Standing waves[1]

Part I

Part II

John Atwell Moody
Coventry, 2014

---

[1] The javascript mentioned in this article is at `http://spectrograph.uk`

Part I

This note is a discussion of the first part of Schroedinger's 1926 review paper (in English) [2] which arose in beginning to explain spectral lines of hydrogen as frequency differences, and to approach some relativistic ideas of Bruce Westbury.

Schroedinger posited for a an electron of mass μ and charge e at the point (x, y, z) with the nucleus at the origin, a potential function $V = -e^2/r$ with r the distance from the origin. He wishes to have a function $W(x, y, z, t)$ with gradient $(p_x, p_y, p_z, -E)$; and chose

$$W(x, y, z, t) = -Et + S(x, y, z),$$

imagining a standing electromagnetic wave with amplitude $A(x, y, z)$ given

$$\Psi = A(x, y, z)sin(\frac{2\pi}{h}W(x, y, z, t))$$

with A, S are real functions, h Planck's constant. He stated that the 'standard wave equation' it should satisfy has

$$\Delta\Psi = \frac{1}{u^2}(\frac{\partial}{\partial t})^2\Psi$$

with u the speed of motion of the level sets given by $Et = S(x, y, z)$.

Here u is the ratio between the time partial derivative and the magnitude of the spacial gradient $E/|grad(W)|$ which calculates to $E/\sqrt{2\mu(E-V)}$ if μ is the electron mass.

If we define constants

$$\beta = \frac{-8\pi^2 \mu e^2}{h^2}$$

$$\alpha = \frac{-8\pi^2 \mu E}{h^2}$$

the condition they must satisfy, therefore, is that $\alpha + \beta/r$ is an eigenfunction of the Laplacian.

The connected rotation group of three space operates naturally on the Riemann sphere, which can be viewed as the cosets of a Borel subgroup, and all the representations we will look at extend to the full connected automorphism group, the group holomorphic automorphisms of the Riemann sphere, after complexification if necessary.

The vector bundles $\mathcal{O}(j)$ for j an even number are completely natural, they are equivariant for the full automorphism group of the Riemann sphere, because they are tensor powers of the canonical line bundle. Moreover, again for even values $j = 2l$, the global sections are the complexification of the $2l+1$-dimensional space of real harmonic polynomials which are homogeneous of degree l.

Note that this implies that the complex polynomials of degree $2l$ in two variables are the complexification of a space of real polynomials of degree l in three variables. To see that the dimensions are right, you can use the fact that any homogeneous polynomial of degree l in three variables is uniquely a a sum of powers of r^2 times homogeneous harmonic polynomials of lower degree [1].

Thus the sequence of dimensions of the homogeneous harmonic polynomials of degree l is

$$1, \binom{3}{2}, \binom{4}{2}-1, \binom{5}{2}-\binom{3}{2}, \binom{6}{2}-(\binom{4}{2}-1)-1, \ldots$$

which is indeed the sequence of odd numbers. It follows that all are irreducible.

$\mathcal{O}(j)$ is not fully equivariant if j is odd.

There is no similar interpretation of the global sections of $\mathcal{O}(j)$ when j is odd, and indeed the automorphism group of the projective line, nor even the special orthogonal group which preserves the Riemannian metric, do not act in a natural way on the total space of the line bundle with section sheaf $\mathcal{O}(j)$ for j odd.

The automorphism group of any line bundle maps to the automorphism group of the base manifold with kernel automorphisms of the line bundle which fix the zero section, just nonzero scalars under multiplication in the case of a projective variety, resulting in a central extension group acting on the line bundle, not the original group; the resulting central extension is nontrivial when j is odd.

Each automorphism g does lift to a pair of linear automorphisms of determinant one of $\mathbb{C}^2$, negatives of each other, and choosing to label one of them $s(g)$ one has $s(g)s(h) = z(g,h)s(gh)$ for the appropriate central cocycle z taking values in $\{1, -1\}$. This gives an action on global sections of $\mathcal{O}(1)$ which induces an action on the vector bundle itself and therefore all tensor powers. Such a cocycle adjusts what is called the 'gauge' in Weyl's book. Or, another way of viewing the global sections of $\mathcal{O}(j)$ for odd j as representations having to do with the Riemann sphere is to interpret them as representations of the Lie algebra rather than the Lie group, that is, representations of the global sections of the anticanonical line bundle.

The complex vector spaces $\Gamma(\mathbb{P}^1, \mathcal{O}(j))$ for j odd, however, are even dimensional, and if we interpret them as representations of the three dimensional Lie algebra of vector fields of $\mathbb{P}^1$ they restrict to real irreducible representations of twice the dimension $2(j+1)$ (a multiple of 4) whose endomorphism algebra is just the field $\mathbb{C}$. That is, the complex number field could arise as the endomorphism ring of the global sections of $\mathcal{O}(1)$ as a representation of the vector field Lie algebra of the Riemann sphere, and this is so even if initially we do not use complex numbers, and consider vector fields preserving the Riemannian metric. We will see later a more natural way that complex numbers will arise in this context.

Representations of so_3

Although this is trivial, it makes sense to go through some of the representation spaces just to settle the notational conventions. As one lists the orbitals according to values of $l = 0,\ \frac{1}{2},\ 1,\ \frac{3}{2}$ ... the names $s, p, d, f, ...$ are given to the integral values of l. The wave functions for $l = 0$, those type s, are the constants.

For $l = \frac{1}{2}$ they need a cocycle $z(g, h)$ or can be interpreted as representations of the Lie algebra; and belong to a four dimensional vector space with a complex structure.

For $l = 1$, those of type p correspond to just real linear forms on three space (of dimension three), and the complexification is the space of holomorphic vector fields on the Riemann sphere (dual to the canonical line bundle).

For $l = 3/2$, they need a cocycle and belong to an eight-dimensional real vector space, with a complex structure.

For $l = 2$ the so-called type d, are the five-dimensional space of real harmonic functions which are among the homogeneous polynomials of degree two in three variables. This is the orthogonal complement of the line spanned by r^2 where r is the distance from the origin, under an invariant quadratic form, and its complexification is the global sections of $\mathcal{O}(3)$;

For $l = 5/2$ is a representation of dimension 12 with a complex structure.

For $l = 3$ those of type f there is the seven dimensional space of harmonic polynomials which are homogeneous of degree three in three variables, orthogonal to r^2 times haromonic homogeneous of degree one.

For $l = 7/2$ is just a sixteen dimensional representation with a complex structure.

For $l = 4$ those of type g, the nine dimensional space of harmonics polynomials which which are homogeneous of degree four and which are orthognal both to r^4 and to r^2 times the harmonics homogeneous of degree two, and so-on.

Eigenfunctions of the Laplacian

The action of the Laplacian on products $sf(r)$ with s a homogeneous polynomial of degree l which is a harmonic and f analytic in r is easily calculated. The action of Δ on the powers of r in k variables is $\Delta(r^i) = i(i-2+k)r^{i-2}$, and so for s harmonic homogeneous of degree l

$$\Delta(r^i s) = (\ i(i-1)\ + (k-1+2l)\ i\ )r^{i-2}s$$

Then if f is an analytic function of r and s a harmonic analytic function the Laplacian operator acts on the product fs by

$$= (\frac{d}{dr})^2 + \frac{k-1+2l(s)}{r}(\frac{d}{dr}).$$

where the term $l(s)$ can be understood as the Euler derivation acting on the factor s while commuting with functions of r (the actual Casimir operator in that sense is $l(l+1)$).

Now Δ has an eigenfunction of the form $\alpha + \beta/r$ just when $r\Delta$ has eigenfunction $\alpha r + \beta$.

The action of $r\Delta$ on functions sf where where s is harmonic homogeneous of degree l is

$$r(\frac{d}{dr})^2 + (k-1+2l)(\frac{d}{dr}).$$

Take $k = 3$, the number of variables. For any number λ, $r\Delta$ acts on $r^m e^{\lambda r} s$ by

$$\lambda^2 r + 2\lambda n + \text{lower order}$$

for $n = m + l + 1$. If we take $\alpha = \lambda^2$ the difference $r\Delta - \alpha r - \beta$ preserves the filtration by the span of $e^{\lambda r}s, re^{\lambda r}s, ..., r^m e^{\lambda r}s$, acting the associated graded vector space by $2\lambda(m+l+1) - \beta$ in degree m. For any m we may take $\beta = 2\lambda(m+l+1)$ and the span maps onto the span of just $e^{\lambda r}s, ...r^{m-1}e^{\lambda r}s$ with one dimensional kernel spanned by

$$e^{\frac{1}{2n}\beta\ r} \sum_{i=0}^{n-l-1} \binom{n+l}{n-l-1-i} \frac{(\frac{1}{n}\beta\ r)^i}{i!}\ s.$$

The relation $\alpha = \frac{\beta^2}{4n^2}$ above gives energies

$$E = \frac{-2\pi^2 \mu e^4}{h^2 n^2}$$

Note that β is negative.

This determines a space of eigenfunctions of dimension $2l+1$ for each pair of positive integers (l, n) with $l < n$, in which the restriction of the wave function to a sphere centered at the origin depends only on l while the restriction to a radial line depends on both n and l.

Dividing by $(4\pi\epsilon)^2$, since the potential in units of meters, kilograms, seconds is really $-e^2/(4\pi\epsilon r)$, and dividing by h gives the sequence of frequencies in cycles per second

$$\frac{\mu e^4}{8\epsilon^2 h^3 n^2}.$$

Using

$$h = 6.626 * 10^{-34}$$
$$e = 1.602 * 10^{-19}$$
$$\mu = 9.109 * 10^{-31}$$
$$\epsilon = 8.854 * 10^{-12}$$

gives

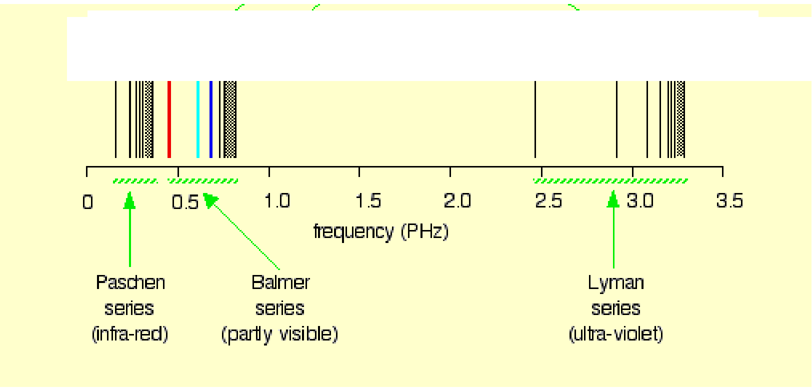
$$3.29/n^2$$

petahertz.

The frequency differences of the $3.29/n^2$ for $n = 1, 2, 3, \ldots$ include the consecutive sequence

$$0.72,\ 0.76,\ 2.45,\ 2.9,\ 3.06,\ 3.13$$

petahertz. These do appear in spectrographs of hydrogen on the internet, of these six in particular the last four in the ultraviolet Lyman series and the first two in the partly visible (nearly infrared) Ballmer series.



I should say that the equation which Schroedinger derives had been known before empirically by Ballmer, Rydberg, and Bohr; it is, in my opinion, an impressive accomplishment to have found a wave equation which appears to explain this spectrum.

The photo of the spectrum, found in Google Images, is from chemguide.co.uk. It is not an actual spectrum, but is missing the fine structure sometimes attributed to ‘spin-momentum interaction,’ something we’ll talk about later on here.

Another thing we’ll discuss later on is that the solutions presented here are not the most general solution of Schroedinger’s equation, even under the requirement of entire analyticity.

Attempts to explain the periodic table

The numbers n and l are typically called the 'main' and 'azimuthal' quantum numbers, and the shape of the wave function corresponding to each value $l = 0, 1, 2, 3, 4, ...$ are named with the letters $s, p, d, f, g, h, ...$. One very rough interpretation of the periodic table would start with the observation that if we consider Helium to be an Alkaline Earth Metal, and number the Alkaline Earth Metals $m = 1, 2, 3, 4...$ for Helium, Beryllium, Magnesium, Calcium, etc, then the atomic number $a(m)$ of the m'th Alkaline Earth Metal is given by the formula

$$a(m) = \begin{cases} \binom{m+2}{3}, & m \text{ even} \\ \binom{m+1}{3} \quad + \quad 2(\frac{m+1}{2})^2, & m \text{ odd} \end{cases} .$$

Thus, the even-numbered Alkaline Earth Metals have atomic number which is the equal to a number of three-element subsets.

m	$\binom{m+2}{3}$	m'th Alkaline Earth Metal	Atomic number
2	4	Be	4
4	20	Ca	20
6	56	Ba	56
8	120	Ubn	120

Although Ubn, Unbilinium, has not been discovered, the notion that the periodic table is understood this way is supported by articles saying that Unbilinium should be considered to be an Alkaline Earth Metal.

The elements whose atomic number, plus twice a square, is the atomic number of the next Alkaline Earth Metal, are those which occur in the rightmost position in a 'period' of the periodic table. For example the Noble Gasses are those elements whose atomic number is 1^2+1^2 less than an Alkaline Earth Metal, and Zinc, Cadmium, Mercury, and Copernicum have atomic numbers

$$38 - 2^2 - 2^2,\ 56 - 2^2 - 2^2,\ 88 - 2^2 - 2^2,\ 120 - 2^2 - 2^2.$$

For Radium of atomic number 88 the fact that Ytterbium has atomic number $88 - 3^2 - 3^2$ would say it is the last element of its period; in fact it is the next-to-last element in the Lanthanide series, having similar properties to Lutetium; and Wikipeida says of this issue "Actual electronic configurations may be slihtly different than predicted by the Aufbau principle."

What is consistent both with the number theoretic structure of the periodic table and with observed spectral lines is the so-called Aufbau principle, that for each atomic number k and each value of l, the range of values of n that actually occur, which, as we know, must be at least $l+1$, do not in the unexcited state exceed $N-l$ where N is the number of Alkaline Earth Metals (including Helium) with atomic number less than or equal to k, by more than the number δ, where we let $\delta = 0$ if $2(l+1)^2$ does not exceed the atomic number of the next Alkaline Earth Metal, and otherwise $\delta = 1$.

Thinking of $\mathbb{C}^\times$, the multipicative group of $\mathbb{C}$, acting on scalars in $\mathbb{C}^2$ by $T(x,y) = (Tx, T^{-1}y)$, the induced action on global sections of $\mathcal{O}(j)$ of an element $T \in \mathbb{C}^\times$ is equivalent to the action on the isomorphic space of monomials $x^j, x^{j-1}y, ..., y^j$ in which T acts by T on x and T^{-1} on y.

We denote by $e_j(T)$ the trace of this action, and so we are just defining a Laurent polynomial

$$e_j(T) = T^{-j} + T^{-j+2} + ... + T^j. \qquad (1)$$

There are no other irreducible representations of $Sl_2(\mathbb{C})$.

The tensor product of representations induces the product of characters, and so we can determine how a tensor product of two irreducible representations decomposes into a sum of irreducible representations, just by looking at the subring of the Laurent polynomial ring generated by the $e_j(T)$. The structure constants are determined by the rule that for $\beta \leq \alpha$

$$e_\alpha(T)e_\beta(T) = e_{\alpha+\beta}(T) + e_{\alpha+\beta-2}(T) + ... + e_{\alpha-\beta}(T).$$

This rule, which is just an identity in the Laurent polynomial ring, is called the 'Clebsch-Gordan rule.' We can double check this identity by setting $T = 1$, where it says

$$(\alpha+1)(\beta+1) = (\alpha+\beta+1)+(\alpha+\beta-1)+...+(\alpha-\beta+1).$$

This corresponds to the fact that the summands of a tensor product must add up to the product of the dimensions.

An interesting coincidence is that the Clebsch Gordan rule happens to agree with what happens when just two spaces of homogeneous harmonic polynomials are multiplied. That is, if I choose two numbers i, j and consider the spaces $\mathcal{H}_i, \mathcal{H}_j$ of homogeneous real harmonic polynomials of degree i and j, then these occur within the polynomal algebra, and when multiplied, decompose into a direct sum of $\mathcal{H}_\alpha r^{i+j-\alpha}$.

Here r is the radial function, and $i + j - \alpha$ turns out always to be an even number. Moreover when one complexifies, keeping track only of the SO_3 action, which makes sense in these particular complexified representations, the resulting decomposition agrees with the Clebsch-Gordan rule. To see this, all that one has to check is that each number α occurs only once, as we knew that the $\mathcal{H}_i$ complexify to the representation with character $e_{2i}(L)$. It may be this coincidence which led to early attempts to understand atoms using Clebsch-Gordan.

We will later use a slight generalization of Clebsch-Gordan, viewing radial functions as being in our base ring, namely

$$e_\alpha(L)e_\beta(L) = e_{\alpha+\beta}(L) + r^2 e_{\alpha+\beta-2}(L) + ... + r^{2\beta} e_{\alpha-\beta}(L)$$

for $\alpha \geq \beta$.

Schroedinger comments

> 'the so-called azimuthal quantum number ...turns out to be half-integer ... in what way the electron spin has to be taken into account ... is yet unknown.'

Although we'll introduce some motivation for doing this later, let us now, following Weyl's notion of using what he called 'vector valued wave functions,' consider our representations to be really representations of the leftmost factor in the cartesian product $SO_3 \times 1$ in the cartesian product group $SO_3(\mathbb{R}) \times SU_2(\mathbb{C})$. Representations of the larger group are also representations of $SU_2(\mathbb{C}) \times SU_2(\mathbb{C})$, and all extend to representations of $SL_2(\mathbb{C}) \times SL_2(\mathbb{C})$. Restricted to a maximal torus $\mathbb{C}^\times \times \mathbb{C}^\times$, such a representation decomposes into a direct sum of lines upon which a point (L, S) acts by a monomial $L^{2l} S^s$ for integers l, s. In fact the irreducible representations of a cartesian product are the tensor products of separate irreducible representations, so that the characters of the irreducible representations of $SU_2(\mathbb{C}) \times SU_2(\mathbb{C})$ are just the $e_i(L)e_j(S)$ for $i, j \geq 0$.

To be very rigorous, if we are really talking about representations of $SU_2(\mathbb{C}) \times SU_2(\mathbb{C})$ we should consider L and S to belong to the unit circle because the torus is only $U(1) \times U(1) \subset \mathbb{C}^\times \times \mathbb{C}^\times$. This will never cause any difficulty.

The irreducible representations which come from representations of $SO_3(\mathbb{R}) \times SU_2(\mathbb{C})$ are those for which the first subscript is even. Thus they have characters $e_{2l}(L)e_s(S)$ where $s, l \geq 0$ are integers. The Clebsh-Gordan rule of course applies to each factor separately, or one may deduce it by working in the ring of Laurent polynomials $\mathbb{Z}[L^2, L^{-2}, S, S^{-1}]$. No odd powers of L are going to occur anywhere and the use of even powers is perhaps only to remind us that the representations are those of $SO_3(\mathbb{R}) \times SU_2(\mathbb{C})$.

Writing the monomials that occur as $L^{2i}S^j$, the monomial in $e_{2l}(L)e_s(S)$ that occurs with maximum value of i and j is just $L^{2l}S^s$. This is called the 'highest weight character.'

