx\right] \\ &= \frac{2}{(2\ell+1)(2\ell+3)}\frac{(\ell+m+2)!}{(\ell-m)!}.\end{aligned}$$

Thus [★4] becomes

$$\langle n'(\ell+1)(m+1)|x|n\ell m\rangle = \frac{I}{2}\sqrt{(2\ell+3)\frac{(\ell-m)!}{(\ell+m+2)!}}\sqrt{(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}}\,\frac{1}{(2\ell+1)(2\ell+3)}\,\frac{(\ell+m+2)!}{(\ell-m)!}$$

$$= \frac{I}{2}\sqrt{\frac{(\ell+m+2)(\ell+m+1)}{(2\ell+1)(2\ell+3)}}. \qquad [★6]$$

Now we do the same for $m' = m-1$:

$$\langle n'\ell'(m-1)|x|n\ell m\rangle = \int R_{n'\ell'}(Y_{\ell'}^{m-1})^* r\sin\theta\cos\phi\, R_{n\ell}Y_\ell^m\, r^2\, dr\, \sin\theta\, d\theta\, d\phi$$

$$= I\sqrt{\frac{(2\ell'+1)}{4\pi}\frac{(\ell'-m+1)!}{(\ell'+m-1)!}}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\int_0^\pi P_{\ell'}^{m-1}P_\ell^m\sin^2\theta\, d\theta\int_0^{2\pi}\cos\phi\, e^{-i(m-1)\phi}e^{im\phi}\, d\phi. [★7]$$

$$\text{Int}_\phi = \frac{1}{2}\int_0^{2\pi}(e^{i\phi}+e^{-i\phi})e^{i\phi}\, d\phi = \frac{1}{2}\int_0^{2\pi}(e^{2i\phi}+1)\, d\phi = \pi. \qquad [★8]$$

Changing variables ($x \equiv \cos\theta$), and using Eqs. 11.135 and [★2]:

$$\text{Int}_\theta = \int_{-1}^{1}\sqrt{1-x^2}\, P_{\ell+1}^{m-1}(x)P_\ell^m(x)\, dx = \frac{1}{(2\ell+3)}\left[\int_{-1}^{1}P_{\ell+2}^m P_\ell^m\, dx - \int_{-1}^{1}P_\ell^m P_\ell^m\, dx\right]$$

$$= -\frac{2}{(2\ell+1)(2\ell+3)}\frac{(\ell+m)!}{(\ell-m)!},$$

and [★7] becomes

$$\langle n'(\ell+1)(m-1)|x|n\ell m\rangle = -\frac{I}{4}\sqrt{(2\ell+3)\frac{(\ell-m+2)!}{(\ell+m)!}}\sqrt{(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}}\,\frac{2}{(2\ell+1)(2\ell+3)}\,\frac{(\ell+m)!}{(\ell-m)!}$$

$$= -\frac{I}{2}\sqrt{\frac{(\ell-m+2)(\ell-m+1)}{(2\ell+1)(2\ell+3)}}. \qquad [★9]$$

Meanwhile, Eq. 11.76 says $|\langle n'\ell'm'|y|n\ell m\rangle|^2 = |\langle n'\ell'm'|y|n\ell m\rangle|^2$, so

$$|\langle n'(\ell+1)(m+1)|\mathbf{r}|n\ell m\rangle|^2 + |\langle n'(\ell+1)m|\mathbf{r}|n\ell m\rangle|^2 + |\langle n'(\ell+1)(m-1)|\mathbf{r}|n\ell m\rangle|^2$$

$$= 2\left[\frac{I}{2}\sqrt{\frac{(\ell+m+2)(\ell+m+1)}{(2\ell+1)(2\ell+3)}}\right]^2 + \left[I\sqrt{\frac{(\ell+1)^2-m^2}{(2\ell+1)(2\ell+3)}}\right]^2 + 2\left[-\frac{I}{2}\sqrt{\frac{(\ell-m+2)(\ell-m+1)}{(2\ell+1)(2\ell+3)}}\right]^2$$

$$= \frac{I^2}{2}\left\{\frac{(\ell+m+2)(\ell+m+1)+2[(\ell+1)^2-m^2]+(\ell-m+2)(\ell-m+1)}{(2\ell+1)(2\ell+3)}\right\}$$

$$= I^2\frac{(2\ell^2+5\ell+3)}{(2\ell+1)(2\ell+3)} = I^2\frac{(\ell+1)}{(2\ell+1)}. \qquad [★10]$$

Therefore, $|\boldsymbol{\wp}|^2$ (summed over the three allowed transitions) is $e^2I^2(\ell+1)/(2\ell+1)$, and the spontaneous emission rate (Eq. 11.63) is

$$\boxed{A_{\ell\to\ell+1} = \frac{e^2\omega^3I^2}{3\pi\epsilon_0\hbar c^3}\frac{(\ell+1)}{(2\ell+1)}.} \qquad [★11]$$

<u>$\ell' = \ell - 1$</u>

Return to Eq. [★1]. This time the integral is

$$\begin{aligned}
\mathrm{Int}_\theta &= \int_{-1}^{1} x\, P_{\ell-1}^m(x) P_\ell^m(x)\, dx = \frac{1}{(2\ell+1)}\left[(\ell+m)\int_{-1}^{1} P_{\ell-1}^m P_{\ell-1}^m\, dx + (\ell-m+1)\int_{-1}^{1} P_{\ell-1}^m P_{\ell+1}^m\, dx\right] \\
&= \frac{(\ell+m)}{(2\ell+1)}\frac{2}{(2\ell-1)}\frac{(\ell-1+m)!}{(\ell-1-m)!} = \frac{2}{(2\ell-1)(2\ell+1)}\frac{(\ell+m)!}{(\ell-m-1)!}.
\end{aligned}$$

Therefore

$$\begin{aligned}
\langle n'(\ell-1)m|z|n\ell m\rangle &= \frac{I}{2}\sqrt{(2\ell-1)\frac{(\ell-1-m)!}{(\ell-1+m)!}}\sqrt{(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}}\,\frac{2}{(2\ell-1)(2\ell+1)}\frac{(\ell+m)!}{(\ell-m-1)!} \\
&= I\sqrt{\frac{\ell^2-m^2}{(2\ell-1)(2\ell+1)}}. \qquad [★12]
\end{aligned}$$

From $\langle n'\ell'm'|x|n\ell m\rangle$ with $m' = m+1$, Eqs. [★4] and [★5] are unchanged; this time

$$\begin{aligned}
\mathrm{Int}_\theta &= \int_{-1}^{1} \sqrt{1-x^2}\, P_{\ell-1}^{m+1}(x) P_\ell^m(x)\, dx = \frac{1}{(2\ell+1)}\left[\int_{-1}^{1} P_{\ell-1}^{m+1} P_{\ell+1}^{m+1}\, dx - \int_{-1}^{1} P_{\ell-1}^{m+1} P_{\ell-1}^{m+1}\, dx\right] \\
&= -\frac{2}{(2\ell-1)(2\ell+1)}\frac{(\ell+m)!}{(\ell-m-2)!},
\end{aligned}$$

and [★4] becomes

$$\begin{aligned}
\langle n'(\ell-1)(m+1)|x|n\ell m\rangle &= -\frac{I}{2}\sqrt{(2\ell-1)\frac{(\ell-m-2)!}{(\ell+m)!}}\sqrt{(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}}\,\frac{1}{(2\ell-1)(2\ell+1)}\frac{(\ell+m)!}{(\ell-m-2)!} \\
&= -\frac{I}{2}\sqrt{\frac{(\ell-m)(\ell-m-1)}{(2\ell-1)(2\ell+1)}}. \qquad [★13]
\end{aligned}$$

Now we do the same for $m' = m-1$. Eqs. [★7] and [★8] are unchanged, the θ integral is

$$\begin{aligned}
\mathrm{Int}_\theta &= \int_{-1}^{1} \sqrt{1-x^2}\, P_{\ell-1}^{m-1}(x) P_\ell^m(x)\, dx = \frac{1}{(2\ell-1)}\left[\int_{-1}^{1} P_\ell^m P_\ell^m\, dx - \int_{-1}^{1} P_{\ell-2}^m P_\ell^m\, dx\right] \\
&= \frac{2}{(2\ell-1)(2\ell+1)}\frac{(\ell+m)!}{(\ell-m)!},
\end{aligned}$$

and [★7] becomes

$$\begin{aligned}
\langle n'(\ell-1)(m-1)|x|n\ell m\rangle &= \frac{I}{2}\sqrt{(2\ell-1)\frac{(\ell-m)!}{(\ell+m-2)!}}\sqrt{(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}}\,\frac{1}{(2\ell-1)(2\ell+1)}\frac{(\ell+m)!}{(\ell-m)!} \\
&= \frac{I}{2}\sqrt{\frac{(\ell+m)(\ell+m-1)}{(2\ell-1)(2\ell+1)}}. \qquad [★14]
\end{aligned}$$

Thus

$$\begin{aligned}
&|\langle n'(\ell-1)(m+1)|\mathbf{r}|n\ell m\rangle|^2 + |\langle n'(\ell-1)m|\mathbf{r}|n\ell m\rangle|^2 + |\langle n'(\ell-1)(m-1)|\mathbf{r}|n\ell m\rangle|^2 \\
&= 2\left[-\frac{I}{2}\sqrt{\frac{(\ell-m)(\ell-m-1)}{(2\ell-1)(2\ell+1)}}\right]^2 + \left[I\sqrt{\frac{\ell^2-m^2}{(2\ell-1)(2\ell+1)}}\right]^2 + 2\left[\frac{I}{2}\sqrt{\frac{(\ell+m)(\ell+m-1)}{(2\ell-1)(2\ell+1)}}.\right]^2 \\
&= \frac{I^2}{2}\left\{\frac{(\ell-m)(\ell-m-1) + 2(\ell^2-m^2) + (\ell+m)(\ell+m-1)}{(2\ell-1)(2\ell+1)}\right\} \\
&= I^2\frac{(2\ell^2-\ell)}{(2\ell-1)(2\ell+1)} = I^2\frac{\ell}{(2\ell+1)}, \qquad [★15]
\end{aligned}$$

and the emission rate is

$$\boxed{A_{\ell\to\ell-1} = \frac{e^2\omega^3 I^2}{3\pi\epsilon_0\hbar c^3}\frac{\ell}{(2\ell+1)}.} \qquad [\bigstar 16]$$

(Of course, I is different for the two cases $\ell \to \ell \pm 1$.)

Problem 11.33

Choosing the triplet configuration $|1\rangle = |\uparrow_e\uparrow_p\rangle$ we have

$$\langle 1\,|\,\mathbf{S}_e\,|\,0\rangle = \frac{1}{\sqrt{2}}\left[\langle\uparrow_e\uparrow_p\,|\,\mathbf{S}_e\,|\,\uparrow_e\downarrow_p\rangle - \langle\uparrow_e\uparrow_p\,|\,\mathbf{S}\,|\,\downarrow_e\uparrow_p\rangle\right].$$

Since $\mathbf{S}_e$ doesn't effect the spin of the proton the first term vanishes and we have

$$\begin{aligned}
\langle 1\,|\,\mathbf{S}_e\,|\,0\rangle &= -\frac{1}{\sqrt{2}}\,\langle\uparrow_e\,|\,\mathbf{S}_e\,|\,\downarrow_e\rangle \\
&= -\frac{1}{\sqrt{2}}\begin{pmatrix} \frac{1}{2}\,\langle\uparrow_e\,|\,S_e^+ + S_e^-\,|\,\downarrow_e\rangle \\ \frac{1}{2\,i}\,\langle\uparrow_e\,|\,S_e^+ - S_e^-\,|\,\downarrow_e\rangle \\ \langle\uparrow_e\,|\,S_e^z\,|\,\downarrow_e\rangle \end{pmatrix} \\
&= \frac{i\,\hbar}{2\sqrt{2}}\begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix}.
\end{aligned}$$

We can then compute

$$|\langle 1\,|\,\mathbf{S}_e\,|\,0\rangle|^2 = \frac{\hbar^2}{8}\,(1+1) = \frac{\hbar^2}{4}.$$

Using the expression given in the problem we then have

$$A = \frac{\omega_0^3\,e^2}{3\,\pi\,\epsilon_0\,\hbar\,c^5\,m_e^2}\,\frac{\hbar^2}{4}$$

The frequency ω_0 is that of the 21cm line transition (see Equation 7.97),

$$\omega_0 = \frac{\Delta E}{\hbar} = \frac{4\,g_p\,\hbar^3}{3\,m_p\,m_e^2\,c^2\,a^4},$$

giving

$$\boxed{\tau = \frac{1}{A} = \frac{81}{64}\frac{1}{\alpha^{13}}\frac{1}{g_p^3}\left(\frac{m_p}{m_e}\right)^3\frac{\hbar}{m_e c^2} = 1.1\times 10^7\,\mathrm{yr}.}$$

Problem 11.34

(a) Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \quad \text{or} \quad \frac{d^2\psi}{dx^2} = -k^2\psi \quad (k \equiv \sqrt{2mE}/\hbar) \quad \begin{cases} 0 < x < \frac{1}{2}a + \epsilon, \\ \frac{1}{2}a + \epsilon < x < a. \end{cases}$$

Boundary conditions: $\psi(0) = \psi(\frac{1}{2}a + \epsilon) = \psi(a) = 0.$

Solution:

(1) $0 < x < \frac{1}{2}a + \epsilon :$ $\psi(x) = A \sin kx + B \cos kx.$ But $\psi(0) = 0 \Rightarrow B = 0,$ and

$$\psi(\tfrac{1}{2}a + \epsilon) = 0 \Rightarrow \begin{cases} k(\frac{1}{2}a + \epsilon) = n\pi \quad (n = 1, 2, 3, \ldots) \Rightarrow E_n = n^2\pi^2\hbar^2/2m(a/2 + \epsilon)^2, \\ \text{or else} \quad A = 0. \end{cases}$$

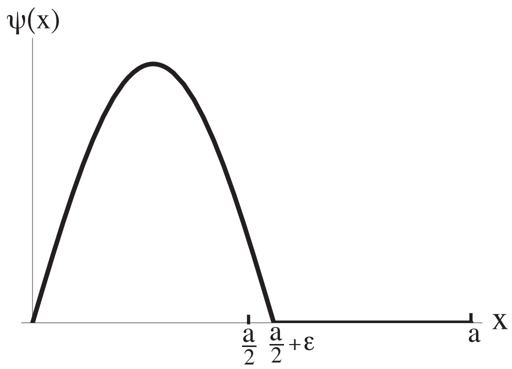
(2) $\frac{1}{2}a + \epsilon < x < a :$ $\psi(x) = F \sin k(a - x) + G \cos k(a - x).$ But $\psi(a) = 0 \Rightarrow G = 0,$ and

$$\psi(\tfrac{1}{2}a + \epsilon) = 0 \Rightarrow \begin{cases} k(\frac{1}{2}a - \epsilon) = n'\pi \quad (n' = 1, 2, 3, \ldots) \Rightarrow E_{n'} = (n')^2\pi^2\hbar^2/2m(a/2 - \epsilon)^2, \\ \text{or else} \quad F = 0. \end{cases}$$

$$\text{The ground state energy is} \begin{cases} \text{either} \quad E_1 = \dfrac{\pi^2\hbar^2}{2m(\frac{1}{2}a + \epsilon)^2} \quad (n = 1), \quad \text{with} \quad F = 0, \\ \text{or else} \quad E_{1'} = \dfrac{\pi^2\hbar^2}{2m(\frac{1}{2}a - \epsilon)^2} \quad (n' = 1), \quad \text{with} \quad A = 0. \end{cases}$$

Both are allowed energies, but E_1 is (slightly) lower (assuming ϵ is positive), so the ground state is

$$\boxed{\psi(x) = \begin{cases} \sqrt{\frac{2}{\frac{1}{2}a+\epsilon}} \sin\left(\frac{\pi x}{\frac{1}{2}a+\epsilon}\right), & 0 \le x \le \frac{1}{2}a + \epsilon; \\ 0, & \frac{1}{2}a + \epsilon \le x \le a. \end{cases}}$$



(b)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + f(t)\delta(x - \tfrac{1}{2}a - \epsilon)\psi = E\psi \quad \Rightarrow \quad \psi(x) = \left\{ \begin{array}{ll} A \sin kx, & 0 \le x < \frac{1}{2}a + \epsilon, \\ F \sin k(a - x), & \frac{1}{2}a + \epsilon < x \le a, \end{array} \right\} \quad \text{where} \quad k \equiv \frac{\sqrt{2mE}}{\hbar}.$$

Continuity in ψ at $x = \frac{1}{2}a + \epsilon :$

$$A \sin k\left(\tfrac{1}{2}a + \epsilon\right) = F \sin k\left(a - \tfrac{1}{2}a - \epsilon\right) = F \sin k\left(\tfrac{1}{2}a - \epsilon\right) \quad \Rightarrow F = A\frac{\sin k\left(\frac{1}{2}a + \epsilon\right)}{\sin k\left(\frac{1}{2}a - \epsilon\right)}.$$

Discontinuity in ψ' at $x = \frac{1}{2}a + \epsilon$ (Eq. 2.128):

$$-Fk \cos k(a - x) - Ak \cos kx = \frac{2mf}{\hbar^2} A \sin kx \;\Rightarrow\; F \cos k\left(\tfrac{1}{2}a - \epsilon\right) + A \cos k\left(\tfrac{1}{2}a + \epsilon\right) = -\left(\frac{2mf}{\hbar^2 k}\right) A \sin k\left(\tfrac{1}{2}a + \epsilon\right).$$

$$A\frac{\sin k\left(\frac{1}{2}a+\epsilon\right)}{\sin k\left(\frac{1}{2}a-\epsilon\right)}\cos k\left(\tfrac{1}{2}a-\epsilon\right)+A\cos k\left(\tfrac{1}{2}a+\epsilon\right)=-\left(\frac{2T}{z}\right)A\sin k\left(\tfrac{1}{2}a+\epsilon\right).$$

$$\sin k\left(\tfrac{1}{2}a+\epsilon\right)\cos k\left(\tfrac{1}{2}a-\epsilon\right)+\cos k\left(\tfrac{1}{2}a+\epsilon\right)\sin k\left(\tfrac{1}{2}a-\epsilon\right)=-\left(\frac{2T}{z}\right)\sin k\left(\tfrac{1}{2}a+\epsilon\right)\sin k\left(\tfrac{1}{2}a-\epsilon\right).$$

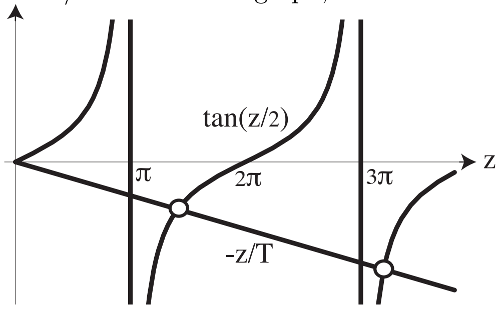
$$\sin k\left(\tfrac{1}{2}a+\epsilon+\tfrac{1}{2}a-\epsilon\right)=-\left(\frac{2T}{z}\right)\frac{1}{2}\left[\cos k\left(\tfrac{1}{2}a+\epsilon-\tfrac{1}{2}a+\epsilon\right)-\cos k\left(\tfrac{1}{2}a+\epsilon+\tfrac{1}{2}a-\epsilon\right)\right].$$

$$\sin ka=-\frac{T}{z}\left(\cos 2k\epsilon-\cos ka\right)\quad\Rightarrow\quad\boxed{z\sin z=T[\cos z-\cos(z\delta)].}$$

(c)

$$\sin z=\frac{T}{z}(\cos z-1)\quad\Rightarrow\quad\frac{z}{T}=\frac{\cos z-1}{\sin z}=-\tan(z/2)\quad\Rightarrow\quad\boxed{\tan(z/2)=-\frac{z}{T}.}$$

Plot $\tan(z/2)$ and $-z/T$ on the same graph, and look for intersections:



As $t:0\to\infty$, $T:0\to\infty$, and the straight line rotates counterclockwise from 6 o'clock to 3 o'clock, so the smallest z goes from π to 2π, and the ground state energy goes from $ka=\pi\Rightarrow E(0)=\dfrac{\hbar^2\pi^2}{2ma^2}$ (appropriate to a well of width a) to $ka=2\pi\Rightarrow E(\infty)=\dfrac{\hbar^2\pi^2}{2m(a/2)^2}$ (appropriate for a well of width $a/2$.