If we are given a Laurent polynomial in L^2 and S, and wish to decompose it as a sum of $e_{2l}(L)e_s(S)$ there is at most one way to do this; it can be done by choosing the highest weight, that is, the monomial $L^{2i}S^j$ that occurs which is maximum for either of the lexicographic orderings on pairs (i, j). One is assured that the character is of the form $e_{2i}(L)e_j(S) + \chi$ and so one can subtract $e_{2i}(L)e_j(S)$, and in this way is an easy inductive method generalizing Clebsch-Gordan, by which any character whatsoever can be decomposed into a sum of irreducible characters.

Although we have not yet attempted to give any explanation of why the group $SO_3(\mathbb{R}) \times SU_2(\mathbb{C})$ should be acting on the space of wave functions (or, as later we may suggest, wave forms), both the Periodic Table, with respect to unexcited atoms, and the individual spectral data, for excited atoms, is consistent with the simple Aufbau principle mentioned above. A little later I'll return to the issue of existing explanations of the principle, arguing that it appears to be unexplained.

Since we may want to consider ions, instead of letting k be the atomic number, let's let k_p be the number of protons and k the number of electrons. If we work using the radial functions as coefficients, replacing the constant β by $k_p\beta$ in the radial eigenfunction (in the sense of eigenvector, not eigenvalue), to account for the fact that the potential function is $-k_pe^2/r$ we have

$$f_{k_p,n,l} = e^{\frac{k_p}{2n}\beta\ r} \sum_{i=0}^{n-l-1} \binom{n+l}{n-l-1-i} \frac{(\frac{k_p}{n}\beta\ r)^i}{i!}. \quad (2)$$

This is the radial solution for the Hydrogen atom but we've multiplied the coefficient β by k_p since now there are k_p protons. The number β is -4.2042; note that $\beta/(4\pi\epsilon) = 3.78 * 10^{10}m^{-1}$ is twice the reciprocal of the Bohr radius of the Hydrogen atom.

Let's first consider the direct sum of the wave functions of individual electrons, and work *over* the ring of analytic functions of r. For k_p fixed, any endomorphism ϕ of the space of Shroedinger solutions which preserves the filtration by n and l and also a filtration compatible with the $\mathbb{C}^\times \times \mathbb{C}^\times$ action has a trace element

$$\chi(S, L, f_{k_p,n,l}, \phi) = \sum_{m_l=-\infty}^{\infty} \sum_{m_s=-\infty}^{\infty} c_{n,l,m_s,m_l}(\phi) S^{2m_l} L^{2m_s} \tag{3}$$

where the c_{n,l,m_s,m_l} are just formal power series (expressions) in all the $f_{k,n,l}$. By including the argument $f_{k_p,n,l}$ on the left I mean that if we interpret these symbols all as numbers, the left side will depend upon their values. The subscripts of l and s on the numbers m_l and m_s have no meaning except to say that m_l and m_s are two possibly different numbers while we've followed the convention of denoting both by m. Also note that by these conventions m_l will be an integer while m_s will be a half-integer.

The first case we'll look at, when ϕ is the identity, is just

$$\chi(S, L, f_{k_p,n,l}, 1) = \sum_{l=0}^{\infty} \sum_{n=l+1}^{\infty} f_{k_p,n,l} e_s(S) e_{2l}(L) \tag{4}$$

While we think of $e_{2l}(L)$ as the character of the the space of homogeneous harmonic polynomials of degree l in the three variables x, y, z; yet $e_s(S)$ still needs to be given a physical interpetation somehow. While the trace element is abstractly the character of the tensor product with the function ring of the space of all homogeneous polynomials of degree s in two complex variables u and v, yet is not justified to write things this way not knowing what the two complex variables u and v may represent; in in a later section I'll return to this mystery.

If we consider only terms where $n \leq M$ with M is an upper bound of our choice, such as the one described by the Aufbau, the result is a Laurent polynomial in S, L and the $f_{k_p,n,l}$ which includes no negative powers of any $f_{k_p,n,l}$.

While there is no great harm in thinking of the $f_{k_p,n,l}$ as analytic functions of a single variable r; then we've specified a linear combination of characters of representations free of finite rank over the ring of analytic functions in the variable r; however, keeping them separate also allows evaluating different choices of the $f_{k_p,n,l}$ at different values of r and describing traces of endomorphisms.

If we now consider the whole space to be a space of differential forms, then we would consider exterior powers of the representation. It follows just from the fact that exterior powers convert sums to tensor products that the series

$$e^{-\sum_{j=0}^{\infty}((-T)^j/j)\chi(S^j, L^j, f^j_{k_p,n,l}, \phi^j)} \qquad (5)$$

is the sum $a_0 + a_1 T + a_2 T^2 ...$ in which a_i is the trace series (4) acting upon the i'th exterior power of the representation whose character is χ.

I presented the expressions in a pretentious way, perhaps. When they are combined, for instance, when ϕ is just the identity, they yield the product $1+f_{k_p,n,l}S^{\epsilon}L^{2\alpha}T$ for and for ϵ, α integers with $\epsilon = \pm 1$ and $-2l \leq \alpha \leq 2l$ and a_k is just the k'th elementary symmetric polynomial in the quantities $f_{k_p,n,l}S^{\epsilon}L^{2\alpha}T$, though this may be an unenlightening way to write it.

Combining (1),(2),(4), and (5) with $k = k_p$ expresses the desired character a_k as an analytic function in S, L, and r, or if we like as an analytic function of S, L and all the $f_{k_p,n,l}$. Using the highest weight method, each coefficient a_k can be written as a polynomial in the $e_s(S)$ and $e_{2l}(L)$ describing then the decomposition of the k'th exterior power of the space of Schroedinger solutions.

For instance for Nitrogen of atomic number 7, with the limit M taken according to the Aufbau restriction the result of combining (1),(2),(4),(5) gives a Laurent polynomial in S, L and the $f_{k,n,l}$; decomposing the result into irreducible characters by the highest weight method gives

$$\begin{aligned}
&f_{7,1,0}^2 f_{7,2,0}^2 f_{7,2,1}^3 (e_3(S) + e_1(S)e_2(L) + e_1(S)e_4(L)) \\
+&f_{7,1,0}^2 f_{7,2,0} f_{7,2,1}^4 (e_3(S)e_2(L) + e_1(S)e_2(L) + e_1(S)e_4(L) + e_1(S)) \\
+&f_{7,1,0}^2 f_{7,2,1}^5 e_1(S)e_2(L).
\end{aligned}$$

If we imagine the electrons do not affect each other, the energy level would be proportional to the (negative) sum of reciprocal squares of the second subscript, and would be the same for wave functions in any of the spaces with these characters. There is no reason to presume that wave functions belonging to the eight irreducible components would have the same energy level if one didn't assume the absence of electron to electron repulsion; hence a more precise version of the Aufbau (which we'll state in the next section) records the observation that this is not true, and that in this case the terms in the first line above have lower energy level than the others, and a rule called Hund's rule says that among these, the term $e_s(S)e_{2l}(L)$ with (s, l) maximum in the lexicographic order has lowest energy.

The Hund rule agrees with Schroedinger's equation, the javascript spectrograph which we'll introduce later can show this, but unlike the Schroedinger equation no such combinatorial rule as the Hund rule extends to a meaningful assertion about the ordering of any but the lowest term. Also the Hund rule can disagree with experiment even for the lowest term symbol of any but the ground electron configuration.

An example the configuration $1s^2 2p^2$ for Beryllium where the Hund rule applied to this excited configuration and the Schroedinger equation both predict the order $e_2(S)e_2(L), e_4(L), 1$ both disagreeing with the order consistent with the spectrum and Stern-Gerlach which is $e_4(L), e_2(S)e_2(L), 1$

There are other cases such as Boron $1s^2 2s^1 2p^2$ where the the Schroedinger equation agrees with the ordering consistent with the spectrum and Stern-Gerlach, which is $e_3(S)e_2(L), e_1(S)e_4(L), e_1(S), e_1(S)e_2(L)$ while the extension of Hund's rule would reverse the last two terms.

An abbreviated notation called ‘term notation’ is used in Chemistry to denote such characters. Each character $e_s(S)$ is described using its dimension, also equal to the value at 1, namely $e_s(1) = s + 1$, as a preceding superscript. Each character $e_{2l}(L)$ is described by attributing to each possible number $l = 0, 1, 2, 3,$ the letter $S, P, D, F, G, H, ...$ And a product character $e_s(S)e_{2l}(L)$ is described by putting the preceding superscript on the letter. Thus the character

$$e_3(S) + e_1(S)e_2(L) + e_1(S)e_4(L)$$

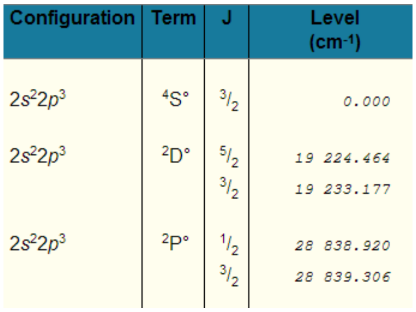
is described as the conjunction of the three ‘terms’

$${}^4S,{}^2P,{}^2D.$$

When as in this case, the sum of the l values of the coefficients $f_{k,n,l}$ is odd, one also appends a superscript letter ‘o’ standing for the word ‘odd’ giving in this case

$${}^4S^\circ,\ {}^2P^\circ,\ {}^2D^\circ.$$

The circle is a useful convention; it indicates of course that the space of wave functions comprising the representation is a space of odd functions with respect to negating x, y, z, and it will turn out that transitions are not observed experimentally except between odd and even functions in this sense.



Configuration	Term	J	Level (cm^{-1})
$2s^2 2p^3$	${}^4S^\circ$	$3/2$	0.000
$2s^2 2p^3$	${}^2D^\circ$	$5/2$	19 224.464
		$3/2$	19 233.177
$2s^2 2p^3$	${}^2P^\circ$	$1/2$	28 838.920
		$3/2$	28 839.306

The preceding superscript on a term symbol is sometimes called the 'multiplicity' of the term symbol; in the most common case when the multiplicity of the corresponding irreducible representation of $SO_3 \times U_2$ is equal to one, it does then describe the multiplicity of the irreducible representation which occurs upon restricting to the subgroup $SO_3 \times 1$, which might be labelled by $S, P, D, F, G, H, ...$ For reasons of consistency we'll reserve the term 'multiplicity' instead for the superscript we'll put on the whole term symbol, using latin numbering 'bis, ter, quater, quinquies, ...' which is the multiplicity with which an irreducible representation of the cartesian product group $SO_3 \times SU_2$ occurs within the representation which we have called an 'electron configuration.'

The numbers shown in the NIST database to the right of the term symbols, when multiplied by the speed of light in centimeters per second, become frequencies in cycles per second. To a first approximation of course these frequencies are proportional to sums of reciprocal squares. In the next sections we'll look at better approximations.

Attempts to explain atomic spectra

The most significant departure of atomic spectra from what would be if atoms were just obtained by coalescing the nuclei of Hydrogen atoms (resulting in a set of frequencies proportional to the differences of two sums of k reciprocal squares) is a displacement of spectral lines which is considered to be due to the electrostatic effect of electron repulsion.

It is sometimes convenient to organize things in terms of what are called 'electron configurations.' One takes the direct sum of functions with k_p fixed

$$V = \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} f_{k_p,n,l}(\mathcal{H}_l\alpha \oplus \mathcal{H}_l\beta)$$

where $\mathcal{H}_l$ is the $l+1$ dimensional vector space of real homogeneous harmonic polynomials of degree l, and α, β formal symbols, and considers the decomposition of the real exterior algebra into the direct sum

$$\oplus(\prod_{i=1}^{n} f^{e_i}_{k_p,l_i,n_i}) \otimes_{i=1}^{n} \Lambda^{e_i}(\mathcal{H}_{l_i}\alpha \oplus \mathcal{H}_{l_i}\beta).$$

(Later we will see that a natural completion of this space occurs as the global holomorphic forms on a complex manifold.) The degree of an exterior power is used as a superscript, and tensor products denoted by juxtaposition; so for example the tensor product

$$\Lambda^2(f_{5,1,0}(\mathcal{H}_0\alpha\oplus\mathcal{H}_0\beta))\otimes\Lambda^1(f_{5,2,0}(\mathcal{H}_0\alpha\oplus\mathcal{H}_0\beta))\otimes\Lambda^2(f_{5,2,1}(\mathcal{H}_1\alpha\oplus\mathcal{H}_1\beta))$$

which occurs as a 30-dimensional subspace of the wave functions for Boron, is denoted $1s^2 2s^1 2p^2$.

When the character is decomposed into irreducibles as we've done before, and these are named according to 'term symbols,' we might include the electron configuration notation alonside the term symbol, and such a symbolic expression really does arise from each isotypical component of the space of Schroedinger wave functions, so here the four isotypical parts of the electron configuration, of dimension 12, 10, 2, 6, can be denoted

$1s^2 2s^1 2p^2\ {}^4P$
$1s^2 2s^1 2p^2\ {}^2D$
$1s^2 2s^1 2p^2\ {}^2S$
$1s^2 2s^1 2p^2\ {}^2P$

It is sometimes said that such notation is describing meaningful physical 'states,' associated to isomorphism types of representations of $SO_3 \times SU_2$, but this would not be quite exactly correct. The isotypical component associated with an electron configuration and term symbol is not always irreducible. This first occurs for the excited Nitrogen electron configuration $1s^2 2s^2 2p^2 3p^1$. Of the eight term symbols, the term symbol ${}^2D^\circ$ occurs with multiplicity two while ${}^2P^\circ$ occurs with multiplicity three; for instance we'll later index the three isomorphic but distinct representations corresponding to the term symbol ${}^2P^\circ$ by the names

$1s^2 2s^2 2p^2 3p^1\ {}^2P^\circ$
$1s^2 2s^2 2p^2 3p^1\ {}^2P^{\circ\ bis}$
$1s^2 2s^2 2p^2 3p^1\ {}^2P^{\circ\ ter}$.

The Aufbau is a more precise principle than I've so far described. What one must do is to imagine the Aufbau as describing a filtration. We consider the number of protons k_p to be fixed, and imagine the atom at first highly ionized, with all electrons pulled away. This gives $k = 0$ and the space V_0 consisting of just the zero function. Then one electron is allowed, $k = 1$, and we have the space V_1 which is the space of Schroedinger's solutions, but with β multiplied by k_p. As k is increased, the number k of electrons vary, and we write

$$V_k = \sum_{l=0}^{\infty} \sum_{n=l+1}^{N-l+\delta} f_{k,n,l}(\mathcal{H}_l\alpha \oplus \mathcal{H}_l\beta).$$

Here α, β are a basis of the two dimensional representation with character $e_1(S)$. Recall that N and δ depend on both k and l, as determined by the Aufbau; to repeat this definition, N is the number of Alkaline Earth Metals including Hydrogen of atomic number less than or equal to k while δ is zero if $2(l+1)^2$ does not exceed the distance to the next Alkaline Earth Metal and 1 if it does. This describes a filtration

$$0 = V_0 \subset V_1 \subset V_2 ... \subset V$$

of the space V of Schroedinger solutions with k_p protons, and with no mutual electron repulsion, as k ranges.

The difference $k_p - k$ is sometimes called the ionization number, and $k_p - k + 1$ is usually denoted by a roman numeral, so for instance when $k_p = 9$ and $k = 8$ we are talking about $F \quad II$ the first positively ionized Fluorine atom.

For each value of k now, the the exterior power has a filtration with the associated graded space having the direct sum decomposition

$$\Lambda^k V_k \cong \oplus_{j_1+...+j_k=k} \otimes_{i=1}^k \Lambda^{j_i}(V_i/V_{i-1}).$$

Most of the terms have $j_i = 0$ and for these $\Lambda^{j_i}(V_i/V_{i-1})$ is just the real number field because most of the inclusions $V_{i-1} \subset V_i$ are the identity.

Let s be the smallest so that $V_s = V_k$. The Aufbau in the more precise version is the assertion that when the associated graded space of $\Lambda^k V_k$ is decomposed into irreducible components, the only components which can occur at the ground level are those in the summand where we take all but the last j_i as large as possible, that is $j_i = dim(V_i/V_{i-1})$ for $i = 1, 2, ..., s-1$, while then $j_s = k - dim(V_{s-1})$.

This implies that the ground state term symbols correspond to the irreducible parts of an exterior power of a single character $e_{2l}(L)e_s(S)$. It also implies that when we consider the entire solution space corresponding to a whole electron configuration, if we consider this as a representation of $(SO_3 \times SU_2)^v$ where v is the number of orbitals, then when we decompose it for this group, the irreducible components, which are just tensor products of components of the separate irreducible representation with character $e_{2l_i}(L_i)e_{s_i}(S_i)$ for the i'th orbital, are indexed by a sequence, assigning to each orbital a choice of term symbol which is identical to the possibilities it might have if it occurred as the unique 'unfilled orbital' in a ground state.

That is, if we initially consider the representation space associated to an electron configuration, for the action of the whole large group which has a cartesian copy of $SO_3 \times SU_2$ for each orbital, the irreducible components are indexed by a choice of term symbol for each orbital, and this is no different than the choices one would make if one were confronted with a sequence of separate atoms, each having the relevant orbital as the last 'unfilled orbital.'

Later, when we talk a little about polarizations, we'll mention that a polarization for this cartesian product group, with one cartesian factor of $SO_3 \times SU_2$ for each orbital, does determine within each irreducible representation – and so corresponding to each such sequence of term symbols – a wave function which 'has' that polarization, and it is unique up to a choice of complex scale factor affecting both magnitude and phase. And also, however, that it is not even approximately true that every 'energy level' is attained by such a specialized wave function, and it is necessary to accept that there is no such meaningful picture as unlinked orbitals like this, and it is necessary to pass to a smaller subgroup, the diagonal copy of $SO_3 \times SU_2$.

Each irreducible part for the diagonal $SO_3 \times SU_2$, in turn, is not actually irreducible for the natural action of the diagonal subgroup $SU_2 \subset SO_3 \times SU_2$. Later, I will argue that this action of the diagonal subgroup corresponds to rotations of space in the familiar way we understand it (though since it consists of automorphisms of a line bundle rather than any actual ambient complex two-dimensional vector space it must still be an SU_2 rather than an SO_3 factor).[2] Therefore, each irreducible part splits further upon restriction to the diagonal and the number of parts should match the number of actual spectral levels coming from each electron configuration and term symbol, in case the isotypical component is irreducible, and each configuration with a decorated term symbol in any case.

When for example a character like $e_2(S)e_4(L)$, denoted by ${}^3D$, is written upon setting $S = L$ to one variable J as the sum $e_6(J) + e_4(J) + e_2(J)$ the term symbols corresponding to the three summands are denoted ${}^3D_{5/2}, {}^3D_{3/2}, {}^3D_{1/2}$.

---

[2] This will involve understanding that the direct product $SU_2 \times SU_2$ is isomorphic to the *semidirect* product $SU_2 \rtimes SU_2$ via the conjugation action, with the rightmost factor being the rotation action on the line bundle, and corresponding to the diagonal subgroup under the isomorphism to $SU_2 \times SU_2$.

The identification of the term symbols can nearly be treated as a matter of observation. For instance, in the Russell-Saunders scheme here, once the set of frequencies is resolved as differences from one set, each term like ^3D corresponding to a representation $e_2(S)e_4(L)$, has the number of Russell Saunders lines emanating from it being equal to the smaller of the subscripts s, l in each symbol $e_2(S)e_{2l}(L)$. The total dimension $(s+1)(2l+1)$ is the number of levels one would see under a magnetic field, when the rotational symmetry is broken and the space of wave functions decomposed as far as possible, into one dimensional parts. From the minimum value and the product, we know the unordered set $\{s, 2l\}$

Here is one example of a coupling scheme that is different than the Russell-Saunders scheme. The NIST gives an example of labelling a spectral line of Cobalt with the symbol

$$3d^7(^4P)4s4p(^3P^\circ)D^\circ\ ^3[5/2]^\circ_{7/2}.$$

In the language of characters, the part

$$3d^7(^4P)$$

describes extracting from the seventh exterior power of the representation with character $e_1(S)e_4(L)$ the component with character $e_3(S)e_2(L)$.