(d) Mathematica yields the following table:

T	0	1	5	20	100	1000
z	3.14159	3.67303	4.76031	5.72036	6.13523	6.21452

(e) $P_r=\dfrac{I_r}{I_r+I_l}=\dfrac{1}{1+(I_l/I_r)}$, where

$$\begin{aligned}I_l&=\int_0^{a/2+\epsilon}A^2\sin^2 kx\,dx=A^2\left[\frac{1}{2}x-\frac{1}{4k}\sin(2kx)\right]\Bigg|_0^{a/2+\epsilon}\\&=A^2\left\{\frac{1}{2}\left(\frac{a}{2}+\epsilon\right)-\frac{1}{4k}\sin\left[2k\left(\frac{a}{2}+\epsilon\right)\right]\right\}=\frac{a}{4}A^2\left[1+\frac{2\epsilon}{a}-\frac{1}{ka}\sin\left(ka+\frac{2\epsilon}{a}ka\right)\right]\\&=\frac{a}{4}A^2\left[1+\delta-\frac{1}{z}\sin(z+z\delta)\right].\end{aligned}$$

$$\begin{aligned}I_r&=\int_{a/2+\epsilon}^{a}F^2\sin^2 k(a-x)\,dx.\quad\text{Let}\quad u\equiv a-x,\ du=-dx.\\&=-F^2\int_{a/2-\epsilon}^{0}\sin^2 ku\,du=F^2\int_0^{a/2-\epsilon}\sin^2 ku\,du=\frac{a}{4}F^2\left[1-\delta-\frac{1}{z}\sin(z-z\delta)\right].\end{aligned}$$

$$\frac{I_l}{I_r} = \frac{A^2\,[1+\delta-(1/z)\sin(z+z\delta)]}{F^2\,[1-\delta-(1/z)\sin(z-z\delta)]}. \quad \text{But (from (b))} \quad \frac{A^2}{F^2} = \frac{\sin^2 k(a/2-\epsilon)}{\sin^2 k(a/2+\epsilon)} = \frac{\sin^2[z(1-\delta)/2]}{\sin^2[z(1+\delta)/2]}.$$

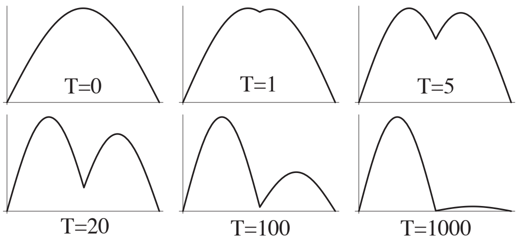
$$= \frac{I_+}{I_-}, \quad \text{where} \quad \boxed{I_\pm \equiv \left[1\pm\delta-\frac{1}{z}\sin z(1\pm\delta)\right]\sin^2[z(1\mp\delta)/2].} \quad \boxed{P_r = \frac{1}{1+(I_+/I_-)}.}$$

Using $\delta = 0.01$ and the z's from (d), Mathematica gives

T	0	1	5	20	100	1000
P_r	0.490001	0.486822	0.471116	0.401313	0.146529	0.00248443

As $t : 0 \to \infty$ (so $T : 0 \to \infty$), the probability of being in the right half drops from almost 1/2 to zero—the particle gets sucked out of the slightly smaller side, as it heads for the ground state in (a).

(f)



Problem 11.35

(a)

$$\text{Let} \quad (mvx^2 - 2E_n^i at)/2\hbar w = \phi(x,t). \quad \Phi_n = \sqrt{\frac{2}{w}}\sin\left(\frac{n\pi}{w}x\right)e^{i\phi}, \quad \text{so}$$

$$\frac{\partial\Phi_n}{\partial t} = \sqrt{2}\left(-\frac{1}{2}\frac{1}{w^{3/2}}v\right)\sin\left(\frac{n\pi}{w}x\right)e^{i\phi} + \sqrt{\frac{2}{w}}\left[-\frac{n\pi x}{w^2}v\cos\left(\frac{n\pi}{w}x\right)\right]e^{i\phi} + \sqrt{\frac{2}{w}}\sin\left(\frac{n\pi}{w}x\right)\left(i\frac{\partial\phi}{\partial t}\right)e^{i\phi}$$

$$= \left[-\frac{v}{2w} - \frac{n\pi xv}{w^2}\cot\left(\frac{n\pi}{w}x\right) + i\frac{\partial\phi}{\partial t}\right]\Phi_n. \quad \frac{\partial\phi}{\partial t} = \frac{1}{2\hbar}\left[-\frac{2E_n^i a}{w} - \frac{v}{w^2}\left(mvx^2 - 2E_n^i at\right)\right] = -\frac{E_n^i a}{\hbar w} - \frac{v}{w}\phi.$$

$$i\hbar\frac{\partial\Phi_n}{\partial t} = -i\hbar\left[\frac{v}{2w} + \frac{n\pi xv}{w^2}\cot\left(\frac{n\pi}{w}x\right) + i\frac{E_n^i a}{\hbar w} + i\frac{v}{w}\phi\right]\Phi_n.$$

$$H\Phi_n = -\frac{\hbar^2}{2m}\frac{\partial^2\Phi_n}{\partial x^2}. \quad \frac{\partial\Phi_n}{\partial x} = \sqrt{\frac{2}{w}}\left[\frac{n\pi}{w}\cos\left(\frac{n\pi}{w}x\right)\right]e^{i\phi} + \sqrt{\frac{2}{w}}\sin\left(\frac{n\pi}{w}x\right)e^{i\phi}\left(i\frac{\partial\phi}{\partial x}\right).$$

$$\frac{\partial\phi}{\partial x} = \frac{mvx}{\hbar w}. \quad \frac{\partial\Phi_n}{\partial x} = \left[\frac{n\pi}{w}\cot\left(\frac{n\pi}{w}x\right) + i\frac{mvx}{\hbar w}\right]\Phi_n.$$

$$\frac{\partial^2\Phi_n}{\partial x^2} = \left[-\left(\frac{n\pi}{w}\right)^2\csc^2\left(\frac{n\pi}{w}x\right) + \frac{imv}{\hbar w}\right]\Phi_n + \left[\frac{n\pi}{w}\cot\left(\frac{n\pi}{w}x\right) + i\frac{mvx}{\hbar w}\right]^2\Phi_n.$$

So the Schrödinger equation ($i\hbar\partial\Phi_n/\partial t = H\Phi_n$) is satisfied $\Leftrightarrow$

$$-i\hbar\left[\frac{v}{2w} + \frac{n\pi xv}{w^2}\cot\left(\frac{n\pi}{w}x\right) + i\frac{E_n^i a}{\hbar w} + i\frac{v}{w}\phi\right]$$

$$= -\frac{\hbar^2}{2m}\left\{-\left(\frac{n\pi}{w}\right)^2 \csc^2\left(\frac{n\pi}{w}x\right) + \frac{imv}{\hbar w} + \left[\frac{n\pi}{w}\cot\left(\frac{n\pi}{w}x\right) + i\frac{mvx}{\hbar w}\right]^2\right\}$$

Cotangent terms: $-i\hbar\left(\frac{n\pi x v}{w^2}\right) \stackrel{?}{=} -\frac{\hbar^2}{2m}\left(2\frac{n\pi}{w}i\frac{mvx}{\hbar w}\right) = -i\hbar\frac{n\pi v x}{w^2}$. ✓

Remaining trig terms on right:

$$-\left(\frac{n\pi}{w}\right)^2 \csc^2\left(\frac{n\pi}{w}x\right) + \left(\frac{n\pi}{w}\right)^2 \cot^2\left(\frac{n\pi}{w}x\right) = -\left(\frac{n\pi}{w}\right)^2\left[\frac{1-\cos^2(n\pi x/w)}{\sin^2(n\pi x/w)}\right] = -\left(\frac{n\pi}{w}\right)^2.$$

This leaves:

$$i\left[\frac{v}{2w} + i\frac{E_n^i a}{\hbar w} + i\frac{v}{w}\left(\frac{mvx^2 - 2E_n^i a t}{2\hbar w}\right)\right] \stackrel{?}{=} \frac{\hbar}{2m}\left[-\left(\frac{n\pi}{w}\right)^2 + \frac{imv}{\hbar w} - \frac{m^2v^2x^2}{\hbar^2 w^2}\right]$$

$$\cancel{\frac{iv}{2}} - \frac{E_n^i a}{\hbar} - \cancel{\frac{mv^2x^2}{2\hbar w}} + \frac{vE_n^i a t}{\hbar w} \stackrel{?}{=} -\frac{\hbar n^2\pi^2}{2mw} + \cancel{\frac{iv}{2}} - \cancel{\frac{mv^2x^2}{2\hbar w}}$$

$$-\frac{E_n^i a}{\hbar w}(w - vt) = -\frac{E_n^i a^2}{\hbar w} \stackrel{?}{=} -\frac{\hbar n^2\pi^2}{2mw} \Leftrightarrow -\frac{n^2\pi^2\hbar^2}{2ma^2}\frac{a^2}{\hbar w} = -\frac{\hbar n^2\pi^2}{2mw} = \text{r.h.s.} \quad ✓$$

So Φ_n *does* satisfy the Schrödinger equation, and since $\Phi_n(x,t) = (\cdots)\sin(n\pi x/w)$, it fits the boundary conditions: $\Phi_n(0,t) = \Phi_n(w,t) = 0$.

(b)

Equation 11.137 $\Longrightarrow \Psi(x,0) = \sum c_n \Phi_n(x,0) = \sum c_n \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)e^{imvx^2/2\hbar a}.$

Multiply by $\sqrt{\frac{2}{a}}\sin\left(\frac{n'\pi}{a}x\right)e^{-imvx^2/2\hbar a}$ and integrate:

$$\sqrt{\frac{2}{a}}\int_0^a \Psi(x,0)\sin\left(\frac{n'\pi}{a}x\right)e^{-imvx^2/2\hbar a}dx = \sum c_n \left[\underbrace{\frac{2}{a}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\sin\left(\frac{n'\pi}{a}x\right)dx}_{\delta_{nn'}}\right] = c_{n'}.$$

So, in general: $\quad c_n = \sqrt{\frac{2}{a}}\int_0^a e^{-imvx^2/2\hbar a}\sin\left(\frac{n\pi}{a}x\right)\Psi(x,0)dx.$ In this particular case,

$$c_n = \frac{2}{a}\int_0^a e^{-imvx^2/2\hbar a}\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{\pi}{a}x\right)dx. \quad \text{Let} \quad \frac{\pi}{a}x \equiv z; \quad dx = \frac{a}{\pi}dz; \quad \frac{mvx^2}{2\hbar a} = \frac{mvz^2}{2\hbar a}\frac{a^2}{\pi^2} = \frac{mva}{2\pi^2\hbar}z^2.$$

$$c_n = \frac{2}{\pi}\int_0^\pi e^{-i\alpha z^2}\sin(nz)\sin(z)\,dz. \quad \text{QED}$$

(c)

$w(T_e) = 2a \Rightarrow a + vT_e = 2a \Rightarrow vT_e = a \Rightarrow \boxed{T_e = a/v;}$ $\quad e^{-iE_1t/\hbar} \Rightarrow \omega = \frac{E_1}{\hbar} \Rightarrow T_i = \frac{2\pi}{\omega} = 2\pi\frac{\hbar}{E_1}$, or

$T_i = \frac{2\pi\hbar}{\pi^2\hbar^2}2ma^2 = \frac{4}{\pi}\frac{ma^2}{\hbar}.$ $\boxed{T_i = \frac{4ma^2}{\pi\hbar}.}$ Adiabatic $\Rightarrow T_e \gg T_i \Rightarrow \frac{a}{v} \gg \frac{4ma^2}{\pi\hbar} \Rightarrow \frac{4}{\pi}\frac{mav}{\hbar} \ll 1$, or

$8\pi\left(\frac{mav}{2\pi^2\hbar}\right) = 8\pi\alpha \ll 1$, so $\alpha \ll 1$. Then $c_n = \frac{2}{\pi}\int_0^\pi \sin(nz)\sin(z)dz = \boxed{\delta_{n1}.}$ Therefore

$$\boxed{\Psi(x,t) = \sqrt{\frac{2}{w}}\sin\left(\frac{\pi x}{w}\right)e^{i(mvx^2-2E_1^i at)/2\hbar w},}$$

which (apart from a phase factor) is the ground state of the instantaneous well, of width w, as required by the adiabatic theorem. (Actually, the first term in the exponent, which is at most $\frac{mv(2a)^2}{2\hbar(2a)} = \frac{mva}{\hbar} \ll 1$ and could be dropped, in the adiabatic regime.)

(d)

$$\theta(t) = -\frac{1}{\hbar}\left(\frac{\pi^2\hbar^2}{2m}\right)\int_0^t \frac{1}{(a+vt')^2}\,dt' = -\frac{\pi^2\hbar}{2m}\left[-\frac{1}{v}\left(\frac{1}{a+vt'}\right)\right]\Bigg|_0^t$$
$$= -\frac{\pi^2\hbar}{2mv}\left(\frac{1}{a}-\frac{1}{w}\right) = -\frac{\pi^2\hbar}{2mv}\left(\frac{vt}{aw}\right) = -\frac{\pi^2\hbar t}{2maw}.$$

So (dropping the $\dfrac{mvx^2}{2\hbar w}$ term, as explained in (c)) $\Psi(x,t) = \sqrt{\dfrac{2}{w}}\sin\left(\dfrac{\pi x}{w}\right)e^{-iE_1^i at/\hbar w}$ can be written (since $-\dfrac{E_1^i at}{\hbar w} = -\dfrac{\pi^2\hbar^2}{2ma^2}\dfrac{at}{\hbar w} = -\dfrac{\pi^2\hbar t}{2maw} = \theta$): $\boxed{\Psi(x,t) = \sqrt{\dfrac{2}{w}}\sin\left(\dfrac{\pi x}{w}\right)e^{i\theta}.}$

This is exactly what one would naively expect: For a *fixed* well (of width a) we'd have $\Psi(x,t) = \Psi_1(x)e^{-iE_1t/\hbar}$; for the (adiabatically) *expanding* well, simply replace a by the (time-dependent) width w, and *integrate* to get the accumulated phase factor, noting that E_1 is now a function of t.

Problem 11.36

(a) Check the answer given: $x_c = \omega\int_0^t f(t')\sin[\omega(t-t')]\,dt' \Longrightarrow x_c(0)=0.$ ✓

$$\dot{x}_c = \omega f(t)\sin[\omega(t-t)] + \omega^2\int_0^t f(t')\cos[\omega(t-t')]\,dt' = \omega^2\int_0^t f(t')\cos[\omega(t-t')]\,dt' \Rightarrow \dot{x}_c(0) = 0. \quad ✓$$

$$\ddot{x}_c = \omega^2 f(t)\cos[\omega(t-t)] - \omega^3\int_0^t f(t')\sin[\omega(t-t')]\,dt' = \omega^2 f(t) - \omega^2 x_c.$$

Now the classical equation of motion is $m(d^2x/dt^2) = -m\omega^2 x + m\omega^2 f$. For the proposed solution, $m(d^2x_c/dt^2) = m\omega^2 f - m\omega^2 x_c$, so it *does* satisfy the equation of motion, with the appropriate boundary conditions.

(b) Let $z \equiv x - x_c$ (so $\psi_n(x-x_c) = \psi_n(z)$, and z depends on t as well as x).

$$\frac{\partial\Psi}{\partial t} = \frac{d\psi_n}{dz}(-\dot{x}_c)e^{i\{\}} + \psi_n e^{i\{\}}\frac{i}{\hbar}\left[-(n+\frac{1}{2})\hbar\omega + m\ddot{x}_c(x-\frac{x_c}{2}) - \frac{m}{2}\dot{x}_c^2 + \frac{m\omega^2}{2}fx_c\right]$$

$$[\,] = -(n+\frac{1}{2})\hbar\omega + \frac{m\omega^2}{2}\left[2x(f-x_c) + x_c^2 - \frac{\dot{x}_c^2}{\omega^2}\right].$$

$$\frac{\partial\Psi}{\partial t} = -\dot{x}_c\frac{d\psi_n}{dz}e^{i\{\}} + i\Psi\left\{-(n+\frac{1}{2})\omega + \frac{m\omega^2}{2\hbar}\left[2x(f-x_c) + x_c^2 - \frac{\dot{x}_c^2}{\omega^2}\right]\right\}.$$

$$\frac{\partial\Psi}{\partial x} = \frac{d\psi_n}{dz}e^{i\{\}} + \psi_n e^{i\{\}}\frac{i}{\hbar}(m\dot{x}_c); \qquad \frac{\partial^2\Psi}{\partial x^2} = \frac{d^2\psi_n}{dz^2}e^{i\{\}} + 2\frac{d\psi_n}{dz}e^{i\{\}}\frac{i}{\hbar}(m\dot{x}_c) - \left(\frac{m\dot{x}_c}{\hbar}\right)^2\psi_n e^{i\{\}}.$$

$$H\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{1}{2}m\omega^2x^2\Psi - m\omega^2 fx\Psi$$
$$= -\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dz^2}e^{i\{\}} - \frac{\hbar^2}{2m}2\frac{d\psi_n}{dz}e^{i\{\}}\frac{im\dot{x}_c}{\hbar} + \frac{\hbar^2}{2m}\left(\frac{m\dot{x}_c}{\hbar}\right)^2\Psi + \frac{1}{2}m\omega^2x^2\Psi - m\omega^2fx\Psi.$$

But $\quad -\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dz^2} + \frac{1}{2}m\omega^2z^2\psi_n = (n+\frac{1}{2})\hbar\omega\psi_n, \quad$ so

$$H\Psi = \cancel{(n+\frac{1}{2})\hbar\omega\Psi} - \frac{1}{2}m\omega^2z^2\Psi - \cancel{i\hbar\dot{x}_c\frac{d\psi_n}{dz}}e^{i\{\}} + \frac{m}{2}\dot{x}_c^2\Psi + \frac{1}{2}m\omega^2x^2\Psi - m\omega^2fx\Psi$$
$$\stackrel{?}{=} i\hbar\frac{\partial\Psi}{\partial t} = \cancel{-i\hbar\dot{x}_c\frac{d\psi_n}{dz}}e^{i\{\}} - \hbar\Psi\left[\cancel{-(n+\frac{1}{2})\omega} + \frac{m\omega^2}{2\hbar}(2xf - 2xx_c + x_c^2 - \frac{1}{\omega^2}\dot{x}_c^2)\right]$$

$$-\frac{1}{2}m\omega^2z^2 + \cancel{\frac{m}{2}\dot{x}_c^2} + \frac{1}{2}m\omega^2x^2 - \cancel{m\omega^2fx} \stackrel{?}{=} -\frac{m\omega^2}{2}\left(\cancel{2xf} - 2xx_c + x_c^2 - \cancel{\frac{1}{\omega^2}\dot{x}_c^2}\right)$$

$$z^2 - x^2 \stackrel{?}{=} -2xx_c + x_c^2; \quad z^2 \stackrel{?}{=} (x^2 - 2xx_c + x_c^2) = (x-x_c)^2. \quad \checkmark$$

(c)

Eq. 11.140 $\Rightarrow H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2\left(x^2 - 2xf + f^2\right) - \frac{1}{2}m\omega^2f^2.$ Shift origin: $\quad u \equiv x - f.$

$$H = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial u^2} + \frac{1}{2}m\omega^2u^2\right] - \left[\frac{1}{2}m\omega^2f^2\right].$$

The first term is a simple harmonic oscillator in the variable u; the second is a *constant* (with respect to position). So the eigenfunctions are $\psi_n(u)$, and the eigenvalues are harmonic oscillator ones, $(n+\frac{1}{2})\hbar\omega$, less the constant: $E_n = (n+\frac{1}{2})\hbar\omega - \frac{1}{2}m\omega^2f^2$.