The part

$$4s4p(^3P^\circ)$$

describes extracting from the tensor product whose character is $e_1(S)e_1(S)e_2(L)$ the component $e_2(S)e_2(L)$ which happens to be the one oflarger dimension. The symbol D° refers to the result of tensoring the right factor of the two extracted representations, and extracting from the representation with character $e_2(L)e_2(L)$ the summand with character $e_4(L)$.

The unusual thing here is that instead of multiplying by the two left factors $e_3(S)$ and $e_2(S)$, we replace S by L in the first of these, and only tensor with that, getting the character

$$e_3(L)e_4(L).$$

Note that when we tensor this with the remaining $e_2(S)$ and set S and L to the same variable J we will obtain just the character that we would have obtained in the Russell Saunders case. However, at this juncture, the symbol ${}^3[5/2]_{7/2}$ refers to the operation of extracting the component $e_5(L)$ from the product $e_3(L)e_4(L)$ and multiplying with the needed $e_2(S)$ to obtain $e_2(S)e_5(L)$.

The subscript 7/2 indicates that when the tensor product is restricted to the diagonal subgroup, using the letter J say for the basic character, we extract just the representation with character $e_7(J)$.

Thus, the notation indexes one of the exact same representations as in Russell Saunders notation is indexed by a different symbol. The set of fine lines that is indexed is the same in both schemes; what is different is the groupings of fine lines into terms.

In some, perhaps historical, ways of understanding things, the actual spectral frequencies calculate to different values depending on what coupling scheme is used. However it is not difficult to describe a single theory that simultaneously generalizes all various the orbit-orbit coupling schemes; that is, they are not really mutually inconsistent.

The situation with what are called spin-orbit or spin-spin or spin-other-orbit coupling schemes, there really is a physical issue. There is a group action, if k is the atomic number (minus degree of ionization), of the k-fold cartesian product $(SU_2 \times SU_2)^k$, and this contains the group we mentioned before (with one diagonal copy for each orbital); but it contains overall $2^k - 1$ different diagonal copies of SU_2, and so there are $2^k - 1$ possible Casimir operators one could use to split the space. These do not all commute with each other; each choice of a commuting set from among the $2^k - 1$ operators gives a different decomposition of the space of wave forms, and each of these gives rise to a possibly different coupling scheme.

In the case of spin-orbit coupling, I will argue later that the use of the main diagonal Casimir is implicit in a correct understanding of the Laplacian operator and its effect on residues on an exceptional divisor. Thus, to explain the effect usually attributed to spin-orbit coupling it is not necessary to include any extra term in Schroedinger's equation, and the equation extended to several variables in the usual way by a product formula suffices to explain the fine structure in spectra equally well. Therefore the considerations in the previous paragraph ought really refer only to 'spin other-orbit' coupling; the ideal would be to understand again a way that just a single partial differential equation already explains the departure of spectra, most notably Helium, from what one sees using only the first diagonal Laplacian. I believe that understanding these further issues amounts to finding a correct formulation of residues.

Now let's talk a bit more about the Aufbau. The more coarse filtration which related to finding the ground level can be interpreted as a partial or, if one wishes, a total ordering on the electron configurations.

If we ignore electron repulsion, so that the frequencies are in proportion of differences of reciprocal squares, then the situation is simple. Each time a new electron is added to an ion, each level becomes an accumulation point of infinitely many nearby levels, the set of accumulation points then remaining always a discrete set below an ionization level.

Thinking of how the Aufbau can reverse levels, then one expects that once electron repulsion is included in the Schroedinger equation, there would be no such meaningful structure of the spectrum, again, apart from questions of intensity. But what is the explanation of the Aufbau?

The Aufbau, if it were explained by the electrostatic term, would need to be considered a consequence of the combination of the fact that one considers subspaces of wave functions, or exterior powers, or the Pauli Exclusion, together with the electrostatic effect. The explanation is that when you perturb the central charge model to take account of electrostatic repulsion, as we have done (or else change it to correctly take account of electrostatic repulsion), then it is like shuffling together two decks of cards. One with a combinatorial structure coming from Pauli Exclusion, or from the notion one is considering k dimensional spaces of wave functions (as by Hartree-Fock). The second coming from the continuous changes that are introduced to energy levels by adding the continuous correction.

That because you compare a combinatorial structure with a continuous structure, you get a changed combinatorial structure when the constraint is applied; so that one should expect further and further complexity in the periodic table if atomic numbers were increased further.

That, it isn't a coincidence that it aligns with numbers of electrons in 'orbitals,' because there are not that many different orbitals overall, and each is considered together for some reason.

And, when you look at the spectrum theoretically produced by just the Schroedinger equation and the electrostatic perturbation, it is indeed as if two decks of cards have been shuffled together.

It may be have been tempting to try to explain this geometrically, as though the orbitals are the things people draw, physical things. So it is like trying to pack oddly shaped balloons into a box, when the vendor has chosen the unique efficient packing. Any other way, and you have to squeeze them in place.

But the drawings of orbitals that some chemistry books make do not make sense. Lecture notes say say things like, you don't need to memorize all of these, but if you want to do well on the exam you should memorize the first five.

Here we know that it is like a person in linear algebra, mistakenly thinking that vector spaces have fixed bases, because *it is that literally.* Someone, at some time, chose a basis of the space of homogeneous harmonic polynomials of each degree. Choosing a basis like that would make sense if a vector space had two quadratic forms. The correspondence between the two quadratic forms will produce in the generic case a preferred basis; one is seeing n points in projective space of dimension $n-1$. But, one does not describe *two* natural quadratic forms on the space of homogeneous haromonic polynomials of degree l for each l. It is usually assumed that the electrostatic effect is the explanation. Let us consider this question.

A bit later on, we'll see that not only a choice of basis causes difficulty, but that a more fundamental difficulty should have been envisaged, that of using considerations of symmetry when considering what essentially really are only angles, versus considering harmonic functions as global functions.

But for now the different question which we'll look at is to what extent the electrostatic effect can really be the explanation of the Aufbau, and for this we can just write down the calculated spectrum of a general atom.

Because it is an exercise in A level or high school integration, we'll write down the integrals explicitly and write down the first order perturbation, to give the 'predicted' energy levels.

Before we start, in the way of simplifying things, it might be helpful to mention that the highest weight calculation is not only an algorithm, there is a direct way to pass from a character to its decomposition, which is determined by the totality of the highest weight terms that *would have* arisen from the algorithm.

These can always be written down directly. In the case at hand, for $SU_2 \times SU_2$, we consider the commutative group homomorphism of projection on the positive weight root space

$$\gamma : \mathbb{Z}[S, S^{-1}, L, L^{-1}] \to \mathbb{Z}[S, L].$$

This acts by the identity on any monomial $S^i L^j$ with $i, j \geq 0$ and otherwise sends any monomial to zero. Now if $\chi(S, L)$ is a character, then it is easy to prove that merely multiplying $\chi(S, L)$ by the finite Laurent series

$$(1 - S^{-2})(1 - L^{-2})$$

and applying the projection γ gives as a result exactly the sum of the highest weight terms in the component characters in the irreducible decomposition of $\chi(S, L)$.

If we want to know whether an irreducible character $e_i(L)e_j(S)$ of $SU_2 \times SU_2$ occurs as a summand of the representation with character $\chi(S, L)$, we can define the positive integer $b_{i,j}$ to be zero if it does not occur, and otherwise to be the multiplicity with which it occurs. Then the totality of the multiplicities $b_{i,j}$ can be assembled a polynomial $\sum_{i,j} b_{i,j} S^i L^j$. We find that the polynomial is determined by the simple equation

$$\sum b_{i,j} S^i L^j = \gamma(\chi(S, L)(1 - S^{-2})(1 - L^{-2})) \qquad (6)$$

which does determine the natural number multiplicity $b_{i,j}$ which counts the number times each summand $e_i(S)e_j(L)$ occurs in $\chi(S, L)$.

More generally, if a vector space endomorphism ϕ acts on the representation as before, giving a more general character $\chi(S, L, \phi)$ and also if we work over the formal power series ring in the $f_{k,n,l}$ the same formula holds, but now $b_{i,j}$ is the formal power series in the $f_{k,n,l}$ giving the trace of ϕ acting on the representation with character $e_i(S)e_j(L)$. If we write Schroedinger's equation in the form

$$(\Delta - \beta/r)\Psi = \alpha\Psi$$

then when we generalize to atomic number k thinking of the $f_{k,n,l}$ for different electrons as being functions of different radial variables, then the left side satisfies a product rule, and the α value converts products to sums. This is another way of seeing that the A values for atomic number k with the central charge assumption are sums of reciprocal squares.

So the left side in this case can be written equivalently, and more precisely

$$\Delta - k_p\beta(\frac{1}{r_1} + ... + \frac{1}{r_k}).$$

with $k_p = k$ the number of protons. Recall that β is a negative number. If we let

$$C = \sum_{i<j} \frac{\beta}{|p_i - p_j|}$$

where p_i denotes the i'th point in three space, then the equation with the new term C times a parameter t

$$(\Delta - k_p\beta(\frac{1}{r_1} + ... + \frac{1}{r_k}) + tC)\Psi = \alpha\Psi$$

generalizes to the case when electrostatic repulsion is considered, if we set $t = 1$, but not if we set $t = 0$. And we have solutions of the equation for $t = 0$.

Let me summarize the idea of perturbation theory, which is nicely explained in [3] for example. This applies to the Schroedinger equation if we bring to one side of the equation all but the constant term. We consider a self-adjoint alinear differential operator

$$\phi : H \to H$$

acting on a Hilbert space H, and a finite-dimensional subspace $V \subset H$ so that ϕ has a single eigenvalue λ on V, that is $\phi(v) = \lambda v$ for $v \in V$.

Suppose now that over time t (or with respect to any parameter t) , the operator ϕ varies in a known way, giving at each time t an operator ϕ_t; and suppose that we know abstractly that there is a space of solutions V_t of the same dimension as V, and we assume that there is a decomposition $V_t = \oplus_{i=1}^r V_{t,r}$ where for each time t $V_{t,i}$ is an eigenspace of ϕ_t with an eigenvalue $\lambda_i(t)$.

Thus $\lambda_i(0) = \lambda$ for all i. One wishes to calculate the mysterious character $\chi_{V_t}(\phi)$ which is the trace of ϕ_t acting on the unknown subspace V_t. One of course can calculate the trace $\chi_V(\pi \circ \phi_t \circ i)$

$$V \xrightarrow{i} W \xrightarrow{\phi_t} W \xrightarrow{\pi} V$$

where i and π are the Hilbert space inclusion and projection. The composite can be represented as a finite matrix, and we can take the trace. The result of perturbation theory is that when ϕ_t is suitably analytic in t that we may meaningfully write and manipulate the relevant Taylor series,

Proposition. The Taylor

$$\sum_{i=0}^{\infty} \frac{t^i}{i!} (\frac{d}{dt}^i \ \chi_{V_t}(\phi_t))_{|t=0}$$

and

$$\sum_{i=0}^{\infty} \frac{t^i}{i!} (\frac{d}{dt}^i \ \chi_V(\pi \circ \phi_t \circ i))_{|t=0}$$

agree in the first terms.

For the proof, there is no harm assuming that the $V_{t,i}$ are one dimensional, and so up to multiplying by a function of t there is a unique way to choose a basis element $e_i(t) \in V_{t,i}$, and we assume that we can extend $e_1(t), ..., e_n(t)$ to a basis $e_1(t), e_2(t), ...$ of H consisting of eigenfunctions for ϕ, so there are now functions λ_i such that $\phi(t)e_i(t) = \lambda_i(t)e_i(t)$.

Then

$$0 = \langle(((\phi_0 - \lambda(0)) + \frac{1}{1!}\frac{d}{dt}(\phi_t - \lambda(t))_{|t=0} + \frac{1}{2!}\frac{d}{dt}^{2}(\phi_t - \lambda(t))_{|t=0}...)e_i(t), \widehat{e_i(0)}\rangle .$$

The first term in the left side, operating on anything at all, sends it into the orthogonal subspace for $\widehat{e_i(0)}$ so the leading terms (of lowest degree in t) will be the degree one term of the operator acting on the degree zero term of $e_i(t)$. The fact that the whole expression is zero gives that when $t = 0$

$$0 = \langle\frac{d}{dt}(\phi_t - \lambda_i(t))e_i(0), \widehat{e_i(0)}\rangle$$

so

$$\frac{d}{dt}\lambda_i(t) = \frac{d}{dt}\langle\phi_t e_i(0), \widehat{e}_i(0)\rangle.$$

The left side summed from 1 to n gives the time derivative of the character of the moving representation V_t while the right side is the time derivative of the trace of the map of finite dimensional vector spaces $V \to W \to W \to V$.

For each individual choice of i it is also true that the series agree up to the first nonzero term, and likewise if one is in a situation where one can invoke linear independence of characters, the same is true for the series in the proposition, being sums of linearly independent parts.

When the proposition applies, unless magically differing eigenvalues later become the same again, the final decomposition of V_t for a finite later time t will respect a decomposition into parts of the same dimension as the eigenspaces of the known linear transformation $\pi \circ \phi \circ i : V \to V$.

Just to be very clear about this, the assumption is *not* that the perturbed operator preserves any particular subspace. Rather, the assumption is that each representation such as the non-irreducible representation we calculated earlier for Nitrogen, which was a sum of irreducible representations, moves and changes with time, as a result of the change in the coefficients of the Schroedinger equation; and that whereas at time zero (when no electrostatic repulsion is considered) the action of multiplication by the potential function preserves the large decomposition and acts with a constant eigenvalue on such large parts as this, as time goes on it is a different, modified, decomposition which is preserved. That what had started out being the original irreducible components move, and become different subspaces, but that at each time the correct subspaces are preserved by the correct operator. That then the subspaces which had started out being the irreducible components each may develop different eigenvalues.

And that the time derivative of the trace of the operator ϕ_t at time zero operating in this way on a moving irreducible component, is the same as the sum of the values of

$$\frac{\langle \phi_t f, f \rangle}{\langle f, f \rangle}$$

for f ranging over a non-moving basis of that irreducible component.

This in turn is the trace of a diagonal operator, the one which just acts on each basis element f by multiplication by the number shown above.

If we let $\chi(S,L)$ in (6) be the trace of that diagonal operator, then the $b_{i,j}$ will be the time derivative at time zero of the character of ϕ_t acting on the component $e_i(S)e_j(L)$ as it moves.

Combining ideas, if we let ϕ be the diagonal operator multiplying each basic f by $\frac{\langle Cf,f\rangle}{\langle f,f\rangle}$ and build the character using $a_0 + a_1 T + ..$ coming from (1), (2), (4), (5) then taking for χ in (6) the coefficient a_k from (5), means that the $b_{i,j}$ on the right side of (6) will be such the first order perturbation of the α eigenvalue for term $e_s(S)e_{2l}(L)$.

In the case at hand, we can let t range from 0 to 1 and so when $t = 1$ the Schroedinger equation includes the electrostatic component of the potential

$$\Delta\Psi = -(\frac{2\pi}{h})^2(2m)(\sum_i \frac{k_p\beta e^2}{4n_i^2} + E_1(t) + \sum_i \frac{k_p e^2}{r_i} - t\sum_{i<j}\frac{e^2}{r_{i,j}})\Psi. \tag{7}$$

The negative number $\sum_i \frac{k_p\beta e^2}{4n_i^2}$ is the energy when $t = 0$ and the term $E_1(t)$ corrects this. The last term on the right when brought to the right side of the equation is the perturbation of the operator; perturbation theory calculates then $\frac{d}{dt}E_1(t)$, the rate of motion of the negative energy away from the ground state. The rate of change of frequency in Hertz as a function of t is the rate of change of the whole term times $\frac{1}{h(4\pi\epsilon)^2}$.

Multiplying by $\frac{1}{h(4\pi\epsilon)^2}$ to convert to MKS units and to a frequency gives the corresponding sum of the rate of change at $t = 0$ of the displacement of the spectral line in cycles per second.

One thing that the proposition implies is that the value of the first two nonzero terms does not depend on the choice of Hilbert space structure which we might put on the vector space of Schroedinger equation solutions, except the choice of complement of the chosen subspace (in practise the subspace associated to an electron configuration). This is quite important as there was no reason that the choice of Hilbert space structure which we made was in any way natural or distinguished. It seems certain that higher terms *do* depend on the choice of Hilbert space structure, so in this sense the theory of first-order perturbations does not naturally extend to a higher order theory.

It is a fun exercise to do the calculation, it leads to a closed expression for the spectrum of any atom in terms of elementary functions (pi and natural logarithms). In the case when the space of Schroedinger solutions is multiplicity-free for the $SU_2 \times SU_2$ action, that is, up cases like the excited 'configuration' and term symbol $1s^2 2s^2 2p^4 3p^1\ {}^2D$ of Fluorine, which specifies an irreducible representation of $SU_2 \times SU_2$ of multiplicity three, or the configuration $1s^2 2s^2 2p^2 3p^1$ of Nitrogen which has a term of multiplicity three and one of multiplicity two, we need only write down the character calculation which we've already explained.

In general, in cases like $1s^2 2s^2 2p^2 3p^1$, we'll explain a further essentially number-theoretic calculation, which comprises intersecting four sub-lattices in an integer lattice and leads to a formula for the spectrum in the general case.

A particular basis of the homogeneous harmonic polynonmials of degree l in x, y, z (which also are mutually orthogonal for the Hilbert space structure) are the

$$P_{l,l+a}(z,r)h_{a,\epsilon}(x,y)$$

for $\epsilon = 0,1$ $a = 0,1,2,,...,l$ with the proviso that ϵ must be zero when $a = l$. Here the first factor is homogeneous of degree $l-a$ and the second of degree a, if we assume $r^2 = x^2 + y^2 + z^2$. Specifically we take

$$h_{a,\epsilon}(x,y) = \sum_{i=0}^{[\frac{a-\epsilon}{2}]} (-1)^i \begin{pmatrix} a \\ 2i+\epsilon \end{pmatrix} x^{a-2i-\epsilon} y^{2i+\epsilon}$$

$$P_{l,u}(z,r) = \sum_{i=0}^{[l-\frac{u}{2}]} (-1)^i \frac{(2l-2i)!}{(2l-2i-u)!} \begin{pmatrix} l \\ i \end{pmatrix} z^{2l-2i-u} r^{2i}.$$

Then a basis of the $2l+1$ dimensional space of solutions of the Schroedinger equation for a single electron and particular value of n and l (and with β replaced by $k_p\beta$) are the products

$$f_{k,n,l}(r)h_{a,\epsilon}(x,y)P_{l,l+a}(z,r),$$

for those values of a, ϵ. These happen to be mutually orthogonal too.

The harmonic function

$$\sum_{i<j} \frac{1}{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}}$$

has Taylor series for the i, j term, if $r_i \geq r_j$ given

$$\sum_{s=0}^{\infty} \frac{1}{s!2^s} \frac{r_j^s}{r_i^{s+1}} P_{s,s}(\frac{x_i x_j + y_i y_j + z_i z_j}{r_i r_j}, 1).$$

This known series expansion is called the 'multipole expansion.' It may be possible to work with harmonic functions in a nice conformal sense, here we are only going to look at initial parts of Taylor series.

By choice of the $h_{a,\epsilon}$ we have that for each a

$$h_{a,0}(x, y) + ih_{a,1}(x, y) = (x + iy)^a.$$

For a basis of the complexification, we could also use

$$h_{a,0}(x, y) + ih_{a,1}(x, y)$$

$$h_{a,0}(x, y) - ih_{a,1}(x, y)$$

for $a = 1, 2, ..., l$ and also the constant 1. The span of each of these is preserved by the action of L if we choose the torus in the obvious way, and therefore we can make complex solutions of the single electron Schroedinger equation with character L^{2m} for $m = -l, -l + 1, ..., l$ as

$$f_{k,n,l} P_{l,l+a}(z, r)(h_{a,0} \pm ih_{a,1})$$

using the negative sign if m is negative, with the convention that $h_{a,1} = 0$ if $a = 0$.

The definite integrals[3]

$$Y_{k,a,b,n_1,l_1,n_2,l_2,n_3,l_3,n_4,l_4}$$

$$= \beta^{a+b+2}\int_0^\infty\int_0^{r_2} f_{k,n_1,l_1}(r_1)f_{k,n_2,l_2}(r_1)f_{k,n_3,l_3}(r_2)f_{k,n_4,l_4}(r_2)r_1^a r_2^b dr_1 dr_2$$

and

$$Z_{s,l_1,a_1,\epsilon_1,l_2,a_2,\epsilon_2,l_3,a_3,\epsilon_3,l_4,a_4,\epsilon_4}$$

$$= \int_{S^2\times S^2} h_{a_1,\epsilon_1}(x_1,y_1)P_{l_1,l_1+a_1}(z_1,r_1)h_{a_2,\epsilon_2}(x_1,y_1)P_{l_2,l_2+a_2}(z_1,r_1)$$
$$h_{a_3,\epsilon_3}(x_2,y_2)P_{l_3,l_3+a_3}(z_2,r_2)h_{a_4,\epsilon_4}(x_2,y_2)P_{l_4,l_4+a_4}(z_r,r_2)$$
$$P_{s,s}(x_1x_2+y_1y_2+z_1z_2,r_1r_2)\sigma,$$

where σ is the standard area form on the two-sphere, are easily determined. We will evaluate both integrals in a minute.

Since we will want to consider the perturbation on the exterior power, we need to choose a Hilbert space structure on the exterior algebra.

If α_i and β_i are elements of the (as yet undefined) representation whose character is $e_1(S)$, and f_i, g_i wave forms or wave functions, we will write

$$\langle f_1\alpha_1\wedge ...\wedge f_k\alpha_k, g_1\beta_1\wedge ...\wedge g_k\beta_k\rangle$$
$$= determinant(\langle f_i\alpha_i, g_j\beta_j\rangle)$$

---

[3] The coefficient β^{a+b+2} makes the value independent of β, it amounts to an inessential change of basis. It is inessential because although removing the coefficient changes the integral, it does not change the overall calculation.

and we take

$$\langle f_i\alpha_i, g_j\beta_j\rangle = \langle f_i, g_j\rangle\langle\alpha_i\beta_j\rangle.$$

Let's take as the Hilbert space structure on our space with character $e_1(S)$, with basis say α, β, just the Euclidean product $\langle\alpha,\beta\rangle = \langle\beta,\alpha\rangle = 0$, $\langle\alpha,\alpha\rangle = \langle\beta,\beta\rangle = 1$. And for the functions we'll take

$$\langle f, g\rangle = \int fg\omega$$

for ω a volume form on three space. In order to apply Perturbation theory we need any reasonable extension of the Hilbert space structure to a space including multiples of our wave forms by L^2 functions; it is not difficult to do this.

Our inner product

$$\langle f_1\alpha_1 \wedge ... \wedge f_k\alpha_k, g_1\beta_1 \wedge ... \wedge g_k\beta_k\rangle$$

$$= \sum_\sigma (-1)^{sgn\ \sigma}\langle\alpha_1, \beta_{\sigma(1)}\rangle ... \langle\alpha_k\beta_{\sigma(k)}\rangle\langle f_1, g_{\sigma(1)}\rangle ... \langle f_k, g_{\sigma(k)}\rangle$$

is of course also equal to

$$\sum_\sigma (-1)^{sgn\ \sigma}\langle\alpha_1, \beta_{\sigma(1)}\rangle ... \langle\alpha_k\beta_{\sigma(k)}\rangle \int f_1 g_{\sigma(1)}\omega ... \int f_k g_{\sigma(k)}\omega$$

and we can rewrite

$$\int f_1 g_{\sigma(1)}\omega ... \int f_k g_{\sigma(k)}\omega = \int f_1(p_1)g_{\sigma(1)}(p_1) ... f_k(p_k)g_{\sigma(k)}(p_k)\omega_k$$

for $(p_1, ..., p_k)$ in $3k$ space and ω_k the volume form in $3k$ space. This is equal to

$$\int f_1(p_1)g_1(p_{\sigma^{-1}(1)}) ... f_k(p_k)g_k(p_{\sigma^{-1}(k)})\omega_k$$

and also to

$$\int f_1(p_{\sigma(1)})g_1(p_1)...f_k(p_{\sigma(k)})g_k(p_k).$$

Thus if ψ and ϕ are any two functions of $(p_1, ..., p_k)$ we may write

$$\langle \psi\alpha_1 \wedge ... \wedge \alpha_k, \phi\beta_1 \wedge ... \wedge \beta_k\rangle$$
$$= \sum_\sigma (-1)^{sgn(\sigma)}\langle \alpha_1, \beta_{\sigma(1)}\rangle ... \langle \alpha_k, \beta_\sigma(k)\rangle \int \psi(p_{\sigma(1)}, ..., p_{\sigma(k)})\overline{\phi(p_1, ..., p_k)}\omega_k.$$

A particular basis of the k'th exterior power of the space of Schroedinger solutions is the wedge products of the

$$f_{k,n,l}(r)P_{l,a}(z,r)(h_{a,0} + ih_{a,1})(x,y)\sigma_s$$

We've reverted to using complex numbers, but not in an essential way. We will write, for $a > 0$

$$h_{-a,0} + ih_{-a,1} = h_{a,0} - ih_{a,1}$$

There is no reason for this choice except if we write

$$h_{a,0} + ih_{a,1} = (x + iy)^a$$

then when $x^2 + y^2 = 1$ we really are talking about the reciprocal. These functions are indexed by l, n, a, σ satisfying

$$0 \le l \le n - 1$$
$$-l \le a \le l$$
$$0 \le \sigma \le 1.$$

Here σ_0, σ_1 are the basis of the as yet undefined representation we are using, whose character is $e_1(S)$

(In other notation the number a is sometimes instead denoted m_l and is sometimes called the 'magnetic quantum number,' and the number s is sometimes given values $1/2$ and $-1/2$ and would be called 'spin.')

If we begin with a vector space spanned by a set of these basis vectors, the matrix of $V \to W \to W \to V$ where $W \to W$ is multiplying by electrostatic potential, is given so that for two such basis vectors (the second indexed by primed subscripts) the matrix entry is for instance if $l_i = l'_i, a_i = a'_i, n_i = n'_i$, and $\sigma_i = \sigma'_i$ and all a_i are positive then

$$
\begin{aligned}
&X_{l_1,\ldots,l_k;a_1,\ldots a_k;n_1,\ldots,n_k;\sigma_1,\ldots,\sigma_k;l'_1,\ldots,l'_k;a'_1,\ldots,a'_k;n'_1,\ldots,n'_k;\sigma'_1,\ldots,\sigma'_k} \\
&= \sum_{i<j} \int f_{k,n_i,l_i}(r_1) P_{l_i,l_i+a_i}(z_1,r_1)(h_{a_i,0} \pm i h_{a_i,1})(x_1,y_1) \\
&f_{k,n_j,l_j}(r_2) P_{l_j,l_j+a_j}(z_2,r_2)(h_{a_j,0} \pm i h_{a_j,1})(x_2,y_2) \\
&\sum_{i<j} \sum_{s=0}^{\infty} \frac{r_{\le}^{s}}{r_{\ge}^{s+1}} \frac{1}{s!2^s} P_{s,s}(\frac{x_1x_2+y_1y_2+z_1z_2}{r_1r_2}, 1) \\
&f_{k,n'_i,l'_i}(r_1) P_{l'_i,l'_i+a'_i}(z_1,r_1)(h_{a_i,0} \mp i h_{a'_i,1})(x_1,y_1) \\
&f_{k,n'_j,l'_j}(r_2) P_{l'_j,l'_j+a'_j}(z_2,r_2)(h_{a_j,0} \mp i h_{a_j,1})(x_2,y_2) \\
&- f_{k,n_i,l_i}(r_1) P_{l_1,l_i+a_i}(z_1,r_1)(h_{a_i,0} \pm i h_{a_i,1})(x_1,y_1) \\
&f_{k,n_j,l_j}(r_2) P_{l_j,l_j+a_j}(z_2,r_2)(h_{a_j,0} \pm i h_{a_j,1})(x_2,y_2) \\
&\sum_{s=0}^{\infty} \frac{r_{\le}^{s}}{r_{\ge}^{s+1}} \frac{1}{s!2^s} P_{s,s}(\frac{x_1x_2+y_1y_2+z_1z_2}{r_1r_2}, 1) \\
&f_{k,n'_i,l'_i}(r_2) P_{l'_i,l_i+a'_i}(z_2,r_2)(h_{a_i,0} \mp i h_{a'_i,1})(x_2,y_2) \\
&f_{k,n'_j,l'_j}(r_1) P_{l'_j,l'_j+a'_j}(z_1,r_1)(h_{a'_j,0} \mp i h_{a'_j,1})(x_1,y_1) \\
&dx_1dy_1dz_1dx_2dy_2dz_2/D
\end{aligned}
$$

with D chosen to correct that our basis elements aren't norm one.

This is an easy calculation which can be done by hand in terms of the definite integrals which we described above, and will calculate a little later in terms of π and the natural log function only.

When some a_i are negative we need to muliply by signs $sgn(a_i)$.

The actual perturbation matrix differs slighty from this in matters of sign when a_i can be negative and we don't assume that the two sets of subscripts are equal. Unlike the character calculation, the actual perturbation matrix is unwieldy for hand calculation, but not too unweildy for a simple javascript. It is

$$X_{l_1,\ldots,l_k;a_1,\ldots a_k;n_1,\ldots,n_k;\sigma_1,\ldots,\sigma_k;l'_1,\ldots,l'_k;a'_1,\ldots,a'_k;n'_1,\ldots,n'_k;\sigma'_1,\ldots,\sigma'_k} = \sum_{i<j}\sum_{i_2<j_2}(-1)^{i-i_2+j-j_2}$$

$$\delta_{l_1,\ldots,\widehat{l_i},\ldots,\widehat{l_j},\ldots,l_k;a_1,\ldots,\widehat{a_i},\ldots,\widehat{a_j},....,a_k;n_1,\ldots,\widehat{n_i},\ldots,\widehat{n_j},\ldots,n_k;\sigma_1,\ldots,\widehat{\sigma_i},\ldots,\widehat{\sigma_j},\ldots,\sigma_k;l'_1,\ldots,\widehat{l'_{i_2}},\ldots,\widehat{l'_{j_2}},\ldots,l'_k;a'_1,\ldots,\widehat{a'_{i_2}},\ldots,\widehat{a'_{j_2}},\ldots,a'_k;n'_1,\ldots,\widehat{n'_{i_2}},\ldots,\widehat{n'_{j_2}},\ldots,n'_k;\sigma'_1,\ldots,\widehat{\sigma'_{i_2}},\ldots,\widehat{\sigma'_{j_2}},\ldots,\sigma'_k}$$

$$\sum_{s=0}^{\infty}\Big(\frac{\delta_{\sigma_i\sigma_{i'}}\delta_{\sigma_j\sigma_{j'}}}{s!2^s}(Y(k,l_i+l'_{i2}+s+2,l_j+l'_{j_2}-s+1,n_i,l_i,n'_{i_2},l'_{i_2},n_j,l_j,n'_{j_2},l'_{j_2})$$

$$+Y(k,l_j+l'_{j_2}+s+2,l_i+l'_{i_2}-s+1,n_j,l_j,n'_{j_2},l'_{j_2},n_i,l_i,n'_{i_2},l'_{i_2}))$$

$$(Z(s,l_i,a_i,0,l'_{i_2},a'_{i_2},0,l_j,a_j,0,l'_{j_2},a'_{j_2},0)-Z(s,l_i,a_i,0,l'_{i_2},a'_{i_2},1,l_j,a_j,0,l'_{j_2},a'_{j_2},1)sgn(a'_{i_2})sgn(a'_{j_2})$$

$$+Z(s,l_i,a_i,0,l'_{i_2},a'_{i_2},0,l_j,a_j,1,l'_{j_2},a'_{j_2},1)sgn(a_j)sgn(a'_{j_2})+Z(s,l_i,a_i,0,l'_{i_2},a'_{i_2},1,l_j,a_j,1,l'_{j_2},a'_{j_2},0)sgn(a_j)sgn(a'_{i_2})$$

$$+Z(s,l_i,a_i,1,l'_{i_2},a'_{i_2},0,l_j,a_j,0,l'_{j_2},a'_{j_2},1)sgn(a_i)sgn(a'_{j_2})+Z(s,l_i,a_i,1,l'_{i_2},a'_{i_2},1,l_j,a_j,0,l'_{j_2},a'_{j_2},0)sgn(a_i)sgn(a'_{i_2})$$

$$-Z(s,l_i,a_i,1,l'_{i_2},a'_{i_2},0,l_j,a_j,1,l'_{j_2},a'_{j_2},0)sgn(a_i)sgn(a_j)+Z(s,l_i,a_i,1,l'_{i_2},a'_{i_2},1,l_j,a_j,1,l'_{j_2},a'_{j_2},1)sgn(a_i)sgn(a_j)sgn(a'_{i_2})sgn(a'_{j_2})$$

$$-\frac{\delta_{\sigma_i\sigma_{j'}}\delta_{\sigma_j\sigma_{i'}}}{s!2^s}(Y(k,l_i+l'_{j_2}+s+2,l_j+l'_{i_2}-s+1,n_i,l_i,n'_{j_2},l'_{j_2},n_j,l_j,n'_{i_2},l'_{i_2})$$

$$+Y(k,l_j+l'_{i_2}+s+2,l_i+l'_{j_2}-s+1,n_j,l_j,n'_{i_2},l'_{i_2},n_i,l_i,n'_{j_2},l'_{j_2}))$$

$$(Z(s,l_i,a_i,0,l'_{j_2},a'_{j_2},0,l_j,a_j,0,l'_{i_2},a'_{i_2},0)$$

$$-Z(s,l_i,a_i,0,l'_{j_2},a'_{j_2},1,l_j,a_j,0,l'_{i_2},a'_{i_2},1)sgn(a'_{i_2})sgn(a'_{j_2})+Z(s,l_i,a_i,0,l'_{j_2},a'_{j_2},1,l_j,a_j,1,l'_{i_2},a'_{i_2},0)sgn(a_j)sgn(a'_{j_2})$$

$$+Z(s,l_i,a_i,0,l'_{j_2},a'_{j_2},0,l_j,a_j,1,l'_{i_2},a'_{i_2},1)sgn(a_j)sgn(a'_{i_2})+Z(s,l_i,a_i,1,l'_{j_2},a'_{j_2},1,l_j,a_j,0,l'_{i_2},a'_{i_2},0)sgn(a_i)sgn(a'_{j_2})$$

$$+Z(s,l_i,a_i,1,l'_{j_2},a'_{j_2},0,l_j,a_j,0,l'_{i_2},a'_{i_2},1)sgn(a_i)sgn(a'_{i_2})-Z(s,l_i,a_i,1,l'_{j_2},a'_{j_2},0,l_j,a_j,1,l'_{i_2},a'_{i_2},0)sgn(a_i)sgn(a_j)$$

$$+Z(s,l_i,a_i,1,l'_{j_2},a'_{j_2},1,l_j,a_j,1,l'_{i_2},a'_{i_2},1)sgn(a_i)sgn(a_j)sgn(a'_{i_2})sgn(a'_{j_2}))\Big)$$

$$\Big/\sqrt{\Big(}((Y(k,l_i+l_i+2,l_j+l_j+2,n_i,l_i,n_i,l_i,n_j,l_j,n_j,l_j)$$

$$+Y(k,l_j+l_j+2,l_i+l_i+2,n_j,l_j,n_j,l_j,n_i,l_i,n_i,l_i))$$

$$(Z(0,l_i,a_i,0,l_i,a_i,0,l_j,a_j,0,l_j,a_j,0)-Z(0,l_i,a_i,0,l_i,a_i,1,l_j,a_j,0,l_j,a_j,1)sgn(a_i)sgn(a_j)$$

$$+Z(0,l_i,a_i,0,l_i,a_i,0,l_j,a_j,1,l_j,a_j,1)sgn(a_j)sgn(a_j)+Z(0,l_i,a_i,0,l_i,a_i,1,l_j,a_j,1,l_j,a_j,0)sgn(a_j)sgn(a_i)$$

$$+Z(0,l_i,a_i,1,l_i,a_i,0,l_j,a_j,0,l_j,a_j,1)sgn(a_i)sgn(a_j)+Z(0,l_i,a_i,1,l_i,a_i,1,l_j,a_j,0,l_j,a_j,0)sgn(a_i)sgn(a_i)$$

$$-Z(0,l_i,a_i,1,l_i,a_i,0,l_j,a_j,1,l_j,a_j,0)sgn(a_i)sgn(a_j)+Z(0,l_i,a_i,1,l_i,a_i,1,l_j,a_j,1,l_j,a_j,1)sgn(a_i)sgn(a_j)sgn(a_i)sgn(a_j))$$

$$(Y(k,l'_{i_2}+l'_{i_2}+2,l'_{j_2}+l'_{j_2}+2,n'_{i_2},l'_{i_2},n'_{i_2},l'_{i_2},n'_{j_2},l'_{j_2},n'_{j_2},l'_{j_2})$$

$$+Y(k,l'_{j_2}+l'_{j_2}+2,l'_{i_2}+l'_{i_2}+2,n'_{j_2},l'_{j_2},n'_{j_2},l'_{j_2},n'_{i_2},l'_{i_2},n'_{i_2},l'_{i_2}))$$

$$(Z(0,l'_{i_2},a'_{i_2},0,l'_{i_2},a'_{i_2},0,l'_{j_2},a'_{j_2},0,l'_{j_2},a'_{j_2},0)-Z(0,l'_{i_2},a'_{i_2},0,l'_{i_2},a'_{i_2},1,l'_{j_2},a'_{j_2},0,l'_{j_2},a'_{j_2},1)sgn(a'_{i_2})sgn(a'_{j_2})$$

$$+Z(0,l'_{i_2},a'_{i_2},0,l'_{i_2},a'_{i_2},0,l'_{j_2},a'_{j_2},1,l'_{j_2},a'_{j_2},1)sgn(a'_{j_2})sgn(a'_{j_2})+Z(0,l'_{i_2},a'_{i_2},0,l'_{i_2},a'_{i_2},1,l'_{j_2},a'_{j_2},1,l'_{j_2},a'_{j_2},0)sgn(a'_{j_2})sgn(a'_{i_2})$$

$$+Z(0,l'_{i_2},a'_{i_2},1,l'_{i_2},a'_{i_2},0,l'_{j_2},a'_{j_2},0,l'_{j_2},a'_{j_2},1)sgn(a'_{i_2})sgn(a'_{j_2})+Z(0,l'_{i_2},a'_{i_2},1,l'_{i_2},a'_{i_2},1,l'_{j_2},a'_{j_2},0,l'_{j_2},a'_{j_2},0)sgn(a'_{i_2})sgn(a'_{i_2})$$

$$-Z(0,l'_{i_2},a'_{i_2},1,l'_{i_2},a'_{i_2},0,l'_{j_2},a'_{j_2},1,l'_{j_2},a'_{j_2},0)sgn(a'_{i_2})sgn(a'_{j_2})+Z(0,l'_{i_2},a'_{i_2},1,l'_{i_2},a'_{i_2},1,l'_{j_2},a'_{j_2},1,l'_{j_2},a'_{j_2},1)sgn(a'_{i_2})sgn(a'_{j_2})sgn(a'_{i_2})sgn(a$$

Here a hat symbol $\widehat{\ }$ indicates that a particular subscript does not actually occur. The number

$$\delta_{l_1,\ldots,\widehat{l_i},\ldots,\widehat{l_j},\ldots,l_k;a_1,\ldots,\widehat{a_i},\ldots,\widehat{a_j},\ldots.,a_k;n_1,\ldots,\widehat{n_i},\ldots,\widehat{n_j},\ldots,n_k;\sigma_1,\ldots,\widehat{\sigma_i},\ldots,\widehat{\sigma_j},\ldots,\sigma_k;l'_1,\ldots,\widehat{l'_{i_2}},\ldots,\widehat{l'_{j_2}},\ldots,l'_k;a'_1,\ldots,\widehat{a'_{i_2}},\ldots,\widehat{a'_{j_2}},\ldots,a'_k;n'_1,\ldots,\widehat{n'_{i_2}},\ldots,\widehat{n'_{j_2}},\ldots,n'_k;\sigma'_1,\ldots,\widehat{\sigma'_{i_2}},\ldots,\widehat{\sigma'_{j_2}},\ldots,\sigma'_k}$$

is just defined to be 0 unles the first set of subscripts equals the second, and otherwise 1. This δ arises when we evaluate a $k-2$-fold iterated integral of products of just two functions obtaining the product of of $k-2$ simpler delta functions just expressing orthogonality of the basic functions which we chose.