(d) Note that $\sin[\omega(t-t')] = \frac{1}{\omega}\frac{d}{dt'}\cos[\omega(t-t')]$, so $x_c(t) = \int_0^t f(t')\frac{d}{dt'}\cos[\omega(t-t')]\,dt'$, or

$$x_c(t) = f(t')\cos[\omega(t-t')]\Big|_0^t - \int_0^t\left(\frac{df}{dt'}\right)\cos[\omega(t-t')]\,dt' = f(t) - \int_0^t\left(\frac{df}{dt'}\right)\cos[\omega(t-t')]\,dt'$$

(since $f(0)=0$). Now, for an *adiabatic* process we want df/dt very small; specifically: $\boxed{\frac{df}{dt'} \ll \omega f(t)}$ $(0 < t' \le t)$. Then the integral is negligible compared to $f(t)$, and we have $\boxed{x_c(t) \approx f(t).}$ (Physically, this says that if you pull on the spring very gently, no fancy oscillations will occur; the mass just moves along as though attached to a *string* of fixed length.)

(e) Put $x_c \approx f$ into Eq. 11.142, using Eq. 11.143:

$$\Psi(x,t) = \psi_n(x,t)e^{\frac{i}{\hbar}\left[-(n+\frac{1}{2})\hbar\omega t + m\dot{f}(x-f/2) + \frac{m\omega^2}{2}\int_0^t f^2(t')dt'\right]}.$$

The dynamic phase (Eq. 11.92) is

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\,dt' = -(n+\frac{1}{2})\omega t + \frac{m\omega^2}{2\hbar}\int_0^t f^2(t')\,dt', \quad \text{so} \quad \Psi(x,t) = \psi_n(x,t)e^{i\theta_n(t)}e^{i\gamma_n(t)},$$

confirming Eq. 11.144, with the geometric phase given (ostensibly) by $\gamma_n(t) = \frac{m}{\hbar}\dot{f}(x-f/2)$. But the eigenfunctions here are *real*, and this means the geometric phase should be *zero*. The point is that (in the adiabatic approximation) $\dot{f}$ is extremely small (see above), and hence in this limit $\frac{m}{\hbar}\dot{f}(x-f/2) \approx 0$ (at least, in the only region of x where $\psi_n(x,t)$ is nonzero).

Problem 11.37

(a) The probability that the system is still in the upper state at time t is

$$P_b(t) = 1 - \alpha\, t^2\,,$$

and after two measurements

$$P_b(t)^2 = \left(1 - \alpha\, t^2\right)^2 \approx 1 - 2\,\alpha\, t^2\,.$$

However, if we make a single measurement at time $2\,t$, the probability that the system is still in the upper state is instead

$$P_b(2\,t) = 1 - \alpha\,(2\,t)^2 = 1 - 4\,\alpha\, t^2\,.$$

So the system is more likely to be in the upper state if we repeatedly measure it.

(b) Now imagine that we make measurements at n intervals of time T/n between 0 and T. The probability that the system is still in the upper state is

$$P_b(T) = \left[1 - \alpha\left(\frac{T}{n}\right)^2\right]^n$$

and by the binomial expansion this is

$$\begin{aligned}\left[1 - \alpha\left(\frac{T}{n}\right)^2\right]^n &= 1 - n\,\alpha\left(\frac{T}{n}\right)^2 + \frac{n\,(n-1)}{2}\,\alpha^2\left(\frac{T}{n}\right)^4 + \ldots \\ &= 1 - \frac{1}{n}\,\alpha\, T^2 + \frac{1}{2}\frac{(n-1)}{n^3}\,\alpha^2\, T^4 + \ldots\end{aligned}$$

In the limit that $n \to \infty$, all terms except the first vanish and the probability is 1.

Problem 11.38

(a) Let $\theta \equiv \Delta t \mathsf{H}/\hbar$. Equation 11.151 (the exact expression) is

$$\mathsf{U} = e^{-i\theta} = 1 - i\theta - \frac{\theta^2}{2} + i\frac{\theta^3}{6} + \frac{\theta^4}{24} + \cdots\,,$$

whereas Eq. 11.153 (the approximation) says

$$\mathsf{U} \approx \frac{1 - i\theta/2}{1 + i\theta/2} = \left(1 - i\frac{\theta}{2}\right)\left(1 - i\frac{\theta}{2} - \frac{\theta^2}{4} + i\frac{\theta^3}{8} + \frac{\theta^4}{16} + \cdots\right) = 1 - i\theta - \frac{\theta^2}{2} + i\frac{\theta^3}{4} + \frac{\theta^4}{8} + \cdots\,,$$

which matches the exact expression up through the θ^2 term. ✓

As for the unitarity of Eq. 11.153, note that θ is hermitian, so

$$\mathsf{U}\mathsf{U}^\dagger = \left(\frac{1 - i\theta/2}{1 + i\theta/2}\right)\left(\frac{1 + i\theta/2}{1 - i\theta/2}\right) = 1. \quad ✓$$

(b) Here's the Mathematica code:

Physical constants

```
In[1]:= m = 1; ω = 1; ℏ = 1;
```

Numerical constants

```
In[2]:= Nx = 100; xmin = -10.; xmax = 10.; dx = (xmax - xmin)/(Nx + 1);
        Nt = 100; dt = (2 π / Ω)/Nt;
```

Construct H

The Identity Matrix

```
In[3]:= OpenOne = SparseArray[{i_, i_} → 1., {Nx, Nx}];
```

The second derivative operator

```
In[4]:= D2 = 1.0/dx^2 SparseArray[{{i_, i_} → -2., {i_, j_} /; Abs[i - j] == 1 → 1.}, {Nx, Nx}];
```

The position operator

```
In[5]:= X = SparseArray[{i_, i_} → xmin + dx i, {Nx, Nx}];
```

The Hamiltonian

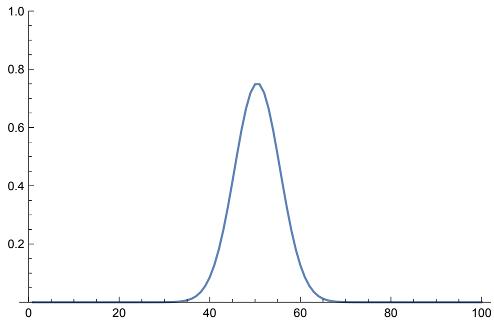
```
In[6]:= H = -1/2 D2 + 1/2 X.X;
```

```
In[9]:= Take[Reverse[Eigenvalues[H]], 2]
Out[9]= {0.498772, 1.49385}
```

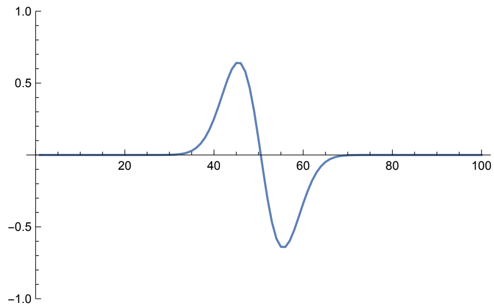
These differ from the exact values of 1/2 and 3/2 by less than 1%.
The ground and first excited states (dividing by Sqrt[dx] normalizes them):

```
In[19]:= EVE = Eigenvectors[H] / Sqrt[dx]
```

```
ListLinePlot[EVE[[100]], PlotRange → {0, 1}]
```




```
ListLinePlot[EVE[[99]], PlotRange → {-1, 1}]
```



(c) Continuing:

Construct U

The denominator in Cayley's form

```
In[24]:= Uplus = OpenOne + 1/2 I H dt;
```

The numerator in Cayley's form

```
In[25]:= Uminus = OpenOne - 1/2 I H dt;
```

Solve the t-dep Schrödinger equation

The ground and first excited states and our wave function at t=0

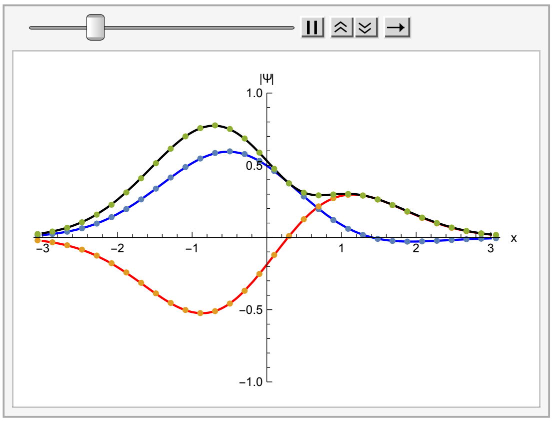
```
In[26]:= ψ0 = Eigenvectors[H][[Nx]] / Sqrt[dx];
ψ1 = Eigenvectors[H][[Nx - 1]] / Sqrt[dx];
Psi0 = (ψ0 + ψ1) / Sqrt[2];
```

Analytical form of eigenstates

$$\texttt{psi[n\_, x\_] :=} \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n\,n!}}\,\texttt{HermiteH}\left[n, \sqrt{\frac{m\,\omega}{\hbar}}\,x\right]\,\texttt{Exp}\left[-\frac{1}{2}\left(\sqrt{\frac{m\,\omega}{\hbar}}\,x\right)^2\right]$$

```
Psi = Psi0;
Data =
  Table[
   (* Step the wave function forward in time *)
   Psi = LinearSolve[Uplus, Uminus.Psi];
   If[
    (* Only Plot 100 frames regardless of number of time steps *)
    Mod[i, Nt / 100] == 0,
    (* The exact solution. Minus sign is due to
     different sign convention in numeric / analytic states *)
    g[x_] = (psi[0, x] Exp[-I ω (i dt) / 2] - psi[1, x] Exp[-3 I ω (i dt) / 2]) /
      Sqrt[2];
    (* Plotting commands *)
    Show[
     {Plot[{Re[g[x]], Im[g[x]], Abs[g[x]]}, {x, -3, 3}, PlotRange → {-1, 1},
       AxesLabel → {"x", "|Ψ|"}, PlotStyle → {Blue, Red, Black}],
      ListPlot[{Re[Psi], Im[Psi], Abs[Psi]}, PlotRange → {-1, 1},
       DataRange → {xmin + dx, xmax - dx},
       PlotStyle → PointSize[Medium]]
     }
    ],
    Nothing
   ],
   {i, 1, Nt}
  ];
```

```
ListAnimate[Data]
```



Problem 11.39

(a) $\Omega = \omega/5$:

The exact solution for the driven oscillator which we'll compare to

```
In[1]:= Clear[m, ω, ℏ, Ω, A];
In[2]:= f[t_] = A Sin[Ω t];
In[3]:= xc[t_] = Simplify[ω Integrate[f[tp] Sin[ω (t - tp)], {tp, 0, t}]];
```

$$\text{In[4]:= psi[n\_, x\_] := } \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n\, n!}} \text{ HermiteH}\left[n, \sqrt{\frac{m\,\omega}{\hbar}}\, x\right] \text{Exp}\left[-\frac{1}{2}\left(\sqrt{\frac{m\,\omega}{\hbar}}\, x\right)^2\right]$$

$$\text{In[5]:= }\Psi\text{[n\_, x\_, t\_] = Simplify}\left[\text{psi[n, x - xc[t]] Exp}\left[\frac{I}{\hbar}\left(-\left(n+\frac{1}{2}\right)\hbar\,\omega\, t + m\, \text{xc}'[t]\left(x - \frac{\text{xc}[t]}{2}\right) + \frac{m\,\omega^2}{2}\text{ Integrate[f[tp] xc[tp], \{tp, 0, t\}]}\right)\right]\right];$$

Numerics $\Omega = \omega / 5$

Physical constants

```
In[6]:= m = 1; ω = 1; ℏ = 1; Ω = .2; A = 1;
```

Numerical constants

$$\text{In[7]:= Nx = 100; xmin = -10.; xmax = 10.; dx = } \frac{\text{xmax - xmin}}{\text{Nx + 1}};$$

$$\text{Nt = 1000; dt = } \frac{2\,\pi\,/\,\Omega}{\text{Nt}};$$

Construct H

The Identity Matrix

```
In[8]:= OpenOne = SparseArray[{i_, i_} → 1., {Nx, Nx}];
```

The second derivative operator

$$\text{In[9]:= D2 = } \frac{1.0}{dx^2}\text{ SparseArray[\{\{i\_, i\_\} → -2., \{i\_, j\_\} /; Abs[i - j] == 1 → 1.\}, \{Nx, Nx\}];}$$

The position operator

```
In[10]:= X = SparseArray[{i_, i_} → xmin + dx i, {Nx, Nx}];
```

The Hamiltonian

$$\text{In[11]:= H[t\_] = } -\frac{\hbar^2}{2\,m}\text{ D2} + \frac{1}{2}\, m\,\omega^2\text{ X.X} - m\,\omega^2\text{ X f[t]};$$

Construct the time-evolution operator

The numerator in Cayley's form

$$\text{In[12]:= Uplus[t\_] = OpenOne + I H}\left[t + \frac{dt}{2}\right]\frac{dt}{2};$$

The denominator in Cayley's form

$$\text{In[13]:= Uminus[t\_] = OpenOne - I H}\left[t + \frac{dt}{2}\right]\frac{dt}{2};$$

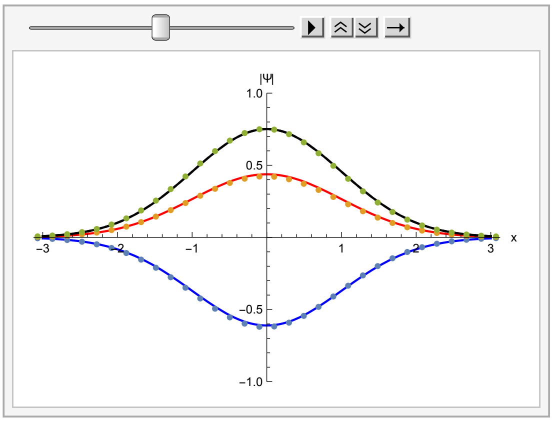
Solve the t-dep Schrödinger equation

In[14]:=
```
Psi0 = Eigenvectors[H[0]][[Nx]] / Sqrt[dx];
```

In[15]:=
```
Psi = Psi0;
Data =
  Table[
   (* Step the wave function forward in time *)
   Psi = LinearSolve[Uplus[(i - 1) dt], Uminus[(i - 1) dt].Psi];
   If[
    (* Only Plot 100 frames regardless of number of time steps *)
    Mod[i, Nt / 100] == 0,
    (* The exact solution *)
    g[x_] = Ψ[0, x, i dt];
    (* The instantaneous ground state *)
    h[x_] = psi[0, x - f[i dt]];
    (* Plotting commands *)
    Show[
     {Plot[{Re[g[x]], Im[g[x]], Abs[g[x]], Abs[h[x]]},
       {x, -3, 3}, PlotRange → {-1, 1}, AxesLabel → {"x", "|Ψ|"},
       PlotStyle → {Blue, Red, Black, {Black, Dashed}}],
      ListPlot[{Re[Psi], Im[Psi], Abs[Psi]}, PlotRange → {-1, 1},
       DataRange → {xmin + dx, xmax - dx},
       PlotStyle → PointSize[Medium]]
     }
    ],
    Nothing
   ],
   {i, 1, Nt}
  ];
```

In[17]:=
```
ListAnimate[Data]
```

Out[17]=



(b) $\Omega = 5\omega$:

Numerics Ω = 5 ω

Physical constants

```
In[18]:= m = 1; ω = 1; ℏ = 1; Ω = 5; A = 1;
```

Numerical constants

$$\texttt{In[19]:= Nx = 100; xmin = -10.; xmax = 10.; dx = } \frac{\texttt{xmax - xmin}}{\texttt{Nx + 1}};$$

$$\texttt{Nt = 1000; dt = } \frac{2\pi / \Omega}{\texttt{Nt}};$$

Construct H

The Identity Matrix

```
In[20]:= OpenOne = SparseArray[{i_, i_} → 1., {Nx, Nx}];
```

The second derivative operator

$$\texttt{In[21]:= D2 = } \frac{1.0}{\texttt{dx}^2}\texttt{ SparseArray[\{\{i\_, i\_\} → -2., \{i\_, j\_\} /; Abs[i - j] == 1 → 1.\}, \{Nx, Nx\}];}$$

The position operator

```
In[22]:= X = SparseArray[{i_, i_} → xmin + dx i, {Nx, Nx}];
```

The Hamiltonian

$$\texttt{In[23]:= H[t\_] := -}\frac{\hbar^2}{2\,\texttt{m}}\texttt{ D2 + }\frac{1}{2}\texttt{ m } \omega^2 \texttt{ X.X - m } \omega^2 \texttt{ X f[t] ;}$$

Construct the time-evolution operator

The numerator in Cayley's form

$$\texttt{In[24]:= Uplus[t\_] := OpenOne + I H}\left[\texttt{t + }\frac{\texttt{dt}}{2}\right]\frac{\texttt{dt}}{2};$$

The denominator in Cayley's form

$$\texttt{In[25]:= Uminus[t\_] := OpenOne - I H}\left[\texttt{t + }\frac{\texttt{dt}}{2}\right]\frac{\texttt{dt}}{2};$$

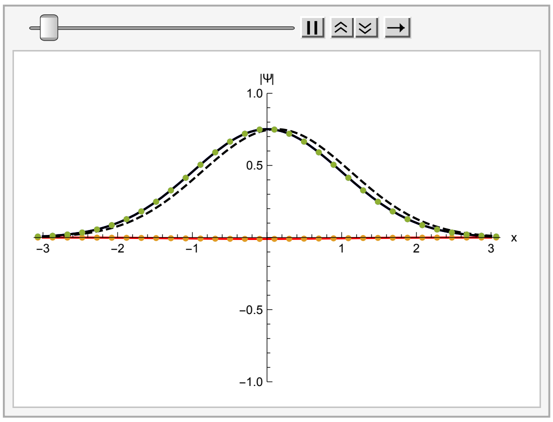
Solve the t-dep Schrödinger equation

```
In[26]:= Psi0 = Eigenvectors[H[0]][[Nx]] / Sqrt[dx];

In[27]:= Psi = Psi0;
         Data =
           Table[
            (* Step the wave function forward in time *)
            Psi = LinearSolve[Uplus[(i - 1) dt], Uminus[(i - 1) dt].Psi];
            If[
             (* Only Plot 100 frames regardless of number of time steps *)
             Mod[i, Nt / 100] == 0,
             (* The exact solution *)
             g[x_] = Ψ[0, x, i dt];
             (* The instantaneous ground state *)
             h[x_] = psi[0, x - f[i dt]];
             (* Plotting commands *)
             Show[
              {Plot[{Re[g[x]], Im[g[x]], Abs[g[x]], Abs[h[x]]},
                {x, -3, 3}, PlotRange → {-1, 1}, AxesLabel → {"x", "|Ψ|"},
                PlotStyle → {Blue, Red, Black, {Black, Dashed}}],
               ListPlot[{Re[Psi], Im[Psi], Abs[Psi]}, PlotRange → {-1, 1},
                DataRange → {xmin + dx, xmax - dx},
                PlotStyle → PointSize[Medium]]
              }
             ],
             Nothing
            ],
            {i, 1, Nt}
           ];

In[29]:= ListAnimate[Data]
```

Out[29]=



(c) $\Omega = 6\omega/5$:

Numerics $\Omega = 6/5\ \omega$

Physical constants

```
In[30]:= m = 1; ω = 1; ℏ = 1; Ω = 6/5; A = 1;
```

Numerical constants

$$\text{In[31]:= Nx = 100; xmin = -10.; xmax = 10.; dx = }\frac{\text{xmax - xmin}}{\text{Nx + 1}};$$

$$\text{Nt = 1000; dt = }\frac{2\pi\ /\ \Omega}{\text{Nt}};$$

Construct H

The Identity Matrix

```
In[32]:= OpenOne = SparseArray[{i_, i_} → 1., {Nx, Nx}];
```

The second derivative operator

$$\text{In[33]:= D2 = }\frac{1.0}{\text{dx}^2}\text{ SparseArray[\{\{i\_, i\_\} → -2., \{i\_, j\_\} /; Abs[i - j] == 1 → 1.\}, \{Nx, Nx\}];}$$

The position operator

```
In[34]:= X = SparseArray[{i_, i_} → xmin + dx i, {Nx, Nx}];
```

The Hamiltonian

$$\text{In[35]:= H[t\_] = }-\frac{\hbar^2}{2\,\text{m}}\text{ D2 + }\frac{1}{2}\text{ m }\omega^2\text{ X.X - m }\omega^2\text{ X f[t] ;}$$

Construct the time-evolution operator

The numerator in Cayley's form

$$\text{In[36]:= Uplus[t\_] = OpenOne + I H}\left[\text{t + }\frac{\text{dt}}{2}\right]\frac{\text{dt}}{2};$$

The denominator in Cayley's form

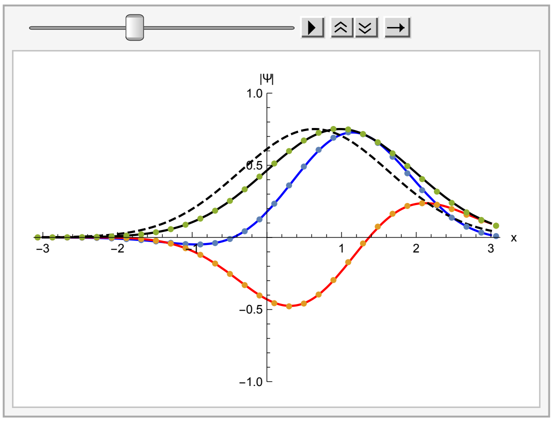
$$\text{In[37]:= Uminus[t\_] = OpenOne - I H}\left[\text{t + }\frac{\text{dt}}{2}\right]\frac{\text{dt}}{2};$$

Solve the t-dep Schrödinger equation

```
In[38]:= Psi0 = Eigenvectors[H[0]][[Nx]] / Sqrt[dx];

In[39]:= Psi = Psi0;
Data =
  Table[
   (* Step the wave function forward in time *)
   Psi = LinearSolve[Uplus[(i - 1) dt], Uminus[(i - 1) dt].Psi];
   If[
    (* Only Plot 100 frames regardless of number of time steps *)
    Mod[i, Nt / 100] == 0,
    (* The exact solution *)
    g[x_] = Ψ[0, x, i dt];
    (* The instantaneous ground state *)
    h[x_] = psi[0, x - f[i dt]];
    (* Plotting commands *)
    Show[
     {Plot[{Re[g[x]], Im[g[x]], Abs[g[x]], Abs[h[x]]},
       {x, -3, 3}, PlotRange → {-1, 1}, AxesLabel → {"x", "|Ψ|"},
       PlotStyle → {Blue, Red, Black, {Black, Dashed}}],
      ListPlot[{Re[Psi], Im[Psi], Abs[Psi]}, PlotRange → {-1, 1},
       DataRange → {xmin + dx, xmax - dx},
       PlotStyle → PointSize[Medium]]
     }
    ],
    Nothing
   ],
   {i, 1, Nt}
  ];

ListAnimate[Data]
```



Chapter 12

Afterword

Problem 12.1

Suppose, on the contrary, that

$$\alpha|\phi_a(1)\rangle|\phi_b(2)\rangle + \beta|\phi_b(1)\rangle|\phi_a(2)\rangle = |\psi_r(1)\rangle|\psi_s(2)\rangle,$$

for some one-particle states $|\psi_r\rangle$ and $|\psi_s\rangle$. Because $|\phi_a\rangle$ and $|\phi_b\rangle$ constitute a complete set of one-particle states (this is a two-level system), any other one-particle state can be expressed as a linear combination of them. In particular,

$$|\psi_r\rangle = A|\phi_a\rangle + B|\phi_b\rangle, \quad \text{and} \quad |\psi_s\rangle = C|\phi_a\rangle + D|\phi_b\rangle,$$

for some complex numbers A, B, C, and D. Thus

$$\begin{aligned}\alpha|\phi_a(1)\rangle|\phi_b(2)\rangle + \beta|\phi_b(1)\rangle|\phi_a(2)\rangle &= \left[A|\phi_a(1)\rangle + B|\phi_b(1)\rangle\right]\left[C|\phi_a(2)\rangle + D|\phi_b(2)\rangle\right] \\ &= AC|\phi_a(1)\rangle|\phi_a(2)\rangle + AD|\phi_a(1)\rangle|\phi_b(2)\rangle + BC|\phi_b(1)\rangle|\phi_a(2)\rangle + BD|\phi_b(1)\rangle|\phi_b(2)\rangle.\end{aligned}$$

(i) Take the inner product with $\langle\phi_a(1)|\langle\phi_b(2)|$: $\alpha = AD$.
(ii) Take the inner product with $\langle\phi_a(1)|\langle\phi_a(2)|$: $0 = AC$.
(iii) Take the inner product with $\langle\phi_b(1)|\langle\phi_a(2)|$: $\beta = BC$.
(iv) Take the inner product with $\langle\phi_b(1)|\langle\phi_b(2)|$: $0 = BD$.

(ii) $\Rightarrow$ either $A = 0$ or $C = 0$. But if $A = 0$, then (i) $\Rightarrow \alpha = 0$, which is excluded by assumption, whereas if $C = 0$, then (iii) $\Rightarrow \beta = 0$, which is likewise excluded. *Conclusion:* It is impossible to express this state as a product of one-particle states. QED

Problem 12.2

(a) "The particle must have been in box B_1 all along, since there is no way that opening B_1 could have instantaneously affected the outcome of opening faraway box B_2."

(b) The measurement at B_1 collapses the wave function to a narrow spike at the particle's measured position; the wave function is now zero everywhere in box B_2, and the box will be empty when it is opened.

Problem 12.3

(a) Reading from the figure, $\mathbf{a} = \hat{\imath}$, $\mathbf{b} = \cos\eta\,\hat{\imath} + \sin\eta\,\hat{\jmath}$, $\quad \mathbf{S}_a = S_a(\sin\theta\,\cos\phi\,\hat{\imath} + \sin\theta\,\sin\phi\,\hat{\jmath} + \cos\theta\,\hat{k}) = -\mathbf{S}_b$, so

$$\begin{aligned}
\mathbf{a}\cdot\mathbf{S}_a &= S_a\,\sin\theta\,\cos\phi,\\
\mathbf{b}\cdot\mathbf{S}_b &= -S_a\,\sin\theta(\cos\phi\,\cos\eta + \sin\phi\,\sin\eta) = -S_a\,\sin\theta\,\cos(\phi-\eta).
\end{aligned}$$

But $\sin\theta \geq 0$ (since θ is between 0 and π), so
$A = \text{sign}(\mathbf{a}\cdot\mathbf{S}_a) = \text{sign}(\cos\phi)$, $B = -\text{sign}((\cos(\phi-\eta))$, and hence $A(\mathbf{a},\lambda)B(\mathbf{b},\lambda) = -\text{sign}\left[\cos\phi\,\cos(\phi-\eta)\right]$. ✓

(b) $P(\mathbf{a},\mathbf{b}) = \langle A(\mathbf{a},\lambda)B(\mathbf{b},\lambda)\rangle = \dfrac{1}{4\pi}\displaystyle\int [A(\mathbf{a},\lambda)B(\mathbf{b},\lambda)]\,\sin\theta\,d\theta\,d\phi = -\frac{2}{4\pi}\int_0^{2\pi}\text{sign}[\cos\phi\,\cos(\phi-\eta)]\,d\phi.$
Now, $\cos\phi$ is positive unless $\frac{\pi}{2} < \phi < \frac{3\pi}{2}$, and $\cos(\phi-\eta)$ is positive unless $\frac{\pi}{2}+\eta < \phi < \frac{3\pi}{2}+\eta$.

Assume first that $0 < \eta < \frac{\pi}{2}$, and chop the integral into eight segments, writing $(++)$ to indicate that $\cos\phi$ is positive and $\cos(\phi-\eta)$ is positive, etc.:

$$\begin{aligned}
P(\mathbf{a},\mathbf{b}) &= -\frac{1}{2\pi}\left\{\int_0^{\eta}(++)\,d\phi + \int_{\eta}^{\pi/2}(++)\,d\phi + \int_{\pi/2}^{\pi/2+\eta}(-+)\,d\phi + \int_{\pi/2+\eta}^{\pi}(--)\,d\phi\right.\\
&\qquad \left. + \int_{\pi}^{\pi+\eta}(--)\,d\phi + \int_{\pi+\eta}^{3\pi/2}(--)\,d\phi + \int_{3\pi/2}^{3\pi/2+\eta}(+-)\,d\phi + \int_{3\pi/2+\eta}^{2\pi}(++)\,d\phi\right\}\\
&= -\frac{1}{2\pi}\left\{(\eta-0) + \left(\frac{\pi}{2}-\eta\right) - \left(\frac{\pi}{2}+\eta-\frac{\pi}{2}\right) + \left(\pi-\frac{\pi}{2}-\eta\right) + (\pi+\eta-\pi) + \left(\frac{3\pi}{2}-\pi-\eta\right)\right.\\
&\qquad \left. - \left(\frac{3\pi}{2}+\eta-\frac{3\pi}{2}\right) + \left(2\pi-\frac{3\pi}{2}-\eta\right)\right\} = -\frac{1}{2\pi}(2\pi-4\eta) = \frac{2\eta}{\pi} - 1.
\end{aligned}$$

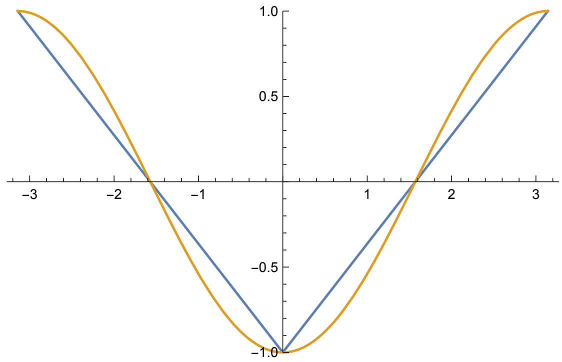
That's for $0 < \eta < \frac{\pi}{2}$; for $\frac{\pi}{2} < \eta < \pi$ we have:

$$\begin{aligned}
P(\mathbf{a},\mathbf{b}) &= -\frac{1}{2\pi}\left\{\int_0^{\eta-\pi/2}(+-)\,d\phi + \int_{\eta-\pi/2}^{\pi/2}(++)\,d\phi + \int_{\pi/2}^{\eta}(-+)\,d\phi + \int_{\eta}^{\pi}(-+)\,d\phi\right.\\
&\qquad \left. + \int_{\pi}^{\eta+\pi/2}(-+)\,d\phi + \int_{\eta+\pi/2}^{3\pi/2}(--)\,d\phi + \int_{3\pi/2}^{\eta+\pi}(+-)\,d\phi + \int_{\eta+\pi}^{2\pi}(+-)\,d\phi\right\}\\
&= -\frac{1}{2\pi}\left\{-\left(\eta-\frac{\pi}{2}-0\right) + \left(\frac{\pi}{2}-\eta+\frac{\pi}{2}\right) - \left(\eta-\frac{\pi}{2}\right) - (\pi-\eta) - \left(\eta+\frac{\pi}{2}-\pi\right) + \left(\frac{3\pi}{2}-\eta-\frac{\pi}{2}\right)\right.\\
&\qquad \left. - \left(\eta+\pi-\frac{3\pi}{2}\right) - (2\pi-\eta-\pi)\right\} = -\frac{1}{2\pi}(2\pi-4\eta) = \frac{2\eta}{\pi} - 1 \text{ (same as before).}
\end{aligned}$$

The average is an even function of η, so the general result (for $-\frac{\pi}{2} < \eta < \frac{\pi}{2}$) is $\boxed{\dfrac{2|\eta|}{\pi} - 1.}$

(c) The quantum prediction (Equation 12.4) is $P(\mathbf{a},\mathbf{b}) = -\cos\eta$; plotting the two:

```
Plot[{2 Abs[x]/π - 1, -Cos[x]}, {x, -π, π}, PlotRange → {-1, 1}]
```



They agree at $\boxed{\eta = 0, \pm\frac{\pi}{2}, \text{ and } \pm\pi.}$

(d) In this example Bell's inequality says $\left|\frac{2}{\pi}|\eta_{ab}| - 1 - \frac{2}{\pi}|\eta_{ac}| + 1\right| \leq 1 + \frac{2}{\pi}|\eta_{bc}| - 1$, or

$$\Big||\eta_{ab}| - |\eta_{ac}|\Big| \leq |\eta_{bc}|,$$

where all angles are in the range $[-\pi, \pi]$. Now, first assume that $|\eta_{ab}| > |\eta_{ac}|$. In that case

$$|\eta_{ab}| \leq |\eta_{ac}| + |\eta_{cb}|\,.$$

On the other hand, if $|\eta_{ac}| > |\eta_{ab}|$

$$|\eta_{ac}| \leq |\eta_{ab}| + |\eta_{bc}|\,.$$

In either case, the equation says that one angle is smaller than the sum of the other two. This is clearly correct: the vectors **a**, **b**, and **c** define points a, b, and c on a unit sphere, and the angles between the vectors are proportional to the lengths of the great arcs connecting those points. So the inequality just expresses the fact that walking "straight" from a to b is shorter than walking from a to c and c to b (unless c happens to lie on your path in which case it is the same distance).

Problem 12.4

(a) Equation 12.17: $\hat{\rho}^2 = |\Psi\rangle\,\langle\Psi\,|\,\Psi\rangle\,\langle\Psi|$, and since Ψ is normalized, $\hat{\rho}^2 = |\Psi\rangle\; 1\;\langle\Psi| = \hat{\rho}$. ✓

Equation 12.18: To find the Hermitian conjugate of an operator in Dirac notation, we reverse the order of the terms, switch bras and kets, place a † on every operator and a ∗ on every number:

$$\hat{\rho}^\dagger = \left(|\Psi\rangle\,\langle\Psi|\right)^\dagger = |\Psi\rangle\,\langle\Psi| = \rho\,. \quad \checkmark$$

Equation 12.19: $\mathrm{Tr}(\rho) = \sum_i \rho_{ii} = \sum_i \langle e_i\,|\,\Psi\rangle\,\langle\Psi\,|\,e_i\rangle = \langle\Psi|\left(\sum_i |e_i\rangle\,\langle e_i|\right)|\Psi\rangle = \langle\Psi\,|\,\Psi\rangle = 1.$ ✓

Equation 12.20:

$$\begin{aligned}
\mathrm{Tr}(\rho\,\mathsf{A}) &= \sum_i (\rho\,\mathsf{A})_{ii} = \sum_i\sum_j \rho_{ij}\,A_{ji} = \sum_i\sum_j \langle e_i\,|\,\Psi\rangle\;\langle\Psi\,|\,e_j\rangle\;\left\langle e_j\,\middle|\,\hat{A}\,\middle|\,e_i\right\rangle \\
&= \sum_i\sum_j \langle\Psi\,|\,e_j\rangle\;\left\langle e_j\,\middle|\,\hat{A}\,\middle|\,e_i\right\rangle\;\langle e_i\,|\,\Psi\rangle = \langle\Psi|\left(\sum_j |e_j\rangle\,\langle e_j|\right)\hat{A}\left(\sum_i |e_i\rangle\,\langle e_i|\right)|\Psi\rangle = \left\langle\Psi\,\middle|\,\hat{A}\,\middle|\,\Psi\right\rangle \\
&= \langle A\rangle\,. \quad \checkmark
\end{aligned}$$

(b) $i\hbar\,\dfrac{d}{dt}\hat{\rho} = i\hbar\left(\left|\dot{\Psi}\right\rangle\langle\Psi| + |\Psi\rangle\left\langle\dot{\Psi}\right|\right)$. From the Schrödinger equation: $i\hbar\,|\dot{\Psi}\rangle = \hat{H}\,|\Psi\rangle$, and, taking the adjoint: $-i\hbar\,\langle\dot{\Psi}| = \langle\Psi|\,\hat{H}$. Thus

$$i\hbar\,\frac{d}{dt}\hat{\rho} = \hat{H}\,|\Psi\rangle\,\langle\Psi| - |\Psi\rangle\,\langle\Psi|\,\hat{H} = \hat{H}\,\hat{\rho} - \hat{\rho}\,\hat{H} = \left[\hat{H},\hat{\rho}\right]. \quad \checkmark$$

Problem 12.5

For an electron with spin-down along the y direction (Problem 4.32(a)):

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}; \quad \langle\Psi| = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & i\end{pmatrix}.$$

So

$$\begin{aligned}
\rho_{11} &= \frac{1}{2}\left[\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\-i\end{pmatrix}\right]\left[\begin{pmatrix}1 & i\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}\right] = \frac{1}{2}(1)(1) = \frac{1}{2}, \\
\rho_{12} &= \frac{1}{2}\left[\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\-i\end{pmatrix}\right]\left[\begin{pmatrix}1 & i\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{2}(1)(i) = \frac{i}{2} \\
\rho_{21} &= \frac{1}{2}\left[\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}1\\-i\end{pmatrix}\right]\left[\begin{pmatrix}1 & i\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}\right] = \frac{1}{2}(-i)(1) = -\frac{i}{2} \\
\rho_{22} &= \frac{1}{2}\left[\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}1\\-i\end{pmatrix}\right]\left[\begin{pmatrix}1 & i\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{2}(-i)(i) = \frac{1}{2}
\end{aligned}$$

and

$$\rho = \frac{1}{2}\begin{pmatrix}1 & i\\-i & 1\end{pmatrix}.$$

Or, more efficiently,

$$\rho = |\Psi\rangle\,\langle\Psi| = \frac{1}{2}\begin{pmatrix}1\\-i\end{pmatrix}\begin{pmatrix}1 & i\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & i\\-i & 1\end{pmatrix}.$$

Problem 12.6

(a) Equation 12.31: As in Problem 12.4(a), $\hat{\rho}^\dagger = \left(\sum_k p_k \,|\Psi_k\rangle\,\langle\Psi_k|\right)^\dagger = \sum_k |\Psi_k\rangle\,\langle\Psi_k|\,p_k^*$. Since p_k is real, $\hat{\rho}^\dagger = \hat{\rho}$, ✓

Equation 12.32:

$$\begin{aligned}\mathrm{Tr}\,[\rho] &= \sum_i \rho_{ii} = \sum_i \sum_k p_k \,\langle e_i \,|\, \Psi_k\rangle\,\langle \Psi_k \,|\, e_i\rangle = \sum_k p_k \left\langle \Psi_k \,\middle|\, \sum_i |e_i\rangle\,\langle e_i| \,\middle|\, \Psi_k \right\rangle \\ &= \sum_k p_k \,\langle \Psi_k \,|\, \Psi_k\rangle = \sum_k p_k = 1\,. \quad ✓\end{aligned}$$

In the last two steps I used the fact that each wave function is normalized, and Equation (12.30).