The denominator can be simplified by removing four pairs of cancelling terms. Since we will just use a simple javascript to evaluate the sum, the extra work will not be difficult and we'll leave the eight cancelling terms in place. Each matrix entry is thus a sum of integrals which we will directly evaluate in terms of natural logs and π, working as if it were a high-school calculus problem. The sum in s (the multipole expansion) only needs to be taken up to $s=4$ (what is called the quadropole term) for good accuracy.

Since the electrostatic repulsion term in the potential is invariant under $SU_2 \times SU_2$ the eigenspaces of this matrix will necessarily be representations of $SU_2 \times SU_2$, and in every generic case will of course be irreducible representations. If the Casimir operators of $SU_2 \times 1$ and $1 \times SU_2$ in the action on the exterior power are written in the relevant basis (not a basis with respect to which one would ordinarily consider the Casimir operator, but, rather involving a change of basis using the coefficient of the Legendre polynomials as a matrix), then the matrix above will commute with both Casimir operators.

For low atomic number, the first case we're considering, where the action of $SU_2 \times SU_2$ on the exterior power is multiplicity-free, one then has a three-way bijection, between eigenspaces for this matrix, versus a set of isomorphism types of irreducible representations of $SU_2 \times SU_2$ (which also correspond to characters), versus what one might call Russell-Saunders configurations of spectral lines, consisting of a term symbol representing a spectral line which, viewed more carefully is seen to consist of Russell-Saunders lines, and each of these which can be further resolved into finer lines by either observing the spectrum in the presence of a magnetic field or perhaps better resolving one spectral line coming from a glass prism by a magnetic prism to generate Stern-Gerlach lines.

For example the term symbol ${}^3D$ corresponding to $e_2(S)e_4(L)$ has three Russell-Saunders lines (three being the minimum of $2+1$ and $4+1$) and the dimensions of the corresponding representations are $7, 5, 3$ corresponding to one of the Russell-Saunders lines splitting into seven parts, one into five parts, one into three parts under magnetism.

Let's now calculate the actual values of the various Z and Y definite integrals, As I just mentioned, these can easily be calculated in terms of π, the natural logarithm function, and rational numbers. The integral of a monomial $x^{2a}y^{2b}z^{2c}$ in (x, y, z) space over the unit two sphere for a, b, c natural numbers (note that a monomial with any odd exponent integrates to zero). For $r^2 = x^2 + y^2 + z^2$,

$$\int \frac{x^{2a}y^{2b}z^{2c}}{r^{2a+2b+2c}} dxdydz \cdot \int_0^\infty e^{-r^2} r^{2a+2b+2c} r^2 dr$$
$$= \int e^{-x^2} x^{2a} e^{-y^2} y^{2b} e^{-z^2} z^{2b} dxdydz$$
$$= \Gamma(a+\frac{1}{2})\Gamma(b+\frac{1}{2})\Gamma(c+\frac{1}{2}),$$

while the second factor is

$$\int_0^\infty e^{-r^2} r^{a+b+c+2} \frac{r}{2} \frac{dr}{r^2}$$
$$= \frac{1}{2}\Gamma(a+b+c+\frac{3}{2}).$$

Thus the integral of the monomial over the unit sphere is

$$2\frac{\Gamma(a+\frac{1}{2})\Gamma(b+\frac{1}{2})\Gamma(c+\frac{1}{2})}{\Gamma(a+b+c+\frac{3}{2})}.$$

$$= \frac{4\pi}{2a+2b+2c+1} \frac{\binom{a+b+c}{a,\ b,\ c}}{\binom{2a+2b+2c}{2a,\ 2b,\ 2c}}$$

where the second factor is the ratio of trinomial coefficients.

Let's then calculate the second integral, taking account of the fact that we can set $r_1 = r_2 = 1$. It evaluates to a rational multiple of π, given

$$Z_{s,l_1,a_1,\epsilon_1,l_2,a_2,\epsilon_2,l_3,a_3,\epsilon_3,l_4,a_4,\epsilon_4}$$

$$= \int_{S^2\times S^2} \sum_{i_1=0}^{[\frac{a_1-\epsilon_1}{2}]} \sum_{i_2=0}^{[\frac{a_2-\epsilon_2}{2}]} \sum_{i_3=0}^{[\frac{a_3-\epsilon_3}{2}]} \sum_{i_4=0}^{[\frac{a_4-\epsilon_4}{2}]} \sum_{j_1=0}^{[\frac{l_1-a_1}{2}]} \sum_{j_2=0}^{[\frac{l_2-a_2}{2}]} \sum_{j_3=0}^{[\frac{l_3-a_3}{2}]} \sum_{j_4=0}^{[\frac{l_4-a_4}{2}]} \sum_{w=0}^{[s-\frac{s}{2}]}$$

$$(-1)^{i_1+i_2+i_3+i_4+j_1+j_2+j_3+j_4+w} \binom{a_1}{2i_1+\epsilon_1} \binom{a_2}{2i_2+\epsilon_2} \binom{a_3}{2i_3+\epsilon_3} \binom{a_4}{2i_4+\epsilon_4}$$

$$\frac{(2l_1-2j_1)!}{(l_1-2j_1-a_1)!} \frac{(2l_2-2j_2)!}{(l_2-2j_2-a_2)!} \frac{(2l_3-2j_3)!}{(l_3-2j_3-a_3)!} \frac{(2l_4-2j_4)!}{(l_4-2j_4-a_4)!}$$

$$\frac{(2s-2w)!}{(2s-2w-s)!} \binom{l_1}{j_1} \binom{l_2}{j_2} \binom{l_3}{j_3} \binom{l_4}{j_4} \binom{s}{w}$$

$$x_1^{a_1-2i_1-\epsilon_1+a_2-2i_2-\epsilon_2} y_1^{2i_1+\epsilon_1+2i_2+\epsilon_2} z_1^{l_1-2j_1-a_1+l_2-2j_2-a_2}$$

$$x_2^{a_3-2i_3-\epsilon_3+a_4-2i_4-\epsilon_4} y_2^{2i_3+\epsilon_3+2i_4+\epsilon_4} z_2^{l_3-2j_3-a_3+l_4-2j_4-a_4}$$

$$(x_1x_2+y_1y_2+z_1z_2)^{(s-2w)}\sigma$$

$$= \sum_{i_1=0}^{[\frac{a_1-\epsilon_1}{2}]} \sum_{i_2=0}^{[\frac{a_2-\epsilon_2}{2}]} \sum_{i_3=0}^{[\frac{a_3-\epsilon_3}{2}]} \sum_{i_4=0}^{[\frac{a_4-\epsilon_4}{2}]} \sum_{j_1=0}^{[\frac{l_1-a_1}{2}]} \sum_{j_2=0}^{[\frac{l_2-a_2}{2}]} \sum_{j_3=0}^{[\frac{l_3-a_3}{2}]} \sum_{j_4=0}^{\frac{[l_4-a_4}{2}]} \sum_{w=0}^{[s-\frac{s}{2}]} (-1)^{i_1+i_2+i_3+i_4+j_1+j_2+j_3+j_4+w}$$

$$\binom{a_1}{2i_1}\binom{a_2}{2i_2}\binom{a_3}{2i_3}\binom{a_4}{2i_4}$$

$$\frac{(2l_1-2j_1)!}{(l_1-2j_1-a_1)!}\frac{(2l_2-2j_2)!}{(l_2-2j_2-a_2)!}\frac{(2l_3-2j_3)!}{(l_3-2j_3-a_3)!}\frac{(2l_4-2j_4)!}{(l_4-2j_4-a_4)!}\frac{(2s-2w)!}{(2s-2w-s)!}$$

$$\binom{l_1}{j_1}\binom{l_2}{j_2}\binom{l_3}{j_3}\binom{l_4}{j_4}$$

$$\sum_{q=0}^{s-2w} \sum_{v=0}^{s-2w-q} \frac{(s-2w)!}{q!v!(s-2w-q-v)!}$$

$$\frac{1}{2}(1+(-1)^{a_1+\epsilon_1+a_2+\epsilon_2+q})\frac{1}{2}(1+(-1)^{\epsilon_1+\epsilon_2+v})\frac{1}{2}(1+(-1)^{a_1+a_2+l_1+l_2+s-2w-q-v})$$

$$\frac{1}{2}(1+(-1)^{a_3+\epsilon_3+a_4+\epsilon_4+q})\frac{1}{2}(1+(-1)^{\epsilon_3+\epsilon_4+v})\frac{1}{2}(1+(-1)^{a_3+a_4+l_3+l_4+s-2w-q-v})$$

$$2\frac{\Gamma\left(\frac{a_1-2i_1-\epsilon_1+a_2-2i_2-\epsilon_2+q+1}{2}\right)\Gamma\left(\frac{2i_1+\epsilon_1+2i_2+\epsilon_2+v+1}{2}\right)\Gamma\left(\frac{l_1-2j_1-a_1+l_2-2j_2-a_2+(s-2w-q-v)+1}{2}\right)}{\Gamma\left(\left(\frac{a_1-2i_1-\epsilon_1+a_2-2i_2-\epsilon_2+q+1}{2}\right)+\left(\frac{2i_1+\epsilon_1+2i_2+\epsilon_2+v+1}{2}\right)+\left(\frac{l_1-2j_1-a_1+l_2-2j_2-a_2+(s-2w-q-v)+1}{2}\right)\right)}$$

$$2\frac{\Gamma\left(\frac{a_3-2i_3-\epsilon_3+a_4-2i_3-\epsilon_3+q+1}{2}\right)\Gamma\left(\frac{2i_3+\epsilon_3+2i_4+\epsilon_4+v+1}{2}\right)\Gamma\left(\frac{l_3-2j_3-a_3+l_4-2j_4-a_4+(s-2w-q-v)+1}{2}\right)}{\Gamma\left(\left(\frac{a_3-2i_3-\epsilon_3+a_4-2i_3-\epsilon_3+q+1}{2}\right)+\left(\frac{2i_3+\epsilon_3+2i_4+\epsilon_4+v+1}{2}\right)+\left(\frac{l_3-2j_3-a_3+l_4-2j_4-a_4+(s-2w-q-v)+1}{2}\right)\right)} \quad (9)$$

and one may substitute then the given values of the gamma function as ratios of trinomial coefficients.

For the first integral,

$$Y_{k,a,b,n_1,l_1,n_2,l_2,n_3,l_3,n_4,l_4}$$

$$= \beta^{a+b+2} \sum_{i_1=0}^{n_1-l_1-1} \sum_{i_2=0}^{n_2-l_2-1} \sum_{i_3=0}^{n_3-l_3-1} \sum_{i_4=0}^{n_4-l_4-1}$$

$$\binom{n_1+l_1}{n_1-l_1-1-i_1} \binom{n_2+l_2}{n_2-l_2-1-i_2} \binom{n_3+l_3}{n_3-l_3-1-i_3} \left(\begin{matrix} n_4+l_4 \\ n_4-4_4-1-i \end{matrix} \right.$$

$$\frac{(\frac{k}{n_1}\beta)^{i_1}}{i_1!} \frac{(\frac{k}{n_2}\beta)^{i_2}}{i_2!} \frac{(\frac{k}{n_3}\beta)^{i_3}}{i_3!} \frac{(\frac{k}{n_4}\beta)^{i_4}}{i_4!}$$

$$\int_0^\infty \int_0^{r_2} e^{k\beta(r_1(\frac{1}{2n_1}+\frac{1}{2n_2})+r_2(\frac{1}{2n_3}+\frac{1}{2n_4}))} r_1^{a+i_1+i_2} r_2^{b+i_3+i_4} dr_1 dr_2$$

$$= \sum_{i_1=0}^{n_1-l_1-1} \sum_{i_2=0}^{n_2-l_2-1} \sum_{i_3=0}^{n_3-l_3-1} \sum_{i_4=0}^{n_4-l_4-1}$$

$$\binom{n_1+l_1}{n_1-l_1-1-i_1} \binom{n_2+l_2}{n_2-l_2-1-i_2} \binom{n_3+l_3}{n_3-l_3-1-i_3} \left(\begin{matrix} n_4+l_4 \\ n_4-4_4-1-i \end{matrix} \right.$$

$$\frac{(\frac{k}{n}\beta)^{i_1}}{i_1!} \frac{(\frac{k}{n}\beta)^{i_2}}{i_2!} \frac{(\frac{k}{n}\beta)^{i_3}}{i_3!} \frac{(\frac{k}{n}\beta)^{i_4}}{i_4!}$$

$$\int_0^\infty e^{k\beta r_2(\frac{1}{2n_3}+\frac{1}{2n_4})} r_2^{i_3+i_4+b} \int_0^{r_2} e^{k\beta r_1(\frac{1}{2n_1}+\frac{1}{2n_2})} r_1^{i_1+i_2+a} dr_1 dr_2$$

We will only be evaluating the original integral when $a \geq 0$ and $a+b \geq 1$. Now there are two cases. If $i_3+i_4+b \geq 0$ we can simply write

$$
\begin{aligned}
&\int_0^\infty e^{k\beta r_2(\frac{1}{2n_3}+\frac{1}{2n_4})} r_2^{i_3+i_4+b} \int_0^{r_2} e^{k\beta r_1(\frac{1}{2n_1}+\frac{1}{2n_2})} r_1^{i_1+i_2+a} dr_1 dr_2 \\
&= \int_0^\infty e^{k\beta r_2(\frac{1}{2n_1}+\frac{1}{2n_2}+\frac{1}{2n_3}+\frac{1}{2n_4})} r_2^{i_3+i_4+b} \\
&\sum_{j=0}^{i_1+i_2+a} (-1)^j \frac{r_2^{i_1+i_2+a-j}}{(k\beta(\frac{1}{2n_1}+\frac{1}{2n_2}))^{j+1}} \frac{(i_1+i_2+a)!}{(i_1+i_2+a-j)!} \\
&+ \frac{(-1)^{i_1+i_2+a+1}(i_1+i_2+a)!}{(k\beta(\frac{1}{2n_1}+\frac{1}{2n_2}))^{i_1+i_2+a+1}} e^{k\beta r_2(\frac{1}{2n_3}+\frac{1}{2n_4})} dr_2 \\
&= \sum_{j=0}^{i_1+i_2+a} (-1)^j \frac{1}{(k\beta(\frac{1}{2n_1}+\frac{1}{2n_2}))^{j+1}} \frac{(i_1+i_2+a)!}{(i_1+i_2+a-j)!} \\
&(-1)^{i_1+i_2+i_3+i_4+a+b-j+1} \frac{(i_1+i_2+i_3+i_4+a+b-j)!}{(k\beta(\frac{1}{2n_1}+\frac{1}{2n_2}+\frac{1}{2n_3}+\frac{1}{2n_4}))^{i_1+i_2+i_3+i_4+a+b-j+1}} \\
&+ \frac{(-1)^{i_1+i_2+a+1+i_3+i_4+b+1}}{(k\beta(\frac{1}{2n_1}+\frac{1}{2n_2}))^{i_1+i_2+a+1}} \frac{(i_3+i_4+b)!}{k\beta(\frac{1}{2n_3}+\frac{1}{2n_4})^{i_3+i_4+b+1}} (i_1+i_2+a)!) \\
&= \sum_{j=0}^{i_1+i_2+a} (-1)^{i_1+i_2+i_3+i_4+a+b+1} \frac{1}{(k\beta(\frac{1}{2n_1}+\frac{1}{2n_2}))^{j+1}} \frac{(i_1+i_2+a)!}{(i_1+i_2+a-j)!} \\
&\frac{(i_1+i_2+i_3+i_4+a+b-j)!}{(k\beta(\frac{1}{2n_1}+\frac{1}{2n_2}+\frac{1}{2n_3}+\frac{1}{2n_4}))^{i_1+i_2+i_3+i_4+a+b-j+1}} \\
&+ \frac{(-1)^{i_1+i_2+a+1+i_3+i_4+b+1}}{(k\beta(\frac{1}{2n_1}+\frac{1}{2n_2}))^{i_1+i_2+a+1}} \frac{(i_3+i_4+b)!}{(k\beta(\frac{1}{2n_3}+\frac{1}{2n_4}))^{i_3+i_4+b+1}} (i_1+i_2+a)!
\end{aligned}
\tag{10}
$$

If on the other hand $i_1 + i_2 + b < 0$ we can use the integral equation which I found in the integral tables on the NIST website [5]

$$\int_0^\infty xe^{-qx}E_1(wx)dx = \frac{1}{q^2}[ln(1+\frac{q}{w}) - \frac{q}{q+w}]. \quad (11)$$

Setting $q = k\beta(\frac{1}{2n_3} + \frac{1}{2n_4})$ and $w = k\beta(\frac{1}{2n_1} + \frac{1}{2n_2})$ this gives the desired integral for the case $a = 1, b = -1$. We always have $a + b \geq 2$ to begin with, and so integration by parts can certainly always reduce to the calculation of this one integral.

That is, if we write

$$I_1(q, m) = \int_0^\infty e^{-qx}x^m dx$$

$$I_2(q, w, a, b) = \int_0^\infty \int_x^\infty e^{-qx-wy}\frac{x^a}{y^b} \quad (12)$$

we can write an expression for $I_1(q, m)$ by recursively using the rules

$$I_1(q, 0) = 1/q$$

$$I_1(q, m) = \frac{m}{q}I_1(q, m-1)$$

and for I_2 the recursive rules that for $b \geq 2$

$$I_2(q, w, a, b) = \frac{-1}{1-b}I_1(q+w, a+1-b) + \frac{w}{1-b}I_2(q, w, b-1),$$

if $b = 1$ and $a \geq 1$

$$I_2(q, w, a, b) = \frac{a}{q}I_2(q, w, a-1, b) - \frac{1}{q}I_1(w+q, a-b)$$

and finally if $a = b = 1$ $I_2(q, w, a, b)$ is given by the right side of (11).

Now that we've calculated each individual eigenvalue, the perturbation character is below (where the subscripts on X are not repeated, but they only refer to the diagonal matrix entries, we have not yet used the full matrix).

$$\sum_{\phi=0}^{\infty}\sum_{\psi=0}^{\infty}\sum_{w=0}^{\infty}\ \sum_{\substack{a_1+...+a_w=k\\ a_1<a_2<...<a_k}}\ \sum_{l_1=\lceil\frac{a_1-1}{2}\rceil}^{\infty}\cdots\sum_{l_w=\lceil\frac{a_1-1}{2}\rceil}^{\infty}\ \sum_{i_1+j_1=a_1}\cdots\sum_{i_w+j_w=a_w}$$

$$\sum_{l_1+1\leq n_{1,1}<...<n_{1,i_1}<\infty}\cdots\sum_{l_w+1\leq n_{w,1}<...<n_{w,i_w}<\infty}$$

$$\sum_{-l_1\leq m_{1,1}\leq...\leq m_{1,i_1}\leq l_1}\ \sum_{-l_1\leq m'_{1,1}\leq...\leq m'_{1,j_1}\leq l_1}\cdots\sum_{-l_w\leq m_{w,1}\leq...\leq m_{w,i_w}\leq l_w}\ \sum_{-l_w\leq m'_{w,1}\leq...\leq m'_{w,j_w}\leq l_w}$$

$$\sum_{i_1+...+i_w-(j_1+...+j_w)=\phi}\ \sum_{\sum m_{\alpha,\beta}+\sum n_{\alpha\beta}=\psi} Q_{k_p,l_1,m_{1,1},n_{1,1},l_1,m_{1,2},n_{1,2},...l_1,m_{1,i_1},n_{1,i_1},}$$

$$_{l_1,m'_{1,1},n_{1,1},...,l_1,m'_{1,j_1},n_{1,j_1},l_2,m_{2,1},n_{2,1},l_2,m_{2,2},n_{2,2},...,l_2,m_{2,i_2},n_{2,i_2},l_2,m'_{2,1},n_{2,1},l2,m'_{2,2},n_{2,2},...,l_2,m'_{2,j_2},n_{2,j_2},}$$

$$_{...,l_w,m'_{w,j_w},n_{w,j_w},\delta}\ S^{\phi}L^{2\psi}.$$

where the symbol Q here denotes just the *diagonal* element of the matrix X which we calculated, in which a spin number of 1 is inserted after each primed occurrence of m and 0 after each unprimed (and the index sequence repeated to get a diagonal entry).

Multiplying by $(1-S^{-2})(1-L^{-2})$ and projecting to the positive weight space converts the time derivative of the trace of the operator on the moving eigensapces into just the sum of the eigenvalues on highest weight monomials. If the first order perturbation were completely accurate, the trace on each highest weight line would be the perturbation of the eigenvalue which applies to the whole corresponding representation. The coefficients in this character are specific numbers, calculated by (1) through (12) above.

This finishes an explicit closed formula for the spectrum of every atom up to the first case when wave forms for that atom develop multiplicities, in terms of natural logarithms, rational numbers, and the number π, assuming that the quadropole expansion and first order perturbation are accurate.

In cases when the representation is multiplicity free, it describes the energy levels of Schroedinger's equation including the first order electrostatic perturbation.

It is a hand calculation to solve the integrals and term symbols above.

Let's go through the character calculation for an excited configuration of Carbon, the first one with many term symbols, that is $1s^2 2s^2 2p^1 3p^1$. Substituting all the previous equations into the equation above expcicitly gives the perturbation character in units of THz. It has positive part $158464 + 105487\ L^2 + 528020\ L^4 + 790714\ S^2 + 527184\ L^2S^2 + 263039\ L^4S^2$. Multiplying by $(1-L^{-2})(1-S^{-2})$ as though we were finding highest weights of a character (although we are not) gives

$$266234+262712\,L^2+264980\,L^4+263530S^2+264144L^2S^2+263040L^4S^2.$$

The actual character of the space of wave functions with respect to $SU_2\times SU_2$ is by the earlier type of calculation

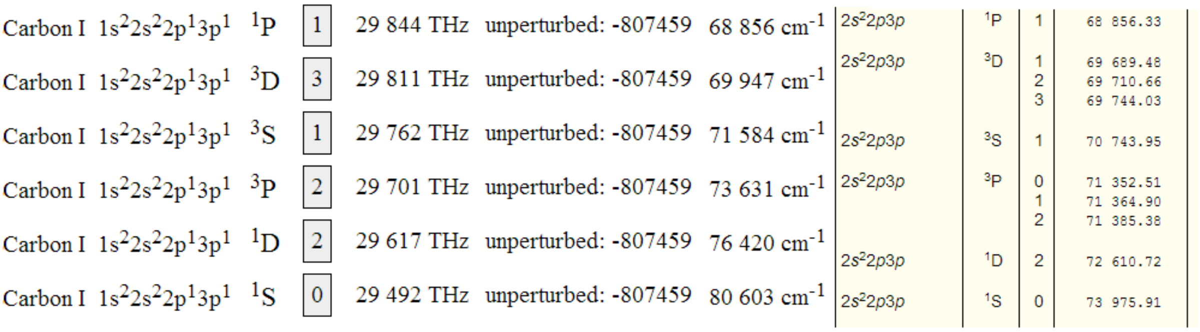
$$6+4L^2+2L^4+3S^2+2L^2S^2+L^4S^2.$$

Now here multiplying by $(1-L^{-2})(1-S^{-2})$ and taking the positive part gives the sum of highest weight monomials

$$1+L^2+L^4+S^2+L^2S^2+L^4S^2,$$

and the frequency displacements are taken to be the the terms of the second expression which occur in the six positions indicated by the fourth expression (in this case all of them).

The term symbols produced by the character calculation are in the order agreeing with the NIST database



Carbon I	$1s^2 2s^2 2p^1 3p^1$	^1P	1	29 844 THz	unperturbed: -807459	68 856 cm^{-1}	$2s^2 2p3p$	^1P	1	68 856.33
Carbon I	$1s^2 2s^2 2p^1 3p^1$	^3D	3	29 811 THz	unperturbed: -807459	69 947 cm^{-1}	$2s^2 2p3p$	^3D	1 2 3	69 689.48 69 710.66 69 744.03
Carbon I	$1s^2 2s^2 2p^1 3p^1$	^3S	1	29 762 THz	unperturbed: -807459	71 584 cm^{-1}	$2s^2 2p3p$	^3S	1	70 743.95
Carbon I	$1s^2 2s^2 2p^1 3p^1$	^3P	2	29 701 THz	unperturbed: -807459	73 631 cm^{-1}	$2s^2 2p3p$	^3P	0 1 2	71 352.51 71 364.90 71 385.38
Carbon I	$1s^2 2s^2 2p^1 3p^1$	^1D	2	29 617 THz	unperturbed: -807459	76 420 cm^{-1}	$2s^2 2p3p$	^1D	2	72 610.72
Carbon I	$1s^2 2s^2 2p^1 3p^1$	^1S	0	29 492 THz	unperturbed: -807459	80 603 cm^{-1}	$2s^2 2p3p$	^1S	0	73 975.91

The six numbers in units of cm^{-1} just result by dividing each of the six coefficients in the character formula by the speed of light in centimeters per second.

The right one-third of the image is a photocopy of data from the NIST database. On the left I have added a reference constant to all the values to make the first values coincide.

The calculation for the trace of just the identity map for the vector space associated to the same the 'electron configuration' $1s^2 2s^2 2p^1 3p^1$ shows that it is actually multiplicity-free. When we multiplied the character of the representation $6+4L^2+2L^4+3S^2+2L^2S^2+L^4S^2$ by $(1-L^2)(1-S^2)$ and deleted all but the positive degree terms, the result $1+L^2+L^4+S^2+L^2S^2+L^4S^2$ had all nonzero coefficients equal to 1, showing us that each irreducible summand occurs with multiplicity one.

The ordering in the NIST database agrees with the energy levels coming from the character calculation, while both are significantly different than extending the the Hund rule ordering for the ground state, unchanged to higher states (as it had originally been envisioned in Hund's first paper) which would have been ${}^3D$, ${}^3P$, ${}^3S{}^1D$, ${}^1P$, ${}^1S$.

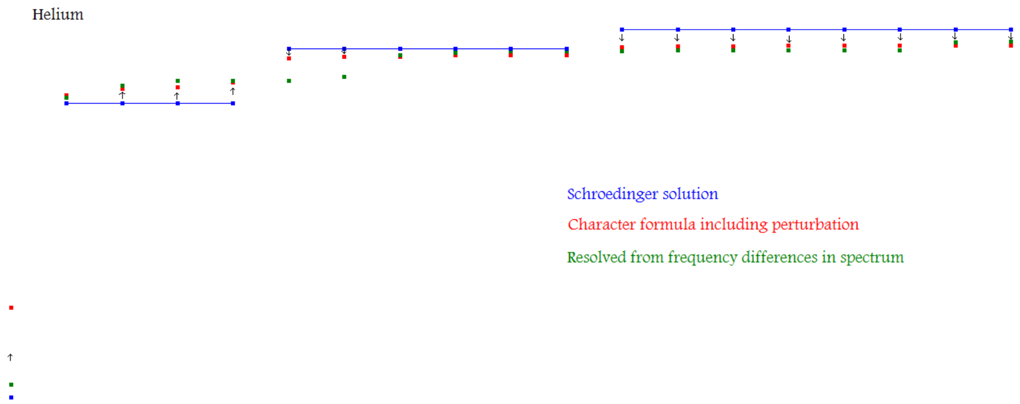
Since the identification of term symbols is a matter of spectrographic observation, it is also true that the character calculation agrees with experimental observation to some extent.

Recall, as I mentioned, that the number of of fine lines coming from each irreducible representation must equal either the preceding superscript in the term symbol minus one, a number which we've called s, or else it must equal $2l$ where $l = 0, 1, 2, ...$ is the number corresponding to the letter $S, P, ...$ whichever is the smaller; while the total number of magnetic lines coming from all RS lines combined must equal $(s+1)(2l+1)$. Actually there is a little ambiguity as such observation cannot detect interchanging the two factors. the character calculation agrees with experiment also.

Clearly action of $SU_2 \times SU_2$ commutes with the perturbation operator, as the electrostatic potential function is invariant for that whole group. Therefore the first order electrostatic perturbation merely acts as a scalar on each (irreducible) isotypical component for the action of $SU_2 \times SU_2$ in the case when the whole representation is multiplicity free. A little later I'll mention how to extend the calculation to the case of arbitrary multiplicity, and and also to obtain the frequencies of the fine spectral lines (the fine structure of the spectrum).

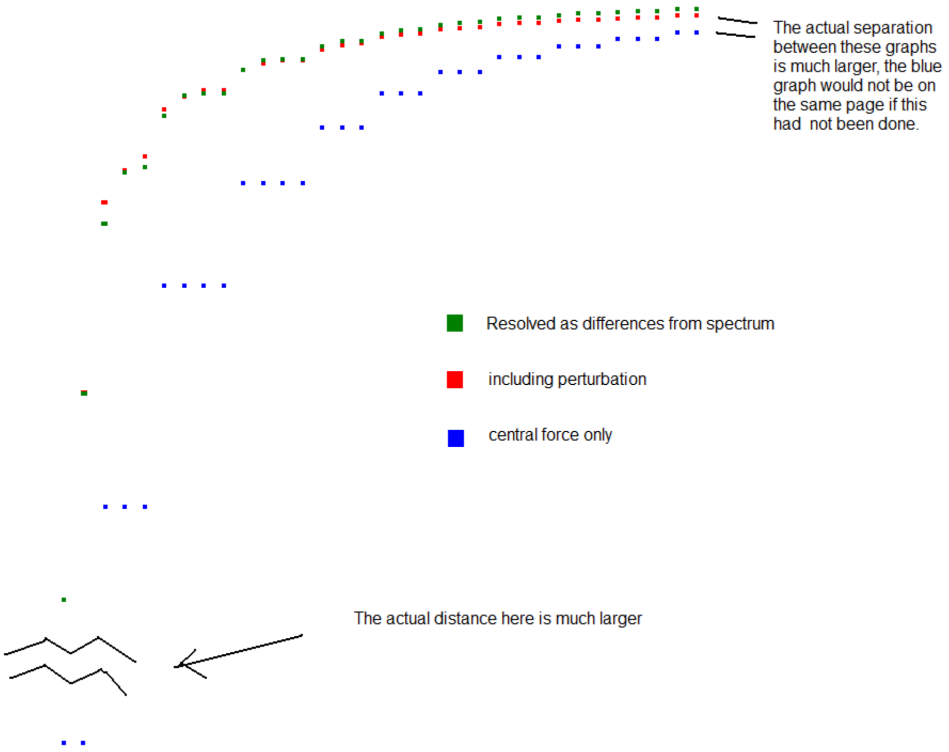
It probably is important though to stress that as elegant as the character-theoretic interpretation is, it is describing nothing theoretically any deeper than the eigenspaces and eigenvalues of the matrix X described a few pages earlier, in this case a size 36 matrix. The coefficients of that character are the eigenvalues of eigenspaces whose dimensions are $15, 9, 5, 3, 3, 1$. At the same time, having a direct description (up to a complex scalar magnitude and phase) of one explicit pair of highest weight wave functions corresponding to each spectral line makes a connection between geometry and physics.

Here are a few levels for Helium and Lithium. There was no attempt to discover the base energy of He III or Li IV; in each case I've translated all three graphs vertically to match. The vertical axis is frequency.

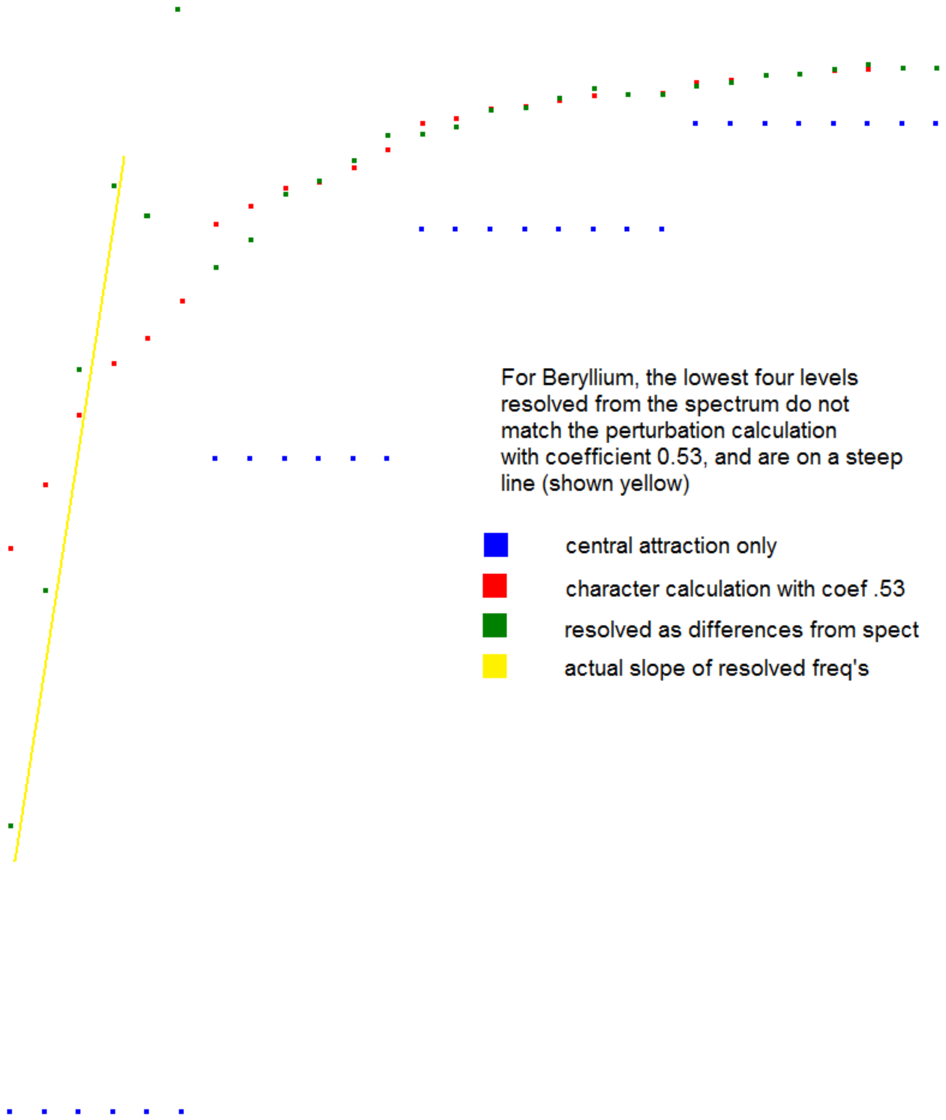


For Lithium, the graph shows using the perturbation coefficient of 0.69865 for the first excited level, and 0.741 for all the remaining levels. The translation made the first pair of data points coincide, and the first perturbation coefficient really only changed the translation for all subsequent points. It might have made more sense to have done a careful adjustment of the 0.741 perturbation coefficient that was used for all subsequent points, so that the overall slope of the green curve would be exactly the same as the red curve.

The perturbation had the effect of moving the blue curve up considerably (the actual displacement is too large to fit both curves on the page, as the legend explains). The step-function behaviour of the blue curve is cancelled by an opposite step-function behaviour of the perturbation, so that what remains is only the amount of step-wise behaviour that actually occurs when differences are resolved from the spectrum.



For the next atom, Beryllium, the perturbation coefficient of 0.53 matches most levels resolved from the spectrum, but the actual first four levels resolved from the spectrum are on a much steeper line, not matching that calculation at all



For Beryllium, the lowest four levels resolved from the spectrum do not match the perturbation calculation with coefficient 0.53, and are on a steep line (shown yellow)

I should explain what I mean by saying that the observed levels are on a steep slope! What I mean is, we have given the electron configurations and term symbols the ordering which the perturbation calculation says that they should have. That is, in the sequence

$$1s^2 2s^2\ {}^1S,\ 1s^2 2s^1 2p^1\ {}^3P^\circ,\ 1s^2 2s^1 2p^1\ {}^1P^\circ,\ 1s^2 2s^2 2p^2\ {}^3P,\ 1s^2 2p^2\ {}^1D,\ 1s^2 2p^2\ {}^1S, \ldots$$

The same levels resolved as frequency differences are spaced out differently, covering the whole range, so that in the NIST database $1s^2 2s^2\ {}^1S$ is even considered to be above the ionization limit.