Equation 12.33:

$$\begin{aligned}\mathrm{Tr}(\rho\,\mathsf{A}) &= \sum_i (\rho\,\mathsf{A})_{ii} = \sum_i \sum_j \rho_{ij}\,A_{ji} = \sum_i \sum_j \sum_k p_k\,\langle e_i \,|\, \Psi_k\rangle\,\langle \Psi_k \,|\, e_j\rangle\,\left\langle e_j \,\middle|\, \hat{A} \,\middle|\, e_i \right\rangle \\ &= \sum_k p_k\,\langle \Psi_k|\,\left(\sum_j |e_j\rangle\,\langle e_j|\right)\hat{A}\left(\sum_i |e_i\rangle\,\langle e_i|\right)|\Psi_k\rangle = \sum_k p_k\,\left\langle \Psi_k \,\middle|\, \hat{A} \,\middle|\, \Psi_k \right\rangle = \langle A\rangle\,. \quad ✓\end{aligned}$$

Equation 12.34: As in Problem 12.4(b):

$$\begin{aligned}i\hbar\,\frac{d}{dt}\hat{\rho} &= i\hbar \sum_k p_k\left(\left|\dot{\Psi}_k\right\rangle\,\langle\Psi_k| + |\Psi_k\rangle\,\left\langle\dot{\Psi}_k\right|\right) = \sum_k p_k\left(\hat{H}\,|\Psi_k\rangle\,\langle\Psi_k| - |\Psi_k\rangle\,\langle\Psi_k|\,\hat{H}\right) \\ &= \hat{H}\,\hat{\rho} - \hat{\rho}\,\hat{H} = \left[\hat{H},\hat{\rho}\right]\,. \quad ✓\end{aligned}$$

(b)

$$\begin{aligned}\mathrm{Tr}\left(\rho^2\right) &= \sum_i \left(\rho^2\right)_{ii} = \sum_i \sum_k \sum_j p_k\,p_j\,\langle e_i \,|\, \Psi_k\rangle\,\langle \Psi_k \,|\, \Psi_j\rangle\,\langle \Psi_j \,|\, e_i\rangle \\ &= \sum_k \sum_j p_k\,p_j\,\langle\Psi_j|\left(\sum_i |e_i\rangle\,\langle e_i|\right)|\Psi_k\rangle\,\langle \Psi_k \,|\, \Psi_j\rangle = \sum_k \sum_j p_k\,p_j|\langle \Psi_k \,|\, \Psi_j\rangle|^2\end{aligned}$$

The wave functions are normalized, so $|\langle\Psi_k|\Psi_j\rangle| \le 1$, with equality if and only if $k = j$. Therefore, unless this is a pure state

$$\mathrm{Tr}\left(\rho^2\right) < \sum_k \sum_j p_k\,p_j = \sum_k p_k \sum_j p_j = 1\,. \quad \text{QED}$$

(c) We already know that $\rho^2 = \rho$ for a pure state. In part (b) we proved that $\mathrm{Tr}\left(\rho^2\right) < 1$ for a non-pure state, whereas from (a) $\mathrm{Tr}(\rho) = 1$ for *any* density matrix. Therefore, for a non-pure state $\rho^2 \neq \rho$ (they have different traces). QED

Problem 12.7

(a) From Example 12.1, the density matrix for an electron in the state spin up along x is

$$\rho_{x+} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix};$$

from Problem 12.5 the density matrix for an electron in the state spin down along y is

$$\rho_{y-} = \begin{pmatrix} 1/2 & i/2 \\ -i/2 & 1/2 \end{pmatrix}.$$

Therefore the density matrix for the state in question is

$$\rho = \frac{1}{3}\,\rho_{x+} + \frac{2}{3}\,\rho_{y-} = \begin{pmatrix} 1/2 & 1/6 + i/3 \\ 1/6 - i/3 & 1/2 \end{pmatrix}.$$

(b) From Equation 4.147,

$$\mathsf{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

so

$$\langle S_y \rangle = \mathrm{Tr}(\rho \mathsf{S}_y) = \frac{\hbar}{2}\mathrm{Tr}\left[\begin{pmatrix} 1/2 & 1/6 + i/3 \\ 1/6 - i/3 & 1/2 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\right] = \frac{\hbar}{2}\mathrm{Tr}\begin{pmatrix} i/6 - 1/3 & -i/2 \\ i/2 & -i/6 - 1/3 \end{pmatrix}$$
$$= \frac{\hbar}{2}\left(\frac{i}{6} - \frac{1}{3} - \frac{i}{6} - \frac{1}{3}\right) = \frac{\hbar}{2}\left(-\frac{2}{3}\right) = \boxed{-\frac{\hbar}{3}.}$$

Problem 12.8

(a) The density matrix for a spin-1/2 state is a two by two matrix which can be written

$$\rho = \begin{pmatrix} c_1 & c_2 \\ c_3 & c_4 \end{pmatrix}$$

for complex numbers c_1, c_2, c_3, c_4. Because the matrix is Hermitian we know that c_1 and c_4 must be real and c_2 and c_3 must be complex conjugates. Thus

$$\rho = \begin{pmatrix} b_1 & b_2 - i\,b_3 \\ b_2 + i\,b_3 & b_4 \end{pmatrix}$$

for *real* numbers b_1, b_2, b_3, b_4. In addition, since the trace is 1 we know that $b_4 = 1 - b_1$. Defining $a_1 = 2\,b_2$, $a_2 = 2\,b_3$, and $a_3 = 2\,b_1 - 1$ then gives

$$\rho = \frac{1}{2}\begin{pmatrix} 1 + a_3 & a_1 - i\,a_2 \\ a_1 + i\,a_2 & 1 - a_3 \end{pmatrix} = \frac{1}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + a_1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + a_2\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + a_3\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]$$
$$= \frac{1}{2}\left(1 + a_1\,\sigma_x + a_2\,\sigma_y + a_3\,\sigma_z\right) = \frac{1}{2}\left(1 + \mathbf{a}\cdot\boldsymbol{\sigma}\right). \quad \checkmark$$

(b)

$$\mathrm{Tr}\big(\rho^2\big) = \mathrm{Tr}\left[\frac{1}{2}\begin{pmatrix} 1 + a_3 & a_1 - i\,a_2 \\ a_1 + i\,a_2 & 1 - a_3 \end{pmatrix}\frac{1}{2}\begin{pmatrix} 1 + a_3 & a_1 - i\,a_2 \\ a_1 + i\,a_2 & 1 - a_3 \end{pmatrix}\right]$$
$$= \frac{1}{4}\,\mathrm{Tr}\left[\begin{pmatrix} a_1^2 + a_2^2 + (1 + a_3)^2 & 2\,(a_1 - i a_2) \\ 2\,(a_1 + i\,a_2) & a_1^2 + a_2^2 + (1 - a_3)^2 \end{pmatrix}\right] = \frac{1}{2}\left(1 + |\mathbf{a}|^2\right).$$

By virtue of Problem 12.6c we see that $|\mathbf{a}| \leq 1$ in order for this to be a density matrix, and it describes a pure state if and only if $|\mathbf{a}| = 1$.

(c) We can calculate the expectation value of S_z and, since there are only two possibilities,

$$\langle S_z \rangle = P_+ \frac{\hbar}{2} + P_- \left(-\frac{\hbar}{2}\right) = P_+ \frac{\hbar}{2} + (1 - P_+) \left(-\frac{\hbar}{2}\right) = \hbar \left(P_+ - \frac{1}{2}\right).$$

This tells us the probability that a measurement will return spin up along z. Now

$$\begin{aligned}\langle S_z \rangle &= \mathrm{Tr}\left(\frac{\hbar}{2}\sigma_z \rho\right) = \frac{\hbar}{2}\mathrm{Tr}\left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{2}\begin{pmatrix} 1+a_3 & a_1 - i\,a_2 \\ a_1 + i\,a_2 & 1-a_3 \end{pmatrix}\right] \\ &= \frac{\hbar}{4}\mathrm{Tr}\left[\begin{pmatrix} 1+a_3 & a_1 - i\,a_2 \\ -a_1 - i\,a_2 & -1+a_3 \end{pmatrix}\right] = \frac{\hbar}{2} a_3.\end{aligned}$$

Combining these two results we have

$$P_+ = \frac{1+a_3}{2}.$$

For the given directions we have: $\boxed{\text{(i) } P_+ = 1, \text{ (ii) } P_+ = 1/2, \text{ and (iii) } P_+ = 0.}$

(d) For a point on the equator at azimuthal angle ϕ, we have $a_1 = \cos\phi$, $a_2 = \sin\phi$, $a_3 = 0$, so

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & e^{-i\,\phi} \\ e^{i\,\phi} & 1 \end{pmatrix}.$$

For a spinor $\chi = \begin{pmatrix} a \\ b \end{pmatrix}$ the density matrix is

$$\rho = \chi\,\chi^\dagger = \begin{pmatrix} a \\ b \end{pmatrix} \begin{pmatrix} a^* & b^* \end{pmatrix} = \begin{pmatrix} |a|^2 & a\,b^* \\ b\,a^* & |b|^2 \end{pmatrix},$$

so, up to an arbitrary overall phase,

$$\boxed{\chi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\,\phi} \end{pmatrix}.}$$

Appendix A

Linear Algebra

Problem A.1

(a) $\boxed{\text{Yes; two-dimensional.}}$

(b) $\boxed{\text{No;}}$ the sum of two such vectors has $a_z = 2$, and is not in the subset. Also, the null vector (0,0,0) is not in the subset.

(c) $\boxed{\text{Yes; one-dimensional.}}$

Problem A.2

(a) $\boxed{\text{Yes;} \quad 1, x, x^2, \dots, x^{N-1}}$ is a convenient basis. Dimension: $\boxed{N.}$

(b) $\boxed{\text{Yes;} \quad 1, x^2, x^4, \dots.}$ Dimension $\boxed{N/2}$ (if N is even) or $\boxed{(N+1)/2}$ (if N is odd).

(c) $\boxed{\text{No.}}$ The sum of two such "vectors" is not in the space.

(d) $\boxed{\text{Yes;} \quad (x-1), (x-1)^2, (x-1)^3, \dots, (x-1)^{N-1}.}$ Dimension: $\boxed{N-1.}$

(e) $\boxed{\text{No.}}$ The sum of two such "vectors" would have value 2 at $x = 0$.

Problem A.3

Suppose $|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \cdots a_n|e_n\rangle$ and $|\alpha\rangle = b_1|e_1\rangle + b_2|e_2\rangle + \cdots + b_n|e_n\rangle$. Subtract: $0 = (a_1 - b_1)|e_1\rangle + (a_2 - b_2)|e_2\rangle + \cdots + (a_n - b_n)|e_n\rangle$. Suppose $a_j \neq b_j$ for some j; then we can divide by $(a_j - b_j)$ to get:

$$|e_j\rangle = -\frac{(a_1 - b_1)}{(a_j - b_j)}|e_1\rangle - \frac{(a_2 - b_2)}{(a_j - b_j)}|e_2\rangle - \cdots - 0|e_j\rangle - \cdots - \frac{(a_n - b_n)}{(a_j - b_j)}|e_n\rangle,$$

so $|e_j\rangle$ is linearly dependent on the others, and hence $\{|e_j\rangle\}$ is not a basis. If $\{|e_j\rangle\}$ *is* a basis, therefore, the components *must* all be equal ($a_1 = b_1, a_2 = b_2, \dots, a_n = b_n$). QED

Problem A.4

(i)

$$\langle e_1|e_1\rangle = |1+i|^2 + 1 + |i|^2 = (1+i)(1-i) + 1 + (i)(-i) = 1+1+1+1 = 4. \quad \|e_1\| = 2.$$

$$\boxed{|e_1'\rangle = \frac{1}{2}(1+i)\,\hat{\imath} + \frac{1}{2}\,\hat{\jmath} + \frac{i}{2}\,\hat{k}.}$$

(ii)

$$\langle e_1'|e_2\rangle = \frac{1}{2}(1-i)(i) + \frac{1}{2}(3) + \left(\frac{-i}{2}\right)1 = \frac{1}{2}(i+1+3-i) = 2.$$

$$|e_2''\rangle \equiv |e_2\rangle - \langle e_1'|e_2\rangle|e_1'\rangle = (i-1-i)\hat{\imath} + (3-1)\hat{\jmath} + (1-i)\hat{k} = (-1)\hat{\imath} + (2)\hat{\jmath} + (1-i)\hat{k}.$$

$$\langle e_2''|e_2''\rangle = 1+4+2 = 7. \quad \boxed{|e_2'\rangle = \frac{1}{\sqrt{7}}[-\hat{\imath} + 2\hat{\jmath} + (1-i)\hat{k}].}$$

(iii)

$$\langle e_1'|e_3\rangle = \frac{1}{2}28 = 14; \quad \langle e_2'|e_3\rangle = \frac{2}{\sqrt{7}}28 = 8\sqrt{7}.$$

$$\begin{aligned} |e_3''\rangle &= |e_3\rangle - \langle e_1'|e_3\rangle|e_1'\rangle - \langle e_2'|e_3\rangle|e_2'\rangle = |e_3\rangle - 7|e_1\rangle - 8|e_2''\rangle \\ &= (0-7-7i+8)\hat{\imath} + (28-7-16)\hat{\jmath} + (0-7i-8+8i)\hat{k} = (1-7i)\hat{\imath} + 5\hat{\jmath} + (-8+i)\hat{k}. \end{aligned}$$

$$\|e_3''\|^2 = 1+49+25+64+1 = 140. \quad \boxed{|e_3'\rangle = \frac{1}{2\sqrt{35}}[(1-7i)\hat{\imath} + 5\hat{\jmath} + (-8+i)\hat{k}].}$$

Problem A.5

From Eq. A.21: $\langle\gamma|\gamma\rangle = \langle\gamma|\left(|\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}|\alpha\rangle\right) = \langle\gamma|\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}\langle\gamma|\alpha\rangle.$ From Eq. A.19:

$$\langle\gamma|\beta\rangle^* = \langle\beta|\gamma\rangle = \langle\beta|\left(|\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}|\alpha\rangle\right) = \langle\beta|\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}\langle\beta|\alpha\rangle = \langle\beta|\beta\rangle - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\alpha|\alpha\rangle}, \text{ which is } \textit{real}.$$

$$\langle\gamma|\alpha\rangle^* = \langle\alpha|\gamma\rangle = \langle\alpha|\left(|\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}|\alpha\rangle\right) = \langle\alpha|\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}\langle\alpha|\alpha\rangle = 0. \quad \langle\gamma|\alpha\rangle = 0. \quad \text{So (Eq. A.20)}:$$

$$\langle\gamma|\gamma\rangle = \langle\beta|\beta\rangle - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\alpha|\alpha\rangle} \geq 0, \text{ and hence } |\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle. \quad \text{QED}$$

Problem A.6

$$\langle\alpha|\beta\rangle = (1-i)(4-i) + (1)(0) + (-i)(2-2i) = 4-5i-1-2i-2 = 1-7i; \quad \langle\beta|\alpha\rangle = 1+7i;$$

$$\langle\alpha|\alpha\rangle = 1+1+1+1 = 4; \quad \langle\beta|\beta\rangle = 16+1+4+4 = 25; \quad \cos\theta = \sqrt{\frac{1+49}{4\cdot 25}} = \frac{1}{\sqrt{2}}; \quad \boxed{\theta = 45^\circ.}$$

Problem A.7

Let $|\gamma\rangle \equiv |\alpha\rangle + |\beta\rangle; \quad \langle\gamma|\gamma\rangle = \langle\gamma|\alpha\rangle + \langle\gamma|\beta\rangle.$

$\langle\gamma|\alpha\rangle^* = \langle\alpha|\gamma\rangle = \langle\alpha|\alpha\rangle + \langle\alpha|\beta\rangle \Longrightarrow \langle\gamma|\alpha\rangle = \langle\alpha|\alpha\rangle + \langle\beta|\alpha\rangle.$
$\langle\gamma|\beta\rangle^* = \langle\beta|\gamma\rangle = \langle\beta|\alpha\rangle + \langle\beta|\beta\rangle \Longrightarrow \langle\gamma|\beta\rangle = \langle\alpha|\beta\rangle + \langle\beta|\beta\rangle.$

$\|(|\alpha\rangle + |\beta\rangle)\|^2 = \langle\gamma|\gamma\rangle = \langle\alpha|\alpha\rangle + \langle\beta|\beta\rangle + \langle\alpha|\beta\rangle + \langle\beta|\alpha\rangle.$

But $\langle\alpha|\beta\rangle + \langle\beta|\alpha\rangle = 2\mathrm{Re}(\langle\alpha|\beta\rangle) \le 2|\langle\alpha|\beta\rangle| \le 2\sqrt{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle}$ (by Schwarz inequality), so $\|(|\alpha\rangle + |\beta\rangle)\|^2 \le \|\alpha\|^2 + \|\beta\|^2 + 2\|\alpha\|\|\beta\| = (\|\alpha\| + \|\beta\|)^2,$ and hence $\|(|\alpha\rangle + |\beta\rangle)\| \le \|\alpha\| + \|\beta\|.$ QED

Problem A.8

(a) $\boxed{\begin{pmatrix} 1 & 1 & 0 \\ 2 & 1 & 3 \\ 3i & (3-2i) & 4 \end{pmatrix}}.$

(b) $\begin{pmatrix} (-2+0-1) & (0+1+3i) & (i+0+2i) \\ (4+0+3i) & (0+0+9) & (-2i+0+6) \\ (4i+0+2i) & (0-2i+6) & (2+0+4) \end{pmatrix} = \boxed{\begin{pmatrix} -3 & (1+3i) & 3i \\ (4+3i) & 9 & (6-2i) \\ 6i & (6-2i) & 6 \end{pmatrix}}.$

(c) $\mathsf{BA} = \begin{pmatrix} (-2+0+2) & (2+0-2) & (2i+0-2i) \\ (0+2+0) & (0+0+0) & (0+3+0) \\ (-i+6+4i) & (i+0-4i) & (-1+9+4) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 2 & 0 & 3 \\ (6+3i) & -3i & 12 \end{pmatrix}.$

$[\mathsf{A}, \mathsf{B}] = \mathsf{AB} - \mathsf{BA} = \boxed{\begin{pmatrix} -3 & (1+3i) & 3i \\ (2+3i) & 9 & (3-2i) \\ (-6+3i) & (6+i) & -6 \end{pmatrix}}.$

(d) $\boxed{\begin{pmatrix} -1 & 2 & 2i \\ 1 & 0 & -2i \\ i & 3 & 2 \end{pmatrix}}.$

(e) $\boxed{\begin{pmatrix} -1 & 1 & -i \\ 2 & 0 & 3 \\ -2i & 2i & 2 \end{pmatrix}}.$

(f) $\boxed{\begin{pmatrix} -1 & 2 & -2i \\ 1 & 0 & 2i \\ -i & 3 & 2 \end{pmatrix}}.$

(g) $4+0+0-1-0-0 = \boxed{3.}$

(h)

$$\mathsf{B}^{-1} = \frac{1}{3}\tilde{\mathsf{C}}; \quad \mathsf{C} = \begin{pmatrix} \begin{vmatrix} 1 & 0 \\ 3 & 2 \end{vmatrix} & -\begin{vmatrix} 0 & 0 \\ i & 2 \end{vmatrix} & \begin{vmatrix} 0 & 1 \\ i & 3 \end{vmatrix} \\ -\begin{vmatrix} 0 & -i \\ 3 & 2 \end{vmatrix} & \begin{vmatrix} 2 & -i \\ i & 2 \end{vmatrix} & -\begin{vmatrix} 2 & 0 \\ i & 3 \end{vmatrix} \\ \begin{vmatrix} 0 & -i \\ 1 & 0 \end{vmatrix} & -\begin{vmatrix} 2 & -i \\ 0 & 0 \end{vmatrix} & \begin{vmatrix} 2 & 0 \\ 0 & 1 \end{vmatrix} \end{pmatrix} = \begin{pmatrix} 2 & 0 & -i \\ -3i & 3 & -6 \\ i & 0 & 2 \end{pmatrix}. \quad \boxed{\mathsf{B}^{-1} = \frac{1}{3}\begin{pmatrix} 2 & -3i & i \\ 0 & 3 & 0 \\ -i & -6 & 2 \end{pmatrix}}.$$

$$\mathsf{B}\mathsf{B}^{-1} = \frac{1}{3}\begin{pmatrix} (4+0-1) & (-6i+0+6i) & (2i+0-2i) \\ (0+0+0) & (0+3+0) & (0+0+0) \\ (2i+0-2i) & (3+9-12) & (-1+0+4) \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad \checkmark$$

$\det \mathsf{A} = 0 + 6i + 4 - 0 - 6i - 4 = 0.$ $\boxed{\text{No;}}$ A does *not* have an inverse.

Problem A.9

(a)

$$\begin{pmatrix} -i+2i+2i \\ 2i+0+6 \\ -2+4+4 \end{pmatrix} = \boxed{\begin{pmatrix} 3i \\ 6+2i \\ 6 \end{pmatrix}}.$$

(b)

$$\begin{pmatrix} -i & -2i & 2 \end{pmatrix}\begin{pmatrix} 2 \\ 1-i \\ 0 \end{pmatrix} = -2i - 2i(1-i) + 0 = \boxed{-2-4i.}$$

(c)

$$\begin{pmatrix} i & 2i & 2 \end{pmatrix}\begin{pmatrix} 2 & 0 & -i \\ 0 & 1 & 0 \\ i & 3 & 2 \end{pmatrix}\begin{pmatrix} 2 \\ 1-i \\ 0 \end{pmatrix} = \begin{pmatrix} i & 2i & 2 \end{pmatrix}\begin{pmatrix} 4 \\ 1-i \\ 3-i \end{pmatrix} = 4i + 2i(1-i) + 2(3-i) = \boxed{8+4i.}$$

(d)

$$\begin{pmatrix} i \\ 2i \\ 2 \end{pmatrix}\begin{pmatrix} 2 & (1+i) & 0 \end{pmatrix} = \boxed{\begin{pmatrix} 2i & (-1+i) & 0 \\ 4i & (-2+2i) & 0 \\ 4 & (2+2i) & 0 \end{pmatrix}}.$$

Problem A.10

(a) $\boxed{\mathsf{S} = \frac{1}{2}(\mathsf{T} + \tilde{\mathsf{T}});}$ $\boxed{\mathsf{A} = \frac{1}{2}(\mathsf{T} - \tilde{\mathsf{T}}).}$

(b) $\boxed{\mathsf{R} = \frac{1}{2}(\mathsf{T} + \mathsf{T}^*);}$ $\boxed{\mathsf{M} = \frac{1}{2}(\mathsf{T} - \mathsf{T}^*).}$

(c) $\boxed{\mathsf{H} = \frac{1}{2}(\mathsf{T} + \mathsf{T}^\dagger);}$ $\boxed{\mathsf{K} = \frac{1}{2}(\mathsf{T} - \mathsf{T}^\dagger).}$

Problem A.11

$$
\begin{aligned}
(\widetilde{\mathsf{ST}})_{ki} &= (\mathsf{ST})_{ik} = \sum_{j=1}^{n} S_{ij}T_{jk} = \sum_{j=1}^{n} \tilde{T}_{kj}\tilde{S}_{ji} = (\tilde{\mathsf{T}}\tilde{\mathsf{S}})_{ki} \;\Rightarrow\; \widetilde{\mathsf{ST}} = \tilde{\mathsf{T}}\tilde{\mathsf{S}}. \quad \text{QED} \\
(\mathsf{ST})^\dagger &= (\widetilde{\mathsf{ST}})^* = (\tilde{\mathsf{T}}\tilde{\mathsf{S}})^* = \tilde{\mathsf{T}}^*\tilde{\mathsf{S}}^* = \mathsf{T}^\dagger\mathsf{S}^\dagger. \quad \text{QED} \\
(\mathsf{T}^{-1}\mathsf{S}^{-1})(\mathsf{ST}) &= \mathsf{T}^{-1}(\mathsf{S}^{-1}\mathsf{S})\mathsf{T} = \mathsf{T}^{-1}\mathsf{T} = \mathsf{I} \quad\Rightarrow\; (\mathsf{ST})^{-1} = \mathsf{T}^{-1}\mathsf{S}^{-1}. \quad \text{QED} \\
\mathsf{U}^\dagger &= \mathsf{U}^{-1},\ \mathsf{W}^\dagger = \mathsf{W}^{-1} \;\Rightarrow (\mathsf{WU})^\dagger = \mathsf{U}^\dagger\mathsf{W}^\dagger = \mathsf{U}^{-1}\mathsf{W}^{-1} = (\mathsf{WU})^{-1} \Rightarrow \mathsf{WU} \text{ is unitary.} \\
\mathsf{H} &= \mathsf{H}^\dagger,\ \mathsf{J} = \mathsf{J}^\dagger \;\Rightarrow (\mathsf{HJ})^\dagger = \mathsf{J}^\dagger\mathsf{H}^\dagger = \mathsf{JH}; \\
&\quad \text{the product is hermitian } \Leftrightarrow \text{this is } \mathsf{HJ}, \text{ i.e.} \Leftrightarrow \boxed{[\mathsf{H},\mathsf{J}] = 0} \text{ (they } \textit{commute}\text{).} \\
(\mathsf{U}+\mathsf{W})^\dagger &= \mathsf{U}^\dagger + \mathsf{W}^\dagger = \mathsf{U}^{-1} + \mathsf{W}^{-1} \stackrel{?}{=} (\mathsf{U}+\mathsf{W})^{-1}. \quad \boxed{\text{No;}} \text{ the sum of two unitary matrices is } \textit{not} \text{ unitary.} \\
(\mathsf{H}+\mathsf{J})^\dagger &= \mathsf{H}^\dagger + \mathsf{J}^\dagger = \mathsf{H}+\mathsf{J}. \; \boxed{\text{Yes;}} \text{ the sum of two hermitian matrices } \textit{is} \text{ hermitian.}
\end{aligned}
$$

Problem A.12

$$\mathsf{U}^\dagger\mathsf{U} = \mathsf{I} \quad\Longrightarrow\quad (\mathsf{U}^\dagger\mathsf{U})_{ik} = \delta_{ik} \Longrightarrow \sum_{j=1}^{n} U^\dagger_{ij}U_{jk} = \sum_{j=1}^{n} U^*_{ji}U_{jk} = \delta_{ik}.$$

Construct the set of n vectors $a^{(j)}{}_i \equiv U_{ij}$ ($\mathsf{a}^{(j)}$ is the j-th column of U; its i-th component is U_{ij}). Then

$$\mathsf{a}^{(i)\dagger}\mathsf{a}^{(k)} = \sum_{j=1}^{n} a^{(i)}{}^*_j\, a^{(k)}{}_j = \sum_{j=1}^{n} U^*_{ji}U_{jk} = \delta_{ik},$$

so these vectors are orthonormal. Similarly,

$$\mathsf{U}\mathsf{U}^\dagger = \mathsf{I} \quad\Longrightarrow\quad (\mathsf{U}\mathsf{U}^\dagger)_{ik} = \delta_{ik} \quad\Longrightarrow\quad \sum_{j=1}^{n} U_{ij}U^\dagger_{jk} = \sum_{j=1}^{n} U^*_{kj}U_{ij} = \delta_{ki}.$$

This time let the vectors $\mathsf{b}^{(j)}$ be the *rows* of U: $b^{(j)}{}_i \equiv U_{ji}$. Then

$$\mathsf{b}^{(k)\dagger}\mathsf{b}^{(i)} = \sum_{j=1}^{n} b^{(k)}{}^*_j\, b^{(i)}{}_j = \sum_{j=1}^{n} U^*_{kj}U_{ij} = \delta_{ki},$$

so the rows are also orthonormal.

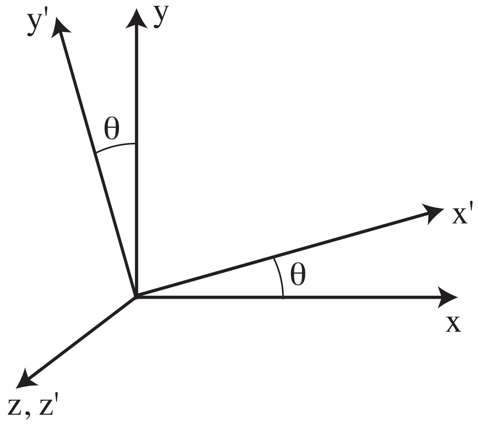
Problem A.13

$$
\begin{aligned}
\mathsf{H}^\dagger &= \mathsf{H} \text{ (hermitian)} \Rightarrow \det\mathsf{H} = \det(\mathsf{H}^\dagger) = \det(\tilde{\mathsf{H}}^*) = (\det\tilde{\mathsf{H}})^* = (\det\mathsf{H})^* \;\Rightarrow \det\mathsf{H} \text{ is real.} \quad \checkmark \\
\mathsf{U}^\dagger &= \mathsf{U}^{-1} \text{ (unitary)} \Rightarrow \det(\mathsf{U}\mathsf{U}^\dagger) = (\det\mathsf{U})(\det\mathsf{U}^\dagger) = (\det\mathsf{U})(\det\tilde{\mathsf{U}})^* = |\det\mathsf{U}|^2 = \det\mathsf{I} = 1, \text{ so } |\det\mathsf{U}| = 1. \quad \checkmark \\
\tilde{\mathsf{S}} &= \mathsf{S}^{-1} \text{ (orthogonal)} \Rightarrow \det(\mathsf{S}\tilde{\mathsf{S}}) = (\det\mathsf{S})(\det\tilde{\mathsf{S}}) = (\det\mathsf{S})^2 = 1, \text{ so } \det\mathsf{S} = \pm 1. \quad \checkmark
\end{aligned}
$$

Problem A.14

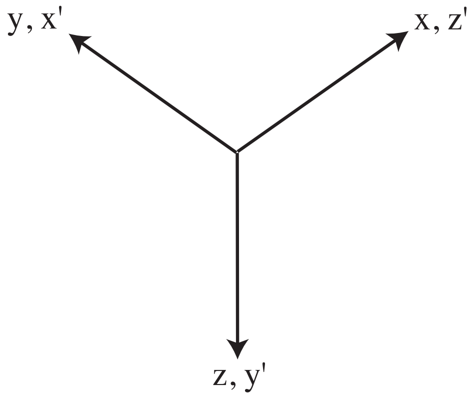
(a)

$$\hat{\imath}' = \cos\theta\,\hat{\imath} + \sin\theta\,\hat{\jmath}; \quad \hat{\jmath}' = -\sin\theta\,\hat{\imath} + \cos\theta\,\hat{\jmath}; \quad \hat{k}' = \hat{k}. \quad \boxed{\mathsf{T}_a = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.}$$



(b)

$$\hat{\imath}' = \hat{\jmath}; \quad \hat{\jmath}' = \hat{k}; \quad \hat{k}' = \hat{\imath}. \quad \boxed{\mathsf{T}_b = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.}$$



(c)

$$\hat{\imath}' = \hat{\imath}; \quad \hat{\jmath}' = \hat{\jmath}; \quad \hat{k}' = -\hat{k}. \quad \boxed{\mathsf{T}_c = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.}$$

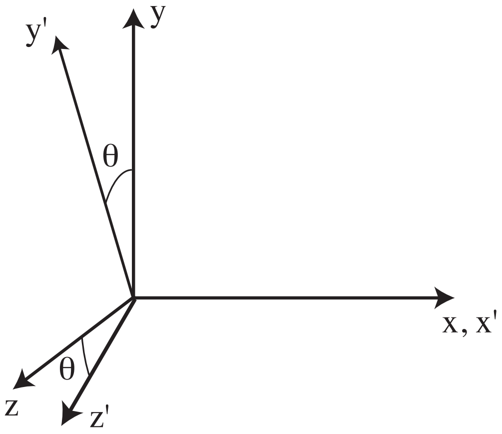
(d)

$$\tilde{\mathsf{T}}_a \mathsf{T}_a = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad \checkmark$$

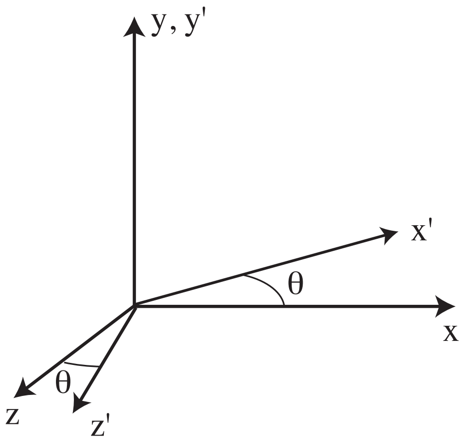
$$\tilde{\mathsf{T}}_b \mathsf{T}_b = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad \checkmark \quad \tilde{\mathsf{T}}_c \mathsf{T}_c = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad \checkmark$$

$$\det \mathsf{T}_a = \cos^2\theta + \sin^2\theta = \boxed{1.} \quad \det \mathsf{T}_b = \boxed{1.} \quad \det \mathsf{T}_c = \boxed{\text{-1.}}$$

Problem A.15



$$\hat{\imath}' = \hat{\imath}; \quad \hat{\jmath}' = \cos\theta\,\hat{\jmath} + \sin\theta\,\hat{k}; \quad \hat{k}' = \cos\theta\,\hat{k} - \sin\theta\,\hat{\jmath}. \quad \boxed{\mathsf{T}_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}.}$$



$$\hat{\imath}' = \cos\theta\,\hat{\imath} - \sin\theta\,\hat{k}; \quad \hat{\jmath}' = \hat{\jmath}; \quad \hat{k}' = \cos\theta\,\hat{k} + \sin\theta\,\hat{\imath}. \quad \boxed{\mathsf{T}_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}.}$$

$$\hat{\imath} = -\hat{\jmath}'; \quad \hat{\jmath} = \hat{\imath}'; \quad \hat{k} = \hat{k}', \quad \text{so (Eq. A.61)} \quad \boxed{\mathsf{S} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix};} \quad \mathsf{S}^{-1} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

$$\begin{aligned} \mathsf{ST}_x\mathsf{S}^{-1} &= \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & -1 & 0 \\ \cos\theta & 0 & -\sin\theta \\ \sin\theta & 0 & \cos\theta \end{pmatrix} = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix} = \mathsf{T}_y(-\theta). \end{aligned}$$

$$\begin{aligned} \mathsf{ST}_y\mathsf{S}^{-1} &= \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & -\cos\theta & \sin\theta \\ 1 & 0 & 0 \\ 0 & \sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} = \mathsf{T}_x(\theta). \end{aligned}$$

Is this what we would expect? Yes, for rotation about the x axis now means rotation about the $-y'$ axis, and rotation about the y axis has become rotation about the x' axis.

Problem A.16

From Eq. A.64 we have

$$\mathsf{A}^f\mathsf{B}^f = \mathsf{SA}^e\mathsf{S}^{-1}\mathsf{SB}^e\mathsf{S}^{-1} = \mathsf{S}(\mathsf{A}^e\mathsf{B}^e)\mathsf{S}^{-1} = \mathsf{SC}^e\mathsf{S}^{-1} = \mathsf{C}^f. \quad \checkmark$$

Suppose $\mathsf{S}^\dagger = \mathsf{S}^{-1}$ and $\mathsf{H}^e = \mathsf{H}^{e\dagger}$ (S unitary, H^e hermitian). Then

$$\mathsf{H}^{f\dagger} = (\mathsf{SH}^e\mathsf{S}^{-1})^\dagger = (\mathsf{S}^{-1})^\dagger\mathsf{H}^{e\dagger}\mathsf{S}^\dagger = \mathsf{SH}^e\mathsf{S}^{-1} = \mathsf{H}^f, \text{ so } \mathsf{H}^f \text{ is hermitian.} \quad \checkmark$$

In an orthonormal basis, $\langle\alpha|\beta\rangle = \mathsf{a}^\dagger\mathsf{b}$ (Eq. A.50). So if $\{|f_i\rangle\}$ is orthonormal, $\langle\alpha|\beta\rangle = \mathsf{a}^{f\dagger}\mathsf{b}^f$. But $\mathsf{b}^f = \mathsf{Sb}^e$ (Eq. A.63), and also $\mathsf{a}^{f\dagger} = \mathsf{a}^{e\dagger}\mathsf{S}^\dagger$. So $\langle\alpha|\beta\rangle = \mathsf{a}^{e\dagger}\mathsf{S}^\dagger\mathsf{Sb}^e$. This is equal to $\mathsf{a}^{e\dagger}\mathsf{b}^e$ (and hence $\{|e_i\rangle\}$ is also orthonormal), for all vectors $|\alpha\rangle$ and $|\beta\rangle \Leftrightarrow \mathsf{S}^\dagger\mathsf{S} = \mathsf{I}$, i.e. S is unitary.

Problem A.17

$$\mathrm{Tr}(\mathsf{T}_1\mathsf{T}_2) = \sum_{i=1}^n(\mathsf{T}_1\mathsf{T}_2)_{ii} = \sum_{i=1}^n\sum_{j=1}^n(\mathsf{T}_1)_{ij}(\mathsf{T}_2)_{ji} = \sum_{j=1}^n\sum_{i=1}^n(\mathsf{T}_2)_{ji}(\mathsf{T}_1)_{ij} = \sum_{j=1}^n(\mathsf{T}_2\mathsf{T}_1)_{jj} = \mathrm{Tr}(\mathsf{T}_2\mathsf{T}_1).$$

Is $\mathrm{Tr}(\mathsf{T}_1\mathsf{T}_2\mathsf{T}_3) = \mathrm{Tr}(\mathsf{T}_2\mathsf{T}_1\mathsf{T}_3)$? $\boxed{\text{No.}}$ Counterexample:

$$\mathsf{T}_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \mathsf{T}_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \mathsf{T}_3 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

$$\mathsf{T}_1\mathsf{T}_2\mathsf{T}_3 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \implies \mathrm{Tr}(\mathsf{T}_1\mathsf{T}_2\mathsf{T}_3) = 1.$$

$$\mathsf{T}_2\mathsf{T}_1\mathsf{T}_3 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \implies \mathrm{Tr}(\mathsf{T}_2\mathsf{T}_1\mathsf{T}_3) = 0.$$

Problem A.18

Eigenvalues:

$$\begin{vmatrix} (\cos\theta-\lambda) & -\sin\theta \\ \sin\theta & (\cos\theta-\lambda) \end{vmatrix} = (\cos\theta-\lambda)^2+\sin^2\theta = \cos^2\theta - 2\lambda\cos\theta+\lambda^2+\sin^2\theta = 0, \text{ or } \lambda^2-2\lambda\cos\theta+1=0.$$

$$\lambda = \frac{2\cos\theta \pm \sqrt{4\cos^2\theta-4}}{2} = \cos\theta \pm \sqrt{-\sin^2\theta} = \cos\theta \pm i\sin\theta = \boxed{e^{\pm i\theta}.}$$

So there are two eigenvalues, both of them complex. Only if $\sin\theta = 0$ does this matrix possess *real* eigenvalues, i.e., only if $\boxed{\theta = 0 \text{ or } \pi.}$

Eigenvectors:

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = e^{\pm i\theta}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \Longrightarrow \cos\theta\,\alpha - \sin\theta\,\beta = (\cos\theta \pm i\sin\theta)\alpha \Rightarrow \beta = \mp i\alpha. \quad \text{Normalizing:}$$

$$\boxed{\mathsf{a}^{(1)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}; \quad \mathsf{a}^{(2)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}.}$$

Diagonalization:

$$(\mathsf{S}^{-1})_{11} = a_1^{(1)} = \frac{1}{\sqrt{2}}; \quad (\mathsf{S}^{-1})_{12} = a_1^{(2)} = \frac{1}{\sqrt{2}}; \quad (\mathsf{S}^{-1})_{21} = a_2^{(1)} = \frac{-i}{\sqrt{2}}; \quad (\mathsf{S}^{-1})_{22} = a_2^{(2)} = \frac{i}{\sqrt{2}}.$$

$$\mathsf{S}^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}; \quad \text{inverting:} \quad \mathsf{S} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}.$$

$$\begin{aligned}\mathsf{STS}^{-1} &= \frac{1}{2}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}\begin{pmatrix} (\cos\theta+i\sin\theta) & (\cos\theta-i\sin\theta) \\ (\sin\theta-i\cos\theta) & (\sin\theta+i\cos\theta) \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}\begin{pmatrix} e^{i\theta} & e^{-i\theta} \\ -ie^{i\theta} & ie^{-i\theta} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2e^{i\theta} & 0 \\ 0 & 2e^{-i\theta} \end{pmatrix} = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}. \quad \checkmark\end{aligned}$$

Problem A.19

$$\begin{vmatrix} (1-\lambda) & 1 \\ 0 & (1-\lambda) \end{vmatrix} = (1-\lambda)^2 = 0 \Longrightarrow \boxed{\lambda = 1} \quad \text{(only one eigenvalue).}$$

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \Longrightarrow \alpha+\beta = \alpha \Longrightarrow \beta = 0; \quad \boxed{\mathsf{a} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}}$$

(only one eigenvector—up to an arbitrary constant factor). Since the eigenvectors do not span the space, this matrix $\boxed{\text{cannot be diagonalized.}}$ [If it *could* be diagonalized, the diagonal form would have to be $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, since the only eigenvalue is 1. But in that case $\mathsf{I} = \mathsf{SMS}^{-1}$. Multiplying from the left by S^{-1} and on the right by S: $\quad \mathsf{S}^{-1}\mathsf{IS} = \mathsf{S}^{-1}\mathsf{SMS}^{-1}\mathsf{S} = \mathsf{M}$. But $\mathsf{S}^{-1}\mathsf{IS} = \mathsf{S}^{-1}\mathsf{S} = \mathsf{I}$. So $\mathsf{M} = \mathsf{I}$, which is false.]