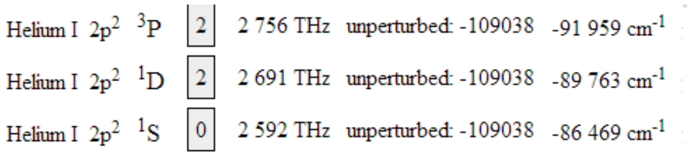
Here is the character calculation determining these particular term symbols and their levels according to the perturbation coefficient of 0.53.

```
based on: 1                                       Extract highest weights: 1                 reduced char: 5211327162727245
based on: 2 + 2 L^2 + S^2 + L^2S^2                Extract highest weights: L^2 + L^2S^2      reduced char: 5581979828294981 L^2 + 5387612548340335 L^2S^2
based on: 2 + 2 L^2 + S^2 + L^2S^2                Extract highest weights: L^2 + L^2S^2      reduced char: 5581979828294981 L^2 + 5387612548340335 L^2S^2
based on: 3 + 2 L^2 + L^4 + S^2 + L^2S^2          Extract highest weights: 1 + L^4 + L^2S^2  reduced char: 5900801219208142 + 5795842888032631 L^4 + 5725870667248959 L^2S^2
based on: 3 + 2 L^2 + L^4 + S^2 + L^2S^2          Extract highest weights: 1 + L^4 + L^2S^2  reduced char: 5900801219208142 + 5795842888032631 L^4 + 5725870667248959 L^2S^2
based on: 3 + 2 L^2 + L^4 + S^2 + L^2S^2          Extract highest weights: 1 + L^4 + L^2S^2  reduced char: 5900801219208142 + 5795842888032631 L^4 + 5725870667248959 L^2S^2
based on: 2 + S^2                                 Extract highest weights: 1 + S^2           reduced char: 4337579215072080 + 4287980289698860 S^2
based on: 2 + S^2                                 Extract highest weights: 1 + S^2           reduced char: 4337579215072080 + 4287980289698860 S^2
based on: 2 + 2 L^2 + S^2 + L^2S^2                Extract highest weights: L^2 + L^2S^2      reduced char: 4407791421214024 L^2 + 4389008396220624 L^2S^2
based on: 2 + 2 L^2 + S^2 + L^2S^2                Extract highest weights: L^2 + L^2S^2      reduced char: 4407791421214024 L^2 + 4389008396220624 L^2S^2
based on: 2 + 2 L^2 + 2 L^4 + S^2 + L^2S^2 + L^4S^2 Extract highest weights: L^4 + L^4S^2    reduced char: 4496421661682106 L^4 + 4447961457199140 L^4S^2
based on: 2 + 2 L^2 + 2 L^4 + S^2 + L^2S^2 + L^4S^2 Extract highest weights: L^4 + L^4S^2    reduced char: 4496421661682106 L^4 + 4447961457199140 L^4S^2
```

With the perturbation coefficient instead set to 1, levels 2,3 and 4 can all be made nearly correct, but not the lowest (ground) level.

Regarding the Aufbau, the first place where the Aufbau actually contradicts considering sums of reciprocal squares is for Potassium, where the Aufbau says $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$ has a lower energy level than $1s^2 2s^2 2p^6 3s^2 3p^6 3d$. The $4p, 4s$ ordering is right for the compensation coefficient at .144 or less, and the $4p, 3d$ ordering is right for values larger than .148. As I'm currently doing things there is no value which puts all the configurations in the correct order.

As a check that we have not made any mistake, and are correctly copying/generalizing what is intended, we can verify one of Condon's statements in his book; that for a p^2 orbital, if you were to ignore inner electrons, the energy ratios of the term symbols would be in the ratio which he denotes $(^1S -^1 D) : (^1D -^3 P) = 3 : 2$. We can give the script a fictitiously high excited level of Helium to test this, and we do find this ratio.



Helium I	$2p^2$	^{3}P	2	2 756 THz	unperturbed: -109038	-91 959 cm^{-1}
Helium I	$2p^2$	^{1}D	2	2 691 THz	unperturbed: -109038	-89 763 cm^{-1}
Helium I	$2p^2$	^{1}S	0	2 592 THz	unperturbed: -109038	-86 469 cm^{-1}

The NIST classification online says that it is taken from Raymond L. Kelly's book, which uses a computer program by R. D. Cowan, and consultations with many spectrographers. As I mentioned, part of the analysis would be experimental, as the actual dimension of each representation is presumed to be the number of lines which the line would split into when the atom is placed in a strong magnetic field, or that it would not split if it is a term with no expected paramegnetism.

The character calculation which I chose above, on the other hand, is an explicitation of Condon's example calculation that
$(^1S -^1 D) : (^1D -^3 P) = 3 : 2$. Condon does not use any group theoretical notation, but his writing is clear, rigorous, and insightful.

Condon dedicated his book to Russell (although likely the two never met), and he permanently resigned from Los Alamos as soon as he learned of the inexplicable secrecy there.

Part II

Three corrections to the fine structure

Before starting our discussion, I cannot resist making at least three independent corrections to what is known as the 'fine structure.' I haven't mentioned how this is understood currently, let me say that for example Condon's book suggests adding to the Schroedinger operator a sum over all the electrons of

$$\frac{1}{2\mu^2 c^2 r}\partial/\partial r U(r) L \cdot S$$

where by $U(r)$ he means the electric potential function, and by $L \cdot S$ he means the product of of $SO_3 \times 1$ and $1 \times SU_2$. Such a calculation is justified by papers of Thomas, Frenkel and others, supported by the approval of Pauli in the literature, and $L \cdot S$ is interpreted as a 'quantized dot product,' the notion to have been that angles themselves are quantized. Here, the letters L and S each ambiguously refer to the tensor operators which describe the action of the Lie algebra and their duals, such that L^2 and S^2 are the Casimirs of $SO_3 \times 1$ and $1 \times SU_2$, and it is not necessary then to use L and S, but only to write $LS = \frac{1}{2}((L+S)^2 - L^2 - S^2)$. Things like how, on wave function which is isotypical for the diagonal subgroup, $(L+S)^2$ acts by $4j(j+1)$ while L^2 and S^2 act by $4l(l+1)$ and $4s(s+1)$ when j, l, s are half-integers indexing the isomorphism types, have led most theorists to a notion that $4l(l+1)$ should be understood as a 'quantized squaring' operator applied to l. Even Weyl believed that.

The results require choosing two ‘gyromagnetic ratios,’ and a ‘Thomas half,’ and even then they disagree with experiment for any atom with more than one electron, though there are cases when it works well.

It is important to understand, as we said earlier, that things which might be called orbit-orbit coupling, are, when correctly understood, merely matters of labelling, and do not actually affect the spectrum. Here, Thomas, Frenkel and others suggest just adding a new term to the Schroedinger equation.

We have been using the letters L and S to denote points in a chosen maximal torus, and let’s temporarily use L^2 and S^2 to denote the Casimir operators. Then, since L^2 and S^2 have a constant effect on the whole collection of spectral frequencies coming from one term symbol (if we consider term symbols to be different in cases of multiplicity), there is no experiment currently done which could possibly make any distinction between any two of the following operators used in place of LS

$\frac{1}{2}(L+S)^2$

$\frac{1}{2}((L+S)^2 - L^2)$

$\frac{1}{2}((L+S)^2 - S^2)$

$\frac{1}{2}((L+S)^2 - L^2 - S^2)$.

Any of these can be used equivalently, as far as agreement with experiments to date, and the preference for the last-listed possibility was likely only to perpetuate the notion of a ‘quantized dot product.’

Now, the second possibility has a different interpretation. It is this: that surely what is called $(L + S)^2$ is the Casimir that corresponds to *actual rotations of three dimensional space.* This requires, by the way, thinking that SU_2 actually is the rotations of space, and so actually I mean the rotations of the line bundle which correspond to rotations of space by a double cover. Surely the fact that each spectral line can be assigned a difference of frequencies each corresponding to exactly one space of wave functions which is an irreducible representation of the diagonal group, is because of this. That is, the diagonal group is the symmetry group which really acts in the final analysis, when no approximations are made, when one is being completely precise.

But when people apply Schroedinger's operator, they do not apply it to the mysterious two-dimensional vector space $\mathbb{C}\alpha \oplus \mathbb{C}\beta$. It acts as the identity there.

If Schroedinger's operator is conjugated with the $1/r^l$ map to cancel out the radial effect, the result seems to be a multiple of the Casimir that is called L^2. But this was the wrong one.

More precisely, what I mean is this: if we take a homogeneous $h(x, y, z)$ of degree l, and write it as $r^l h(\frac{x}{r}, \frac{y}{r}, \frac{z}{r})$ then the Laplacian satsifies Leibniz rule for this product, resulting in an eigenfunction which is a sum of two terms. One of the two terms is $\frac{l(l+1)}{r^2}$ which is the spatial rotational Casimir eigenvalue $(2l)(2l+2)$ times $\frac{1}{4}\frac{1}{r^2}$. If we understand the polynomial as a coefficient in a one-form such as $h(x, y, z)du + g(x, y, z)dv$ and view du and dv as principal parts of $\mathcal{O}(1)$ on the Riemann sphere, then the principal parts exact sequence on global sections (we will describe this in more detail later) filters the vector space by the image under $du \mapsto (x + iy),\ dv \mapsto (x - iy)$ and kernel consisting of homogeneous polynomials of lower degree multiplied by $du \wedge dv$.

Now if the coefficients of $du \wedge dv$ and 1 are re-interpreted as polynomials, and the same substitution is done by which each monomial such as x^i is factorized as $r^i \frac{x}{r}^i$, the eigenfunctions on the two associated graded parts will correspond to the Casimir for the diagonal group. Later we will understand the diagonal group as a subgroup of a semidirect product also, in a way that is more closely related to bundle automorphisms.

Although we have not posed any global equation analagous to Schroedinger's equation which might yield two such different radial coordinates or radial degrees, the fact that the fine structure matches the calculation suggests that Schroedinger's equation ought to be replaced by a simple equation involving coordinates on the tangent space of Euclidean space which would at this point of the analysis lead to a restricted operator in which the action on the single radial coordinate of the spatial rotation Casimir would in this way be replaced by an action of the natural Casimir.

Then, instead of using the last formula, interpreted as a 'quantum dot product,' it seems better to use the second one, interpreted as a 'correction term.'

But then, the function coefficient should not be anything like

$$\frac{1}{2\mu^2c^2r}\partial/\partial rU(r)$$

It should be, as a first guess,

$$(\frac{e^2}{r})(\frac{1}{h})(\frac{1}{r^2}),$$

equivalent to adding to the electrostatic perturbation the sum the of the effects of the Casimir multiplied by

$$(\frac{e^2}{r_i})(\frac{h}{2\pi})^2(\frac{1}{2\mu})(\frac{1}{h})(\frac{1}{4\pi\epsilon})^2(\frac{1}{h})(\frac{1}{r_i^2}).$$

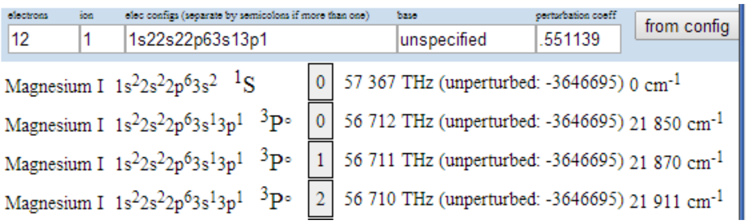
The term involving ϵ and the subsequent one involving h are included just here so that the answer will be in cycles per second. The factors of h cancel.

This is quite a different number, especially as it only involves the first power[4] of the electron mass μ, one would expect this to be off by many many orders of magnitude.

However, we see that if we choose the electrostatic perturbation coefficient of 0.551139 to make the first level of Magnesium correct, it gives not an expected five orders of magnitude of error, but rather, for the two higher fine levels, five orders of decimal digits of accuracy.

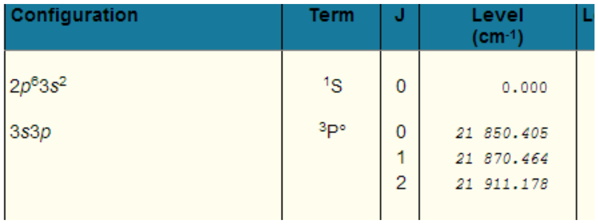
---

[4] and actually the corresponding number involves the zero'th power



electrons	ion	elec configs (separate by semicolons if more than one)	base	perturbation coeff
12	1	1s22s22p63s13p1	unspecified	.551139

```
Magnesium I  1s22s22p63s2  1S     0  57 367 THz (unperturbed: -3646695) 0 cm-1
Magnesium I  1s22s22p63s13p1  3P°  0  56 712 THz (unperturbed: -3646695) 21 850 cm-1
Magnesium I  1s22s22p63s13p1  3P°  1  56 711 THz (unperturbed: -3646695) 21 870 cm-1
Magnesium I  1s22s22p63s13p1  3P°  2  56 710 THz (unperturbed: -3646695) 21 911 cm-1
```



Configuration	Term	J	Level (cm-1)
$2p^6 3s^2$	^1S	0	0.000
$3s3p$	$^3P^\circ$	0	21 850.405
		1	21 870.464
		2	21 911.178

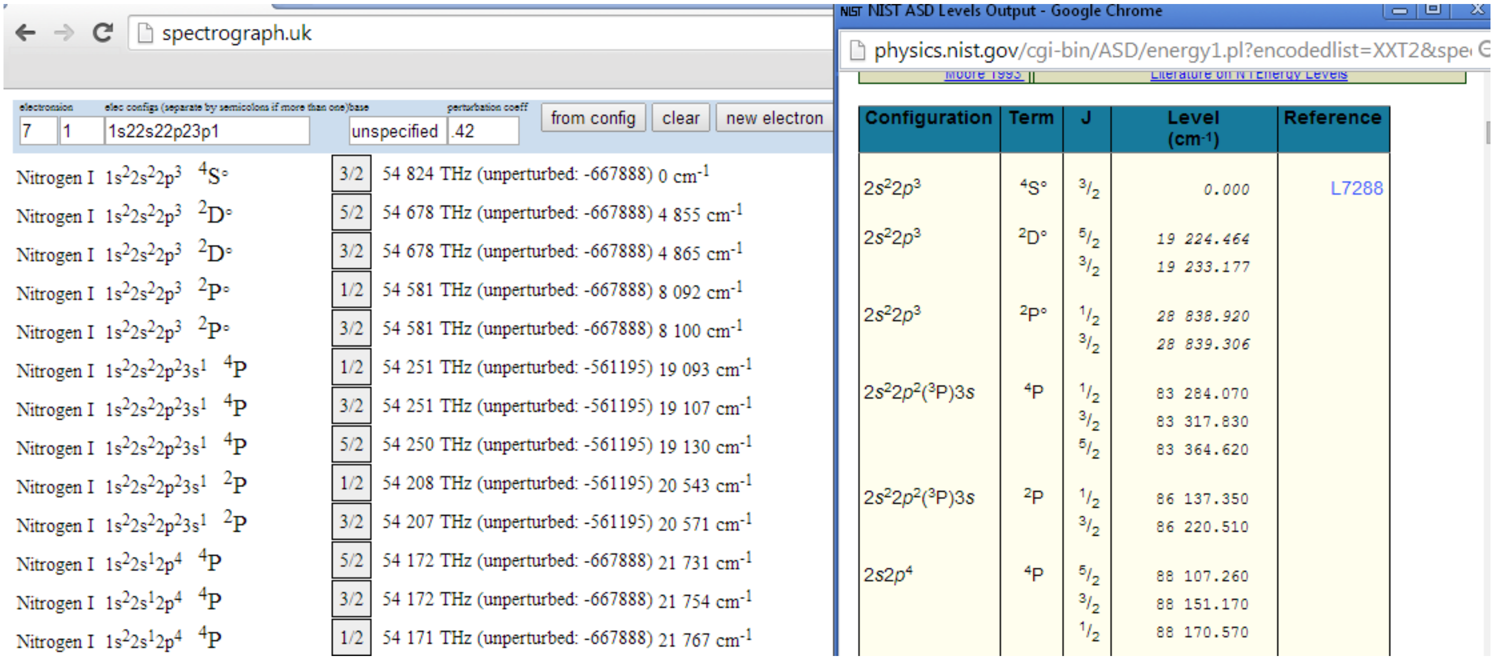
That is, the increases of 20 and 61 are correctly calculated in this case. There are other cases when the calculation is not as good, and it could be a coincidence, though still true, that choosing the perturbation coefficient to make the first level correct regarding the electrostatic perturbation also makes the two higher fine levels correct regarding the fine structure. The calculation can be seen[5]

http://www.spectrograph.uk/index.html?pmult=.551139&fmult=2/pmult&finecorrect.checked=false&autocorre

---

[5] The explanation for the multiplier of $2/pmult$ is that it cancels the effect of the perturbation coefficient on fine structure and re-introduces the coefficient of 2 in the radial eigenfunction of the azimuthal Lie algebra – this coefficient is currently unexplained though

The calculation, setting the electrostatic perturbation coefficient to .42, gives the first 13 fine levels of Nitrogen all in the correct order



electron | ion: 7 | 1
elec configs (separate by semicolons if more than one): 1s22s22p23p1
base: unspecified
perturbation coeff: .42

Nitrogen I $1s^22s^22p^3$	$^4S°$	3/2	54 824 THz (unperturbed: -667888) 0 cm^{-1}
Nitrogen I $1s^22s^22p^3$	$^2D°$	5/2	54 678 THz (unperturbed: -667888) 4 855 cm^{-1}
Nitrogen I $1s^22s^22p^3$	$^2D°$	3/2	54 678 THz (unperturbed: -667888) 4 865 cm^{-1}
Nitrogen I $1s^22s^22p^3$	$^2P°$	1/2	54 581 THz (unperturbed: -667888) 8 092 cm^{-1}
Nitrogen I $1s^22s^22p^3$	$^2P°$	3/2	54 581 THz (unperturbed: -667888) 8 100 cm^{-1}
Nitrogen I $1s^22s^22p^23s^1$	^4P	1/2	54 251 THz (unperturbed: -561195) 19 093 cm^{-1}
Nitrogen I $1s^22s^22p^23s^1$	^4P	3/2	54 251 THz (unperturbed: -561195) 19 107 cm^{-1}
Nitrogen I $1s^22s^22p^23s^1$	^4P	5/2	54 250 THz (unperturbed: -561195) 19 130 cm^{-1}
Nitrogen I $1s^22s^22p^23s^1$	^2P	1/2	54 208 THz (unperturbed: -561195) 20 543 cm^{-1}
Nitrogen I $1s^22s^22p^23s^1$	^2P	3/2	54 207 THz (unperturbed: -561195) 20 571 cm^{-1}
Nitrogen I $1s^22s^12p^4$	^4P	5/2	54 172 THz (unperturbed: -667888) 21 731 cm^{-1}
Nitrogen I $1s^22s^12p^4$	^4P	3/2	54 172 THz (unperturbed: -667888) 21 754 cm^{-1}
Nitrogen I $1s^22s^12p^4$	^4P	1/2	54 171 THz (unperturbed: -667888) 21 767 cm^{-1}

Configuration	Term	J	Level (cm^{-1})	Reference
$2s^22p^3$	$^4S°$	$^3/_2$	0.000	L7288
$2s^22p^3$	$^2D°$	$^5/_2$ $^3/_2$	19 224.464 19 233.177	
$2s^22p^3$	$^2P°$	$^1/_2$ $^3/_2$	28 838.920 28 839.306	
$2s^22p^2(^3P)3s$	^4P	$^1/_2$ $^3/_2$ $^5/_2$	83 284.070 83 317.830 83 364.620	
$2s^22p^2(^3P)3s$	^2P	$^1/_2$ $^3/_2$	86 137.350 86 220.510	
$2s2p^4$	^4P	$^5/_2$ $^3/_2$ $^1/_2$	88 107.260 88 151.170 88 170.570	

including the reversal of the three levels for the $1s^22s^12p^4$ configuration. To see this calculation use `http://spectrograph.uk/index.html?pmult=.42&fmult`

I should explain how this fine calculation can be justified, and then explain why it is really the completely wrong calcuation.