Problem A.20

Expand the determinant (Eq. A.72) by minors, using the first column:

$$\det(\mathsf{T}-\lambda 1) = (T_{11}-\lambda)\begin{vmatrix} (T_{22}-\lambda) & \dots & \dots \\ \vdots & \ddots & \\ \vdots & & (T_{nn}-\lambda) \end{vmatrix} + \sum_{j=2}^{n} T_{j1}\,\text{cofactor}(T_{j1}).$$

But the cofactor of T_{j1} (for $j > 1$) is missing *two* of the original diagonal elements: $(T_{11}-\lambda)$ (from the first column), and $(T_{jj}-\lambda)$ (from the j-th row). So its highest power of λ will be $(n-2)$. Thus terms in λ^n and λ^{n-1} come exclusively from the first term above. Indeed, the same argument applied now to the cofactor of $(T_{11}-\lambda)$ – and repeated as we expand *that* determinant – shows that *only the product of the diagonal elements* contributes to λ^n and λ^{n-1}:

$$(T_{11}-\lambda)(T_{22}-\lambda)\cdots(T_{nn}-\lambda) = (-\lambda)^n + (-\lambda)^{n-1}(T_{11}+T_{22}+\cdots+T_{nn}) + \cdots$$

Evidently then, $C_n = (-1)^n$, and $C_{n-1} = (-1)^{n-1}\,\text{Tr}(\mathsf{T})$. To get C_0 – the term with *no* factors of λ – we simply set $\lambda = 0$. Thus $C_0 = \det(\mathsf{T})$. For a 3×3 matrix:

$$\begin{aligned}
&\begin{vmatrix} (T_{11}-\lambda) & T_{12} & T_{13} \\ T_{21} & (T_{22}-\lambda) & T_{23} \\ T_{31} & T_{32} & (T_{33}-\lambda) \end{vmatrix} \\
&= (T_{11}-\lambda)(T_{22}-\lambda)(T_{33}-\lambda) + T_{12}T_{23}T_{31} + T_{13}T_{21}T_{32} \\
&\quad - T_{31}T_{13}(T_{22}-\lambda) - T_{32}T_{23}(T_{11}-\lambda) - T_{12}T_{21}(T_{33}-\lambda) \\
&= -\lambda^3 + \lambda^2(T_{11}+T_{22}+T_{33}) - \lambda(T_{11}T_{22}+T_{11}T_{33}+T_{22}T_{33}) + \lambda(T_{13}T_{31}+T_{23}T_{32}+T_{12}T_{21}) \\
&\quad + T_{11}T_{22}T_{33} + T_{12}T_{23}T_{31} + T_{13}T_{21}T_{32} - T_{31}T_{13}T_{22} - T_{32}T_{23}T_{11} - T_{12}T_{21}T_{33} \\
&= -\lambda^3 + \lambda^2\,\text{Tr}(\mathsf{T}) + \lambda C_1 + \det(\mathsf{T}), \quad \text{with}
\end{aligned}$$

$$\boxed{C_1 = (T_{13}T_{31}+T_{23}T_{32}+T_{12}T_{21}) - (T_{11}T_{22}+T_{11}T_{33}+T_{22}T_{33}).}$$

Problem A.21

The characteristic equation is an n-th order polynomial, which can be factored in terms of its n (complex) roots:

$$(\lambda_1-\lambda)(\lambda_2-\lambda)\cdots(\lambda_n-\lambda) = (-\lambda)^n + (-\lambda)^{n-1}(\lambda_1+\lambda_2+\cdots+\lambda_n) + \cdots + (\lambda_1\lambda_2\cdots\lambda_n) = 0.$$

Comparing Eq. A.92, it follows that $\text{Tr}(\mathsf{T}) = \lambda_1+\lambda_2+\cdots\lambda_n$ and $\det(\mathsf{T}) = \lambda_1\lambda_2\cdots\lambda_n$. QED

Problem A.22

(a)

$$\mathsf{M}^\dagger = \begin{pmatrix} 1 & 1 \\ 1 & -i \end{pmatrix}; \quad \mathsf{M}\mathsf{M}^\dagger = \begin{pmatrix} 2 & (1-i) \\ (1+i) & 2 \end{pmatrix}, \quad \mathsf{M}^\dagger\mathsf{M} = \begin{pmatrix} 2 & (1+i) \\ (1-i) & 2 \end{pmatrix}; \quad [\mathsf{M},\mathsf{M}^\dagger] = \begin{pmatrix} 0 & -2i \\ 2i & 0 \end{pmatrix} \neq 0. \quad \boxed{\text{No.}}$$

(b) Find the eigenvalues:

$$\begin{vmatrix} (1-\lambda) & 1 \\ 1 & (i-\lambda) \end{vmatrix} = (1-\lambda)(i-\lambda) - 1 = i - \lambda(1+i) + \lambda^2 - 1 = 0;$$

$$\lambda = \frac{(1+i) \pm \sqrt{(1+i)^2 - 4(i-1)}}{2} = \frac{(1+i) \pm \sqrt{4-2i}}{2}.$$

Since there are two distinct eigenvalues, there must be two linearly independent eigenvectors, and that's enough to span the space. So $\boxed{\text{this matrix } \textit{is} \text{ diagonalizable,}}$ even though it is not normal.

Problem A.23

$[\mathsf{T}_1^f, \mathsf{T}_2^f] = \mathsf{T}_1^f\mathsf{T}_2^f - \mathsf{T}_2^f\mathsf{T}_1^f = \mathsf{S}\mathsf{T}_1^e\mathsf{S}^{-1}\mathsf{S}\mathsf{T}_2^e\mathsf{S}^{-1} - \mathsf{S}\mathsf{T}_2^e\mathsf{S}^{-1}\mathsf{S}\mathsf{T}_1^e\mathsf{S}^{-1} = \mathsf{S}\mathsf{T}_1^e\mathsf{T}_2^e\mathsf{S}^{-1} - \mathsf{S}\mathsf{T}_2^e\mathsf{T}_1^e\mathsf{S}^{-1} = \mathsf{S}[\mathsf{T}_1^e, \mathsf{T}_2^e]\mathsf{S}^{-1} = 0.\quad \checkmark$

Problem A.24

$$\begin{aligned}
\mathsf{V}\,\tilde{\mathsf{a}}^{(1)} &= d_{11}\,\mathsf{V}\,\mathsf{a}^{(1)} + d_{21}\,\mathsf{V}\,\mathsf{a}^{(2)} \\
&= d_{11}\left(c_{11}\,\mathsf{a}^{(1)} + c_{21}\,\mathsf{a}^{(2)}\right) + d_{21}\left(c_{12}\,\mathsf{a}^{(1)} + c_{22}\,\mathsf{a}^{(2)}\right) \\
&= (c_{11}\,d_{11} + c_{12}\,d_{21})\ \mathsf{a}^{(1)} + (c_{21}\,d_{11} + c_{22}\,d_{21})\ \mathsf{a}^{(2)} \\
&= \nu_1\,d_{11}\,\mathsf{a}^{(1)} + \nu_1\,d_{21}\,\mathsf{a}^{(2)} = \nu_1\,\tilde{\mathsf{a}}^{(1)}
\end{aligned}$$

(and the same goes for $\tilde{\mathsf{a}}^{(2)}$).

Problem A.25

(a) Since $\mathsf{A}^\dagger = \mathsf{A}$ and $\mathsf{B}^\dagger = \mathsf{B}$, the matrices are clearly normal (Equation A.82), and hence diagonalizable.

$$\begin{aligned}
[\mathsf{A},\mathsf{B}] &= \begin{pmatrix} 1 & 4 & 1 \\ 4 & -2 & 4 \\ 1 & 4 & 1 \end{pmatrix}\begin{pmatrix} 1 & -2 & -1 \\ -2 & 2 & -2 \\ -1 & -2 & 1 \end{pmatrix} - \begin{pmatrix} 1 & -2 & -1 \\ -2 & 2 & -2 \\ -1 & -2 & 1 \end{pmatrix}\begin{pmatrix} 1 & 4 & 1 \\ 4 & -2 & 4 \\ 1 & 4 & 1 \end{pmatrix} \\
&= \begin{pmatrix} -8 & 4 & -8 \\ 4 & -20 & 4 \\ -8 & 4 & -8 \end{pmatrix} - \begin{pmatrix} -8 & 4 & -8 \\ 4 & -20 & 4 \\ -8 & 4 & -8 \end{pmatrix} = 0.\quad \checkmark
\end{aligned}$$

(b) To get the eigenvalues, use the characteristic equation:

$$\begin{aligned}
\det(\mathsf{A} - \lambda 1) &= \begin{vmatrix} 1-\lambda & 4 & 1 \\ 4 & -2-\lambda & 4 \\ 1 & 4 & 1-\lambda \end{vmatrix} = -(1-\lambda)^2(2+\lambda) + 16 + 16 + (2+\lambda) - 16(1-\lambda) - 16(1-\lambda) \\
&= -(1 - 2\lambda + \lambda^2)(2+\lambda) + 2 + 33\lambda = -\lambda^3 + 36\lambda = 0,
\end{aligned}$$

so the eigenvalues are $\boxed{0,\ 6,\ \text{and}\ -6}$ (nondegenerate). As for the eigenvectors:

$$\begin{pmatrix} 1 & 4 & 1 \\ 4 & -2 & 4 \\ 1 & 4 & 1 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \lambda\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \quad \Rightarrow \quad \begin{cases} v_1 + 4v_2 + v_3 = \lambda v_1, \\ 4v_1 - 2v_2 + 4v_3 = \lambda v_2, \\ v_1 + 4v_2 + v_3 = \lambda v_3, \end{cases}$$

(The third equation is redundant, for each of the eigenvalues.)

$$\underline{\lambda = 0} \quad v_1 + 4v_2 + v_3 = 0,\ 4v_1 - 2v_2 + 4v_3 = 0 \quad \Rightarrow \quad v_1 = -v_3,\ v_2 = 0.$$
$$\underline{\lambda = 6} \quad v_1 + 4v_2 + v_3 = 6v_1,\ 4v_1 - 2v_2 + 4v_3 = 6v_2 \quad \Rightarrow \quad v_1 = v_2 = v_3.$$
$$\underline{\lambda = -6} \quad v_1 + 4v_2 + v_3 = -6v_1,\ 4v_1 - 2v_2 + 4v_3 = -6v_2 \quad \Rightarrow \quad v_1 = v_3,\ v_2 = -2v_1.$$

So the (normalized) eigenvectors of A are

$$\boxed{\lambda_1 = 0: \ \mathsf{v}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}} \boxed{\lambda_2 = 6: \ \mathsf{v}_2 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}} \boxed{\lambda_3 = -6: \ \mathsf{v}_3 = \frac{1}{\sqrt{6}}\begin{pmatrix}1\\-2\\1\end{pmatrix}}$$

(c)

$$\mathsf{Bv}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -2 & -1\\-2 & 2 & -2\\-1 & -2 & 1\end{pmatrix}\begin{pmatrix}1\\0\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}2\\0\\-2\end{pmatrix} = 2\mathsf{v}_1,$$
$$\mathsf{Bv}_2 = \frac{1}{\sqrt{3}}\begin{pmatrix}1 & -2 & -1\\-2 & 2 & -2\\-1 & -2 & 1\end{pmatrix}\begin{pmatrix}1\\1\\1\end{pmatrix} = \frac{1}{\sqrt{3}}\begin{pmatrix}-2\\-2\\-2\end{pmatrix} = -2\mathsf{v}_2,$$
$$\mathsf{Bv}_3 = \frac{1}{\sqrt{6}}\begin{pmatrix}1 & -2 & -1\\-2 & 2 & -2\\-1 & -2 & 1\end{pmatrix}\begin{pmatrix}1\\-2\\1\end{pmatrix} = \frac{1}{\sqrt{6}}\begin{pmatrix}4\\-8\\4\end{pmatrix} = 4\mathsf{v}_3.$$

(Evidently the eigenvalues of B are 2, -2, and 4.)

Problem A.26

(a) Since $\mathsf{A}^\dagger = \mathsf{A}$ and $\mathsf{B}^\dagger = \mathsf{B}$, the matrices are normal (Equation A.82), and hence diagonalizable.

$$[\mathsf{A},\mathsf{B}] = \begin{pmatrix}2 & 2 & -1\\2 & -1 & 2\\-1 & 2 & 2\end{pmatrix}\begin{pmatrix}2 & -1 & 2\\-1 & 5 & -1\\2 & -1 & 2\end{pmatrix} - \begin{pmatrix}2 & -1 & 2\\-1 & 5 & -1\\2 & -1 & 2\end{pmatrix}\begin{pmatrix}2 & 2 & -1\\2 & -1 & 2\\-1 & 2 & 2\end{pmatrix}$$
$$= \begin{pmatrix}0 & 9 & 0\\9 & -9 & 9\\0 & 9 & 0\end{pmatrix} - \begin{pmatrix}0 & 9 & 0\\9 & -9 & 9\\0 & 9 & 0\end{pmatrix} = 0. \quad \checkmark$$

(b) To get the eigenvalues, use the characteristic equation:

$$\det(\mathsf{A} - \lambda 1) = \begin{vmatrix}2-\lambda & 2 & -1\\2 & -1-\lambda & 2\\-1 & 2 & 2-\lambda\end{vmatrix} = -(2-\lambda)^2(1+\lambda) - 4 - 4 + (1+\lambda) - 4(2-\lambda) - 4(2-\lambda)$$
$$= -(4 - 4\lambda + \lambda^2)(1+\lambda) - 23 + 9\lambda = -(\lambda+3)(\lambda-3)^2 = 0,$$

so the eigenvalues are $\boxed{\text{3, 3, and -3}}$ (degenerate). As for the eigenvectors:

$$\begin{pmatrix}2 & 2 & -1\\2 & -1 & 2\\-1 & 2 & 2\end{pmatrix}\begin{pmatrix}v_1\\v_2\\v_3\end{pmatrix} = \lambda\begin{pmatrix}v_1\\v_2\\v_3\end{pmatrix} \quad \Rightarrow \quad \begin{cases}2v_1 + 2v_2 - v_3 = \lambda v_1,\\ 2v_1 - v_2 + 2v_3 = \lambda v_2,\\ -v_1 + 2v_2 + 2v_3 = \lambda v_3,\end{cases}$$

(The third equation is redundant, for each of the eigenvalues.)

$$\underline{\lambda = -3} \quad 2v_1 + 2v_2 - v_3 = -3v_1, \; 2v_1 - v_2 + 2v_3 = -3v_2 \quad \Rightarrow \quad v_1 = v_3, \; v_2 = -2v_1.$$
$$\underline{\lambda = 3} \quad 2v_1 + 2v_2 - v_3 = 3v_1, \; 2v_1 - v_2 + 2v_3 = 3v_2 \quad \Rightarrow \quad 2v_2 = v_1 + v_3,$$

but in the latter case there is no condition on v_1 or v_3—*any* vector of the form

$$\mathsf{v} = \begin{pmatrix} 2a \\ a+b \\ 2b \end{pmatrix}$$

is an eigenvector of A, with eigenvalue 3. We might choose the (orthonormal) eigenvectors as follows: So the (normalized) eigenvectors of A are

$$\boxed{\lambda_1 = -3: \; \mathsf{v}_1 = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}} \; \boxed{\lambda_2 = 3: \; \mathsf{v}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}} \; \boxed{\lambda_3 = 3: \; \mathsf{v}_3 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}}$$

(c)

$$\mathsf{Bv}_1 = \frac{1}{\sqrt{6}}\begin{pmatrix} 2 & -1 & 2 \\ -1 & 5 & -1 \\ 2 & -1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{6}}\begin{pmatrix} 6 \\ -12 \\ 6 \end{pmatrix} = 6\,\mathsf{v}_1,$$
$$\mathsf{Bv}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 2 & -1 & 2 \\ -1 & 5 & -1 \\ 2 & -1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = 0\,\mathsf{v}_2,$$
$$\mathsf{Bv}_3 = \frac{1}{\sqrt{3}}\begin{pmatrix} 2 & -1 & 2 \\ -1 & 5 & -1 \\ 2 & -1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{3}}\begin{pmatrix} 3 \\ 3 \\ 3 \end{pmatrix} = 3\,\mathsf{v}_3.$$

I got lucky! It just happens that the v_2 and v_3 I picked *are* also eigenvectors of B (whose eigenvalues are evidently 0, 3, and 6). But the most general eigenvector of A with eigenvalue 3 is *not* an eigenvector of B:

$$\begin{pmatrix} 2 & -1 & 2 \\ -1 & 5 & -1 \\ 2 & -1 & 2 \end{pmatrix}\begin{pmatrix} 2a \\ a+b \\ 2b \end{pmatrix} = \begin{pmatrix} 3(a+b) \\ 3(a+b) \\ 3(a+b) \end{pmatrix} \neq \lambda \begin{pmatrix} 2a \\ a+b \\ 2b \end{pmatrix};$$

the middle line works only if $\lambda = 3$ (in which case the top line requires $a = b$—this is my v_3), or $b = -a$ (this is my v_2).

Problem A.27

Let $|\gamma\rangle = |\alpha\rangle + c|\beta\rangle$, for some complex number c. Then

$$\langle\gamma|\hat{T}\gamma\rangle = \langle\alpha|\hat{T}\alpha\rangle + c\langle\alpha|\hat{T}\beta\rangle + c^*\langle\beta|\hat{T}\alpha\rangle + |c|^2\langle\beta|\hat{T}\beta\rangle, \text{ and}$$
$$\langle\hat{T}\gamma|\gamma\rangle = \langle\hat{T}\alpha|\alpha\rangle + c^*\langle\hat{T}\beta|\alpha\rangle + c\langle\hat{T}\alpha|\beta\rangle + |c|^2\langle\hat{T}\beta|\beta\rangle.$$

Suppose $\langle \hat{T}\gamma|\gamma\rangle = \langle\gamma|\hat{T}\gamma\rangle$ for *all* vectors. For instance, $\langle\hat{T}\alpha|\alpha\rangle = \langle\alpha|\hat{T}\alpha\rangle$ and $\langle\hat{T}\beta|\beta\rangle = \langle\beta|\hat{T}\beta\rangle$), so

$$c\langle\alpha|\hat{T}\beta\rangle + c^*\langle\beta|\hat{T}\alpha\rangle = c\langle\hat{T}\alpha|\beta\rangle + c^*\langle\hat{T}\beta|\alpha\rangle, \text{ and this holds for } any \text{ complex number } \quad c.$$

In particular, for $c = 1$: $\langle\alpha|\hat{T}\beta\rangle + \langle\beta|\hat{T}\alpha\rangle = \langle\hat{T}\alpha|\beta\rangle + \langle\hat{T}\beta|\alpha\rangle$, while for $c = i$: $\langle\alpha|\hat{T}\beta\rangle - \langle\beta|\hat{T}\alpha\rangle = \langle\hat{T}\alpha|\beta\rangle - \langle\hat{T}\beta|\alpha\rangle$. (I canceled the i's). Adding: $\langle\alpha|\hat{T}\beta\rangle = \langle\hat{T}\alpha|\beta\rangle$. QED

Problem A.28

(a)

$$\mathsf{T}^\dagger = \tilde{\mathsf{T}}^* = \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix} = \mathsf{T}. \quad \checkmark$$

(b)

$$\begin{vmatrix} (1-\lambda) & (1-i) \\ (1+i) & (0-\lambda) \end{vmatrix} = -(1-\lambda)\lambda - 1 - 1 = 0;\ \lambda^2 - \lambda - 2 = 0;\ \lambda = \frac{1 \pm \sqrt{1+8}}{2} = \frac{1 \pm 3}{2}. \quad \boxed{\lambda_1 = 2,\ \lambda_2 = -1.}$$

(c)

$$\begin{pmatrix} 1 & (1-i) \\ (1+i) & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 2\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \Longrightarrow \alpha + (1-i)\beta = 2\alpha \Longrightarrow \alpha = (1-i)\beta.$$

$$|\alpha|^2 + |\beta|^2 = 1 \Longrightarrow 2|\beta|^2 + |\beta|^2 = 1 \Longrightarrow \beta = \frac{1}{\sqrt{3}}. \quad \boxed{\mathsf{a}^{(1)} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1-i \\ 1 \end{pmatrix}.}$$

$$\begin{pmatrix} 1 & (1-i) \\ (1+i) & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \Longrightarrow \alpha + (1-i)\beta = -\alpha; \quad \alpha = -\frac{1}{2}(1-i)\beta.$$

$$\frac{1}{4}2|\beta|^2 + |\beta|^2 = 1 \Longrightarrow \frac{3}{2}|\beta|^2 = 1;\ \beta = \sqrt{\frac{2}{3}}. \quad \boxed{\mathsf{a}^{(2)} = \frac{1}{\sqrt{6}}\begin{pmatrix} i-1 \\ 2 \end{pmatrix}.}$$

$$\mathsf{a}^{(1)\dagger}\mathsf{a}^{(2)} = \frac{1}{3\sqrt{2}}\left((1+i)\ \ 1\right)\begin{pmatrix} (i-1) \\ 2 \end{pmatrix} = \frac{1}{3\sqrt{2}}(i - 1 - 1 - i + 2) = 0. \quad \checkmark$$

(d)

$$\text{Eq. A.81} \Longrightarrow (\mathsf{S}^{-1})_{11} = a_1^{(1)} = \frac{1}{\sqrt{3}}(1-i); \quad (\mathsf{S}^{-1})_{12} = a_1^{(2)} = \frac{1}{\sqrt{6}}(i-1);$$

$$(\mathsf{S}^{-1})_{21} = a_2^{(1)} = \frac{1}{\sqrt{3}}; \quad (\mathsf{S}^{-1})_{22} = a_2^{(2)} = \frac{2}{\sqrt{6}}.$$

$$\mathsf{S}^{-1} = \frac{1}{\sqrt{3}}\begin{pmatrix} (1-i) & (i-1)/\sqrt{2} \\ 1 & \sqrt{2} \end{pmatrix}; \quad \mathsf{S} = (\mathsf{S}^{-1})^\dagger = \frac{1}{\sqrt{3}}\begin{pmatrix} (1+i) & 1 \\ (-i-1)/\sqrt{2} & \sqrt{2} \end{pmatrix}.$$

$$\mathsf{STS}^{-1} = \frac{1}{3}\begin{pmatrix} (1+i) & 1 \\ -(1+i)/\sqrt{2} & \sqrt{2} \end{pmatrix}\begin{pmatrix} 1 & (1-i) \\ (1+i) & 0 \end{pmatrix}\begin{pmatrix} (1-i) & (i-1)/\sqrt{2} \\ 1 & \sqrt{2} \end{pmatrix}$$

$$= \frac{1}{3}\begin{pmatrix} (1+i) & 1 \\ -(1+i)/\sqrt{2} & \sqrt{2} \end{pmatrix}\begin{pmatrix} 2(1-i) & (1-i)/\sqrt{2} \\ 2 & -\sqrt{2} \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 6 & 0 \\ 0 & -3 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}. \quad \checkmark$$

(e)

$$\boxed{\mathrm{Tr}(\mathsf{T}) = 1;} \quad \det(\mathsf{T}) = 0 - (1+i)(1-i) = \boxed{-2.} \quad \mathrm{Tr}(\mathsf{STS}^{-1}) = 2 - 1 = 1. \ \checkmark \quad \det(\mathsf{STS}^{-1}) = -2. \ \checkmark$$

Problem A.29

(a)

$$\det(\mathsf{T}) = 8 - 1 - 1 - 2 - 2 - 2 = \boxed{0.} \quad \mathrm{Tr}(\mathsf{T}) = 2 + 2 + 2 = \boxed{6.}$$

(b)

$$\begin{vmatrix} (2-\lambda) & i & 1 \\ -i & (2-\lambda) & i \\ 1 & -i & (2-\lambda) \end{vmatrix} = (2-\lambda)^3 - 1 - 1 - (2-\lambda) - (2-\lambda) - (2-\lambda) = 8 - 12\lambda + 6\lambda^2 - \lambda^3 - 8 + 3\lambda = 0.$$

$$-\lambda^3 + 6\lambda^2 - 9\lambda = -\lambda(\lambda^2 - 6\lambda + 9) = -\lambda(\lambda - 3)^2 = 0. \quad \boxed{\lambda_1 = 0, \ \lambda_2 = \lambda_3 = 3.}$$

$$\lambda_1 + \lambda_2 + \lambda_3 = 6 = \mathrm{Tr}(\mathsf{T}). \ \checkmark \quad \lambda_1\lambda_2\lambda_3 = 0 = \det(\mathsf{T}). \ \checkmark \quad \text{Diagonal form: } \boxed{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3 \end{pmatrix}.}$$

(c)

$$\begin{pmatrix} 2 & i & 1 \\ -i & 2 & i \\ 1 & -i & 2 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = 0 \Longrightarrow \left\{ \begin{array}{l} 2\alpha + i\beta + \gamma = 0 \\ -i\alpha + 2\beta + i\gamma = 0 \Longrightarrow \alpha + 2i\beta - \gamma = 0 \end{array} \right\}.$$

Add the two equations: $3\alpha + 3i\beta = 0 \Longrightarrow \beta = i\alpha$; $\quad 2\alpha - \alpha + \gamma = 0 \Longrightarrow \gamma = -\alpha$.

$$\mathsf{a}^{(1)} = \begin{pmatrix} \alpha \\ i\alpha \\ -\alpha \end{pmatrix}. \quad \text{Normalizing: } |\alpha|^2 + |\alpha|^2 + |\alpha|^2 = 1 \Longrightarrow \alpha = \frac{1}{\sqrt{3}}. \quad \boxed{\mathsf{a}^{(1)} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ i \\ -1 \end{pmatrix}.}$$

$$\begin{pmatrix} 2 & i & 1 \\ -i & 2 & i \\ 1 & -i & 2 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = 3 \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \Longrightarrow \left\{ \begin{array}{ll} 2\alpha + i\beta + \gamma = 3\alpha & \Longrightarrow -\alpha + i\beta + \gamma = 0, \\ -i\alpha + 2\beta + i\gamma = 3\beta & \Longrightarrow \alpha - i\beta - \gamma = 0, \\ \alpha - i\beta + 2\gamma = 3\gamma & \Longrightarrow \alpha - i\beta - \gamma = 0. \end{array} \right.$$

The three equations are redundant – there is only *one* condition here: $\alpha - i\beta - \gamma = 0$. We could pick $\gamma = 0$, $\beta = -i\alpha$, or $\beta = 0$, $\gamma = \alpha$. Then

$$\mathsf{a}_0^{(2)} = \begin{pmatrix} \alpha \\ -i\alpha \\ 0 \end{pmatrix}; \quad \mathsf{a}_0^{(3)} = \begin{pmatrix} \alpha \\ 0 \\ \alpha \end{pmatrix}.$$

But these are not orthogonal, so we use the Gram-Schmidt procedure (Problem A.4); first normalize $\mathsf{a}_0^{(2)}$:

$$\boxed{\mathsf{a}^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}.}$$

$$\mathsf{a}^{(2)\dagger}\mathsf{a}_0^{(3)} = \frac{\alpha}{\sqrt{2}} (1 \ i \ 0) \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \frac{\alpha}{\sqrt{2}}. \quad \text{So} \quad \mathsf{a}_0^{(3)} - (\mathsf{a}^{(2)\dagger}\mathsf{a}_0^{(3)})\,\mathsf{a}^{(2)} = \alpha \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} - \frac{\alpha}{2} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix} = \alpha \begin{pmatrix} 1/2 \\ i/2 \\ 1 \end{pmatrix}.$$

Normalize: $|\alpha|^2\left(\frac{1}{4}+\frac{1}{4}+1\right)=\frac{3}{2}|\alpha|^2=1 \implies \alpha=\sqrt{\frac{2}{3}}.$ $\boxed{\mathsf{a}^{(3)}=\frac{1}{\sqrt{6}}\begin{pmatrix}1\\ i\\ 2\end{pmatrix}.}$

Check orthogonality:

$$\mathsf{a}^{(1)\dagger}\mathsf{a}^{(2)}=\frac{1}{\sqrt{6}}\begin{pmatrix}1 & -i & -1\end{pmatrix}\begin{pmatrix}1\\ -i\\ 0\end{pmatrix}=\frac{1}{\sqrt{6}}(1-1+0)=0. \quad \checkmark$$

$$\mathsf{a}^{(1)\dagger}\mathsf{a}^{(3)}=\frac{1}{3\sqrt{2}}\begin{pmatrix}1 & -i & -1\end{pmatrix}\begin{pmatrix}1\\ i\\ 2\end{pmatrix}=\frac{1}{3\sqrt{2}}(1+1-2)=0. \quad \checkmark$$

(d) S^{-1} is the matrix whose columns are the eigenvectors of T (Eq. A.81):

$$\mathsf{S}^{-1}=\frac{1}{\sqrt{6}}\begin{pmatrix}\sqrt{2} & \sqrt{3} & 1\\ \sqrt{2}\,i & -\sqrt{3}\,i & i\\ -\sqrt{2} & 0 & 2\end{pmatrix}; \quad \mathsf{S}=(\mathsf{S}^{-1})^\dagger=\boxed{\frac{1}{\sqrt{6}}\begin{pmatrix}\sqrt{2} & -\sqrt{2}\,i & -\sqrt{2}\\ \sqrt{3} & \sqrt{3}\,i & 0\\ 1 & -i & 2\end{pmatrix}.}$$

$$\mathsf{STS}^{-1}=\frac{1}{6}\begin{pmatrix}\sqrt{2} & -\sqrt{2}\,i & -\sqrt{2}\\ \sqrt{3} & \sqrt{3}\,i & 0\\ 1 & -i & 2\end{pmatrix}\underbrace{\begin{pmatrix}2 & i & 1\\ -i & 2 & i\\ 1 & -i & 2\end{pmatrix}\begin{pmatrix}\sqrt{2} & \sqrt{3} & 1\\ \sqrt{2}\,i & -\sqrt{3}\,i & i\\ -\sqrt{2} & 0 & 2\end{pmatrix}}_{\begin{pmatrix}0 & 3\sqrt{3} & 3\\ 0 & -3\sqrt{3}\,i & 3i\\ 0 & 0 & 6\end{pmatrix}}=\frac{1}{6}\begin{pmatrix}0 & 0 & 0\\ 0 & 18 & 0\\ 0 & 0 & 18\end{pmatrix}=\begin{pmatrix}0 & 0 & 0\\ 0 & 3 & 0\\ 0 & 0 & 3\end{pmatrix}. \quad \checkmark$$

Problem A.30

(a) $\langle \hat{U}\alpha|\hat{U}\beta\rangle=\langle \hat{U}^\dagger\hat{U}\alpha|\beta\rangle=\langle\alpha|\beta\rangle. \quad \checkmark$

(b) $\hat{U}|\alpha\rangle=\lambda|\alpha\rangle \implies \langle\hat{U}\alpha|\hat{U}\alpha\rangle=|\lambda|^2\langle\alpha|\alpha\rangle$. But from (a) this is also $\langle\alpha|\alpha\rangle$. So $|\lambda|=1$. $\checkmark$

(c) $\hat{U}|\alpha\rangle=\lambda|\alpha\rangle,\ \hat{U}|\beta\rangle=\mu|\beta\rangle \implies |\beta\rangle=\mu\hat{U}^{-1}|\beta\rangle$, so $\hat{U}^\dagger|\beta\rangle=\frac{1}{\mu}|\beta\rangle=\mu^*|\beta\rangle$ (from (b)).

$\langle\beta|\hat{U}\alpha\rangle=\lambda\langle\beta|\alpha\rangle=\langle\hat{U}^\dagger\beta|\alpha\rangle=\mu\langle\beta|\alpha\rangle$, or $(\lambda-\mu)\langle\beta|\alpha\rangle=0$. So if $\lambda\neq\mu$, then $\langle\beta|\alpha\rangle=0$. QED

Problem A.31

(a) (i)

$$\mathsf{M}^2=\begin{pmatrix}0 & 0 & 4\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}; \quad \mathsf{M}^3=\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \quad \text{so}$$

$$e^{\mathsf{M}}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}+\begin{pmatrix}0 & 1 & 3\\ 0 & 0 & 4\\ 0 & 0 & 0\end{pmatrix}+\frac{1}{2}\begin{pmatrix}0 & 0 & 4\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}=\boxed{\begin{pmatrix}1 & 1 & 5\\ 0 & 1 & 4\\ 0 & 0 & 1\end{pmatrix}.}$$

(ii)

$$\mathsf{M}^2 = \begin{pmatrix} -\theta^2 & 0 \\ 0 & -\theta^2 \end{pmatrix} = -\theta^2 \mathsf{I}; \quad \mathsf{M}^3 = -\theta^2 \mathsf{M}; \quad \mathsf{M}^4 = \theta^4 \mathsf{I}; \quad \text{etc.}$$

$$\begin{aligned} e^{\mathsf{M}} &= \mathsf{I} + \theta \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} - \frac{1}{2}\theta^2 \mathsf{I} - \frac{\theta^3}{3!} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + \frac{\theta^4}{4!} \mathsf{I} + \cdots \\ &= \left(1 - \frac{\theta^2}{2} + \frac{\theta^4}{4!} - \cdots \right) \mathsf{I} + \left(\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \cdots \right) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\ &= \cos\theta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sin\theta \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \boxed{\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}.} \end{aligned}$$

(b)

$$\mathsf{SMS}^{-1} = \mathsf{D} = \begin{pmatrix} d_1 & & 0 \\ & \ddots & \\ 0 & & d_n \end{pmatrix} \text{ for some } \mathsf{S}.$$

$$\mathsf{S}e^{\mathsf{M}}\mathsf{S}^{-1} = \mathsf{S}\left(\mathsf{I} + \mathsf{M} + \frac{1}{2}\mathsf{M}^2 + \frac{1}{3!}\mathsf{M}^3 + \cdots \right)\mathsf{S}^{-1}. \quad \text{Insert } \mathsf{SS}^{-1} = \mathsf{I}:$$

$$\begin{aligned} \mathsf{S}e^{\mathsf{M}}\mathsf{S}^{-1} &= \mathsf{I} + \mathsf{SMS}^{-1} + \frac{1}{2}\mathsf{SMS}^{-1}\mathsf{SMS}^{-1} + \frac{1}{3!}\mathsf{SMS}^{-1}\mathsf{SMS}^{-1}\mathsf{SMS}^{-1} + \cdots \\ &= \mathsf{I} + \mathsf{D} + \frac{1}{2}\mathsf{D}^2 + \frac{1}{3!}\mathsf{D}^3 + \cdots = e^{\mathsf{D}}. \quad \text{Evidently} \end{aligned}$$

$$\det(e^{\mathsf{D}}) = \det(\mathsf{S}e^{\mathsf{M}}\mathsf{S}^{-1}) = \det(\mathsf{S})\det(e^{\mathsf{M}})\det(\mathsf{S}^{-1}) = \det(e^{\mathsf{M}}). \quad \text{But}$$

$$\mathsf{D}^2 = \begin{pmatrix} d_1^2 & & 0 \\ & \ddots & \\ 0 & & d_n^2 \end{pmatrix}, \quad \mathsf{D}^3 = \begin{pmatrix} d_1^3 & & 0 \\ & \ddots & \\ 0 & & d_n^3 \end{pmatrix}, \quad \mathsf{D}^k = \begin{pmatrix} d_1^k & & 0 \\ & \ddots & \\ 0 & & d_n^k \end{pmatrix}, \quad \text{so}$$

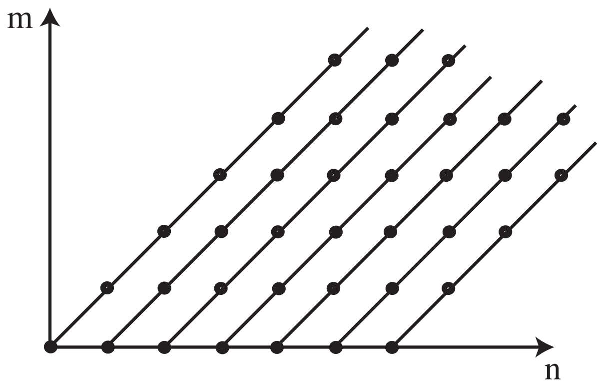
$$e^{\mathsf{D}} = \mathsf{I} + \begin{pmatrix} d_1 & & 0 \\ & \ddots & \\ 0 & & d_n \end{pmatrix} + \frac{1}{2}\begin{pmatrix} d_1^2 & & 0 \\ & \ddots & \\ 0 & & d_n^2 \end{pmatrix} + \frac{1}{3!}\begin{pmatrix} d_1^3 & & 0 \\ & \ddots & \\ 0 & & d_n^3 \end{pmatrix} + \cdots = \begin{pmatrix} e^{d_1} & & 0 \\ & \ddots & \\ 0 & & e^{d_n} \end{pmatrix}.$$

$$\det(e^{\mathsf{D}}) = e^{d_1}e^{d_2}\cdots e^{d_n} = e^{(d_1+d_2+\cdots d_n)} = e^{\operatorname{Tr}\mathsf{D}} = e^{\operatorname{Tr}\mathsf{M}} \text{ (Eq. A.68), so } \det(e^{\mathsf{M}}) = e^{\operatorname{Tr}\mathsf{M}}. \quad \text{QED}$$

(c) Matrices that *commute* obey the same algebraic rules as ordinary *numbers*, so the standard proofs of $e^{x+y} = e^x e^y$ will do the job. Here are two:

(i) Combinatorial Method: Use the binomial theorem (valid if multiplication is commutative):

$$e^{\mathsf{M}+\mathsf{N}} = \sum_{n=0}^{\infty} \frac{1}{n!}(\mathsf{M}+\mathsf{N})^n = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{m=0}^{n} \binom{n}{m} \mathsf{M}^m \mathsf{N}^{n-m} = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{1}{m!(n-m)!} \mathsf{M}^m \mathsf{N}^{n-m}.$$



Instead of summing *vertically* first, for fixed n ($m : 0 \to n$), sum *horizontally* first, for fixed m ($n : m \to \infty$, or $k \equiv n - m : 0 \to \infty$)—see diagram (each dot represents a term in the double sum).

$$e^{\mathsf{M}+\mathsf{N}} = \sum_{m=0}^{\infty} \frac{1}{m!}\mathsf{M}^m \sum_{k=0}^{\infty} \frac{1}{k!}\mathsf{N}^k = e^{\mathsf{M}}e^{\mathsf{N}}. \quad \text{QED}$$

(ii) Analytic Method: Let

$$\mathsf{S}(\lambda) \equiv e^{\lambda\mathsf{M}}e^{\lambda\mathsf{N}}; \quad \frac{d\mathsf{S}}{d\lambda} = \mathsf{M}e^{\lambda\mathsf{M}}e^{\lambda\mathsf{N}} + e^{\lambda\mathsf{M}}\mathsf{N}e^{\lambda\mathsf{N}} = (\mathsf{M}+\mathsf{N})e^{\lambda\mathsf{M}}e^{\lambda\mathsf{N}} = (\mathsf{M}+\mathsf{N})\mathsf{S}.$$

(The second equality, in which we pull N through $e^{\lambda\mathsf{M}}$, would not hold if M and N did not commute.) Solving the differential equation: $\mathsf{S}(\lambda) = Ae^{(\mathsf{M}+\mathsf{N})\lambda}$, for some constant A. But $\mathsf{S}(0) = \mathsf{I}$, so $A = 1$, and hence $e^{\lambda\mathsf{M}}e^{\lambda\mathsf{N}} = e^{\lambda(\mathsf{M}+\mathsf{N})}$, and (setting $\lambda = 1$) we conclude that $e^{\mathsf{M}}e^{\mathsf{N}} = e^{(\mathsf{M}+\mathsf{N})}$. [This method generalizes most easily when M and N do *not* commute—leading to the famous Baker-Campbell-Hausdorf lemma.]

As a counterexample when $[\mathsf{M},\mathsf{N}] \neq 0$, let $\mathsf{M} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $\mathsf{N} = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}$. Then $\mathsf{M}^2 = \mathsf{N}^2 = 0$, so

$$e^{\mathsf{M}} = \mathsf{I} + \mathsf{M} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \; e^{\mathsf{N}} = \mathsf{I} + \mathsf{N} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}; \quad e^{\mathsf{M}}e^{\mathsf{N}} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix}.$$

$$\text{But } (\mathsf{M}+\mathsf{N}) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \text{ so (from a(ii)): } e^{\mathsf{M}+\mathsf{N}} = \begin{pmatrix} \cos(1) & \sin(1) \\ -\sin(1) & \cos(1) \end{pmatrix}.$$

The two are clearly not equal.

(d)

$$e^{i\mathsf{H}} = \sum_{n=0}^{\infty} \frac{1}{n!} i^n \mathsf{H}^n \Longrightarrow (e^{i\mathsf{H}})^\dagger = \sum_{n=0}^{\infty} \frac{1}{n!}(-i)^n(\mathsf{H}^\dagger)^n = \sum_{n=0}^{\infty} \frac{1}{n!}(-i)^n\mathsf{H}^n = e^{-i\mathsf{H}} \text{ (for } \mathsf{H} \text{ hermitian).}$$

$$(e^{i\mathsf{H}})^\dagger(e^{i\mathsf{H}}) = e^{-i\mathsf{H}}e^{i\mathsf{H}} = e^{i(\mathsf{H}-\mathsf{H})} = \mathsf{I}, \text{ using (c). So } e^{i\mathsf{H}} \text{ is unitary.} \quad \checkmark$$

PROBLEM CONCORDANCE
Second and Third Editions
Introduction to Quantum Mechanics

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Chapter 6

All new.

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7.57 (new)	

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Appendix

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