The highest weight space for the diagonal subgroup within an isotypical component for the whole group is approximately determined by an intersection of four integer lattices within one integer lattice. This is just because subspaces of rational vector spaces are the same as saturated sublattices (ones whose quotient is torsion-free). So specifying the isomorphism type for the $SO_3 \times 1$ group, the $1 \times SU_2$ group, and the diagonal of the $SU_2 \times SU_2$ group are choosing three sublattices of a lattice whose rank is equal to the dimension of the space of wave functions which we correspond to one 'electron configuration.' But then to specify the isomorphism type for the action of a chosen diagonal torus, requires intersecting with one further lattice.

In the language of quantum numbers, this last lattice is not determined by a Casimir operator, but is just the total degree of the 'spin' and 'momentum' quantum numbers.

In multiplicity free cases this intersection of four integer lattices is just an integer lattice of rank one, a free abelian group of rank one, and in general it is a free abelian group whose rank is the multiplicity of the term symbol within the 'electron configuration.'

Interpreting the difference above as a correction term that needed to be added to Schroedinger's operator, to correct for the fact that it never acted on 'spin coordinates,' we return to equation (7) where we intend to include in the parentheses on the left side of the equation a coefficient times the Casimir term

$$\frac{C_J - C_L}{r^2}$$

(now writing C_J instead of J^2 for the diagonal Casimir and C_L instead of L^2 for the rotational one). Since this originates from the action of Δ on the left side, as we've explained, the coefficient must include as a factor the reciprocal of the leading coefficient of the parentheses, thus

$$-(\frac{h}{2\pi})^2(\frac{1}{2\mu}).$$

If we interpret the Laplacian acting as we have, in the global equation, we should also have a coefficient factor of $\frac{1}{4}$, because the Laplacian has the eigenfunction term $\frac{l(l+1)}{r^2}$ while rotational Casimir is four times this[6] and an eigenfunction for the radial coordinate of $\frac{(2l)(2l+2)}{r^2}$. However, since it matches experiment not to include the coefficient of $\frac{1}{4}$ we will omit it; and the explanation must be that the operator that is appropriate for a global Schroediger equation has the difference of quantum numbers not half the degree of the canonical divisor on the Riemann sphere, but the full degree. In other words that as the degree in r matches the degree of u^2, uvv^2 there should be some global phenomenon akin to a separate radial function for zero forms and two-forms, which behaves like a square-root of r.

---

[6] This discussion applies to the Casimir scaling which gives eigenvalues of $(2l)(2l+2)$

For some reason it matches the data *not* to cancel out the coefficient of $\frac{e^2}{r_i}$ now, and with little insight as to why, we include this and also $\frac{1}{h}$ to make the additional term independent of the value of h when all is multiplied out (we saw that above, that the occurrences of h all cancel).

And then the coefficient of of the eigenvalue $\frac{l(l+1)}{r^2}$ becomes

$$-(\frac{1}{h})(\frac{e^2}{r_i})(\frac{h}{2\pi})^2(\frac{1}{2\mu})$$

and we can write it into the equation so that (7) becomes modified to be

$$\begin{aligned}\Delta\Psi = -(\frac{2\pi}{h})^2(2\mu)(&\sum_i \frac{k_p\beta e^2}{4n_i^2} + E_1(t)\\ &+\sum_i \frac{e^2}{r_i}(k_p - t\frac{h}{(2\pi)^2}\frac{1}{2\mu}(C_J - C_L)\frac{1}{{r_i}^2})\\ &-t\sum_{i<j}\frac{e^2}{r_{i,j}})\Psi.\end{aligned}$$

When we perform the calculation the terms in the last two lines are multiplied by $\frac{1}{h(4\pi\epsilon)^2}$ to convert to frequency in cycles per second.

The next-to-previous expression gives rise to the perturbation operator that is to be added to the electrostatic perturbation operator before any spectral analysis can be done.

Now let me say how the calculation is still wrong, even while often now appearing giving the right answer.

In the first place, interpreting the added operator as a difference, a correction term, which needed to be added to the Schroedinger operator, to correct for the fact that it never acted on 'spin' coordinates, the corrected constant above, noting that what are called $L^2, S^2, (L+S)^2$ are Casimirs for groups affecting only the coordinates which would describe the position of one electron, then the calculation of the perturbation matrix is done with the extra term included, and *in the same basis.* In the multiplicity free case, the frequency is taken to be the eigenvalue using any nonzero element of the free abelian group as an eigenvector. When there are multiplicities one would look for the spectrum of the operator restricted to the span of the lattice.

In the second place, the occurrence of $\frac{e^2}{hr_i}$ is really unexplained, it should just be 1 if we really are talking about a difference correction term for the Laplacian. One would seek an explanation for why the correction term in the Laplacian should need to become more significant in proportion to the electrostatic attraction. Note that the ratio between E and e^2 is the same as the ratio between α and β, in this regard. In any case it would be wrong for me to dismiss the correction term as describing 'spin-orbit' coupling if I allow it to depend both on the Laplacian and on the electron charge in this way, and it could indeed be describing a coupling.

One explanation for wanting fmult=2/pmult or slightly smaller to make the data match better may be because we should have used $(\frac{2\pi}{h})$ in place of $(\frac{1}{h})$. After all, the constant h without any denominator of π has never occurred except in conjunction with correcting measurement units of the 'permittivity of free space,' whereas $\frac{2\pi}{h}$ occurs whenever we differentiate Ψ with respect to time. Then instead of removing the factor of 1/4 we should have left the factor of 1/4 in place. Thus perhaps the coeffifient which we introduced as our first guess, of

$$(\frac{e^2}{r})(\frac{1}{h})(\frac{1}{r^2})$$

should have the denominator of 2π replaced by 4, becoming

$$(\frac{e^2}{r})(\frac{1}{4})(\frac{2\pi}{h})(\frac{1}{r^2})$$

and the second guess for what our first correction should be, the equation then being

$$\begin{aligned}\Delta\Psi = -(\frac{2\pi}{h})^2(2\mu)(\sum_i \frac{k_p\beta e^2}{4n_i^2} + E_1(t)\\ + \sum_i \frac{e^2}{r_i}(k_p - t(\frac{h}{2\pi})\frac{1}{2\mu}(\frac{C_J - C_L}{4})\frac{1}{{r_i}^2})\\ - t\sum_{i<j}\frac{e^2}{r_{i,j}})\Psi.\end{aligned}$$

Because the javascript implicitly applies the electron charge multiplier *pmult* to this term, the value of $fmult$ that would match this equation in the javascript is $\frac{2\pi}{4\ pmult} = \frac{\pi/2}{pmult}$.

A third, seeming much more likely possibility, for what should be our first correction, is that the factor of $\frac{e^2}{r_i}$ should actually be $\frac{k_p e^2}{r_i}$ meaning the k_p should be outside the parentheses in the second term

$$\begin{aligned}
\Delta\Psi = -(\frac{2\pi}{h})^2(2\mu)(\sum_i \frac{k_p \beta e^2}{4n_i^2} + E_1(t) \\
+ \sum_i \frac{e^2}{r_i} k_p (1 - t(\frac{h}{2\pi})\frac{1}{2\mu}(\frac{C_J - C_L}{4})\frac{1}{{r_i}^2}) \\
- t\sum_{i<j} \frac{e^2}{r_{i,j}})\Psi.
\end{aligned}$$

Actually, here is a possible argument which would in fact *justify making both changes*, including the multipicative factor of k_p in the extra term.

What we might do is perturb a wave function Ψ a little bit, so we can imagine

$$\Psi(t) = \Psi(0) + (\frac{\partial}{\partial t}\Psi)(0).t + ... \qquad (8)$$

and now we also do the perturbation analysis on Ψ, with another parameter s which just adjusts the electrostatic effect.

We write Schroedinger's equation

$$\Delta(\Psi) = (\frac{2\pi}{h})^2(2\mu)(E\Psi - k_p\sum_i \frac{e^2}{r_i}\Psi + s\sum \frac{e^2}{r_{i,j}}\Psi) \qquad (9)$$

with s the perturbation parameter which just multiplies the electrostatic term, so when $s = 1$ it is the 'correct' equation, and we substitute in equation (8), but we are going to ignore the term st as it is 'second order' and will not contribute to the derivative.

Since the equation is totally linear, the derivative should itself be a solution. Then

$$\Delta(\frac{\partial}{\partial t}\Psi) = (\frac{2\pi}{h})^2(2\mu)(E\frac{\partial}{\partial t}(\Psi) - k_p\sum_i \frac{e^2}{r_i}\frac{\partial}{\partial t}(\Psi)),$$

and here we rightfully can ignore the further term (not write it) and solve just for the partial derivative $\frac{\partial}{\partial t}(\Psi)$.

This gives

$$\frac{\partial}{\partial t}(\Psi) = (\frac{h}{2\pi})^2(\frac{1}{2\mu})(\frac{1}{E})\Delta(\frac{\partial}{\partial t}\Psi) + \frac{k_p}{E}\sum_i \frac{e^2}{r_i}\frac{\partial}{\partial t}(\Psi)$$

When we expand Ψ in the Taylor series in t at time 0 in the middle term of (9) we get

$$\Delta(\Psi) = (\frac{2\pi}{h})^2(2\mu)(E\Psi - k_p\sum_i(\frac{e^2}{r_i})[$$

$$\Psi(0)+t(\frac{h}{2\pi})^2(\frac{1}{2\mu})(\frac{1}{E})\Delta(\frac{\partial}{\partial t}(\Psi))+t\frac{k_p}{E}\sum_i\frac{e^2}{r_i}\frac{\partial}{\partial t}(\Psi)+\frac{t^2}{2!}(...)...$$

$$] + s\sum(\frac{e^2}{r_{i,j}}\Psi)$$

We already calculated the derivative with respect to s of E due to the electrostatic effect (the last term) which is turned out to be the number $\frac{e^2}{(4\pi\epsilon)^2}(\frac{1}{h})$ times the perturbation effect of the sum of the $\frac{1}{r_{i,j}}$.

If we look at the middle term in the square parentheses, we write

$$\frac{\partial}{\partial t}(\Psi) = (\frac{2\pi}{h})\Psi$$

and

$$\Delta(\frac{\partial}{\partial t}(\Psi)) = (\frac{2\pi}{h})\Delta(\Psi)$$

and when this acts on a radial coordinate r_i it will contribute then one eigenfunction term

$$(\frac{2\pi}{h})(\frac{1}{4})(\frac{1}{r^2})C_J$$

The 1/4 is there because the eigenvalues it contributes involve $l(l+1)$ where the conventional Casimir involves $(2l)(2l+2)$.

When we multiply everything out, we will multiply this by

$$k_p(\frac{h}{2\pi})^2(\frac{1}{2\mu})(1/E)$$

The magnitude of the derivative, this time with respect to t not s, will be by the same calculation which we already made for sas far as the units of measurement etc and this will mean we are to multiply this by

$$e^2\frac{1}{(4\pi\epsilon)^2}(\frac{1}{h})$$

We also multiply by $\frac{1}{r_i}$, and this just means that the result will be the perturbation matrix for the sum of the r_i^{-3} times the coefficient

$$(\frac{2\pi}{h})(\frac{C_J - C_L}{4})k_p(\frac{h}{2\pi})^2(\frac{1}{2\mu})(\frac{1}{E})e^2(\frac{1}{(4\pi\epsilon)^2})(\frac{1}{h})$$

The h's cancel so let's write it without them, and let's leave off the $e^2(\frac{1}{(4\pi\epsilon)^2})(\frac{1}{h})$ as that is a standard thing (the constant already I multiplied the perturbation matrix of the sum of $\frac{1}{r_{ij}}$ by to get the electrostatic matrix).

And this means the extra factor to put in front of the matrix describing the Hilbert space projection for the *first* exterior power of the sum of the inverse cubes of the r_i, to get one of the components of the perturbation matrix describing the change in time t, is the corresponding matrix entry of

$$(\frac{h}{2\pi})k_p(\frac{C_J - C_L}{4})\frac{1}{2\mu}(\frac{1}{E})$$

For higher exterior powers the perturbation calculation follows from this in a standard way which is also the extension of the projected action by a derivation of the exterior algebra.

The javascript has been using

$$(\frac{h}{2\pi})^2(\frac{1}{2\mu})(\frac{1}{h})(C_J - C_L)$$

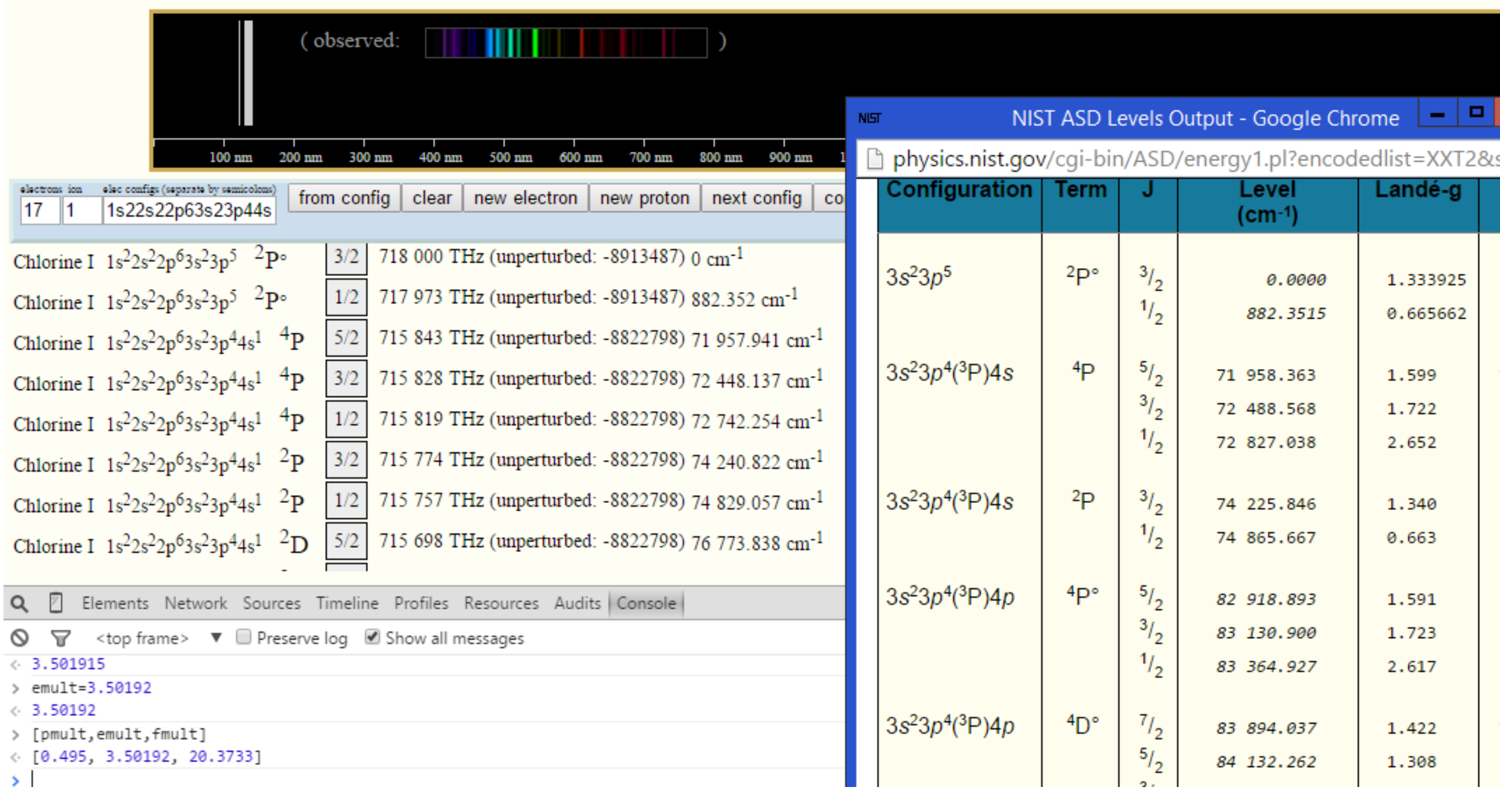
with the 1/h unexplained, times the multiplier $fmult$ which can be set in the url, for example.

Replacing what it is now with what this should suggest amounts to choosing fmult to be

$$k_p(\frac{\pi}{2})(\frac{1}{pmult}).$$

That is, if we could just ignore that $(1/E)$ there!

Such a rough calculation does seem to be justified by the case of Chlorine, where once pmult and emult are chosen, the value of fmult needed is about 20 (for atomic number 17).



17 1 1s22s22p63s23p44s

Chlorine I $1s^22s^22p^63s^23p^5$ $^2P°$ 3/2 718 000 THz (unperturbed: -8913487) 0 cm^{-1}

Chlorine I $1s^22s^22p^63s^23p^5$ $^2P°$ 1/2 717 973 THz (unperturbed: -8913487) 882.352 cm^{-1}

Chlorine I $1s^22s^22p^63s^23p^44s^1$ ^4P 5/2 715 843 THz (unperturbed: -8822798) 71 957.941 cm^{-1}

Chlorine I $1s^22s^22p^63s^23p^44s^1$ ^4P 3/2 715 828 THz (unperturbed: -8822798) 72 448.137 cm^{-1}

Chlorine I $1s^22s^22p^63s^23p^44s^1$ ^4P 1/2 715 819 THz (unperturbed: -8822798) 72 742.254 cm^{-1}

Chlorine I $1s^22s^22p^63s^23p^44s^1$ ^2P 3/2 715 774 THz (unperturbed: -8822798) 74 240.822 cm^{-1}

Chlorine I $1s^22s^22p^63s^23p^44s^1$ ^2P 1/2 715 757 THz (unperturbed: -8822798) 74 829.057 cm^{-1}

Chlorine I $1s^22s^22p^63s^23p^44s^1$ ^2D 5/2 715 698 THz (unperturbed: -8822798) 76 773.838 cm^{-1}

```
< 3.501915
> emult=3.50192
< 3.50192
> [pmult,emult,fmult]
< [0.495, 3.50192, 20.3733]
> |
```

Configuration	Term	J	Level (cm^{-1})	Landé-g
$3s^23p^5$	$^2P°$	3/2	0.0000	1.333925
		1/2	882.3515	0.665662
$3s^23p^4(^3P)4s$	^4P	5/2	71 958.363	1.599
		3/2	72 488.568	1.722
		1/2	72 827.038	2.652
$3s^23p^4(^3P)4s$	^2P	3/2	74 225.846	1.340
		1/2	74 865.667	0.663
$3s^23p^4(^3P)4p$	$^4P°$	5/2	82 918.893	1.591
		3/2	83 130.900	1.723
		1/2	83 364.927	2.617
$3s^23p^4(^3P)4p$	$^4D°$	7/2	83 894.037	1.422
		5/2	84 132.262	1.308

One can repeat the calculation with this link `http://spectrograph.uk/index` and pressing 'compare external.'

For most atoms (particularly the metals) it gives a fine structure about ten times larger than the observed structure.[7]

---

[7] A checkbox called 'other' in the explorer sets fmult to one with this particular theoretical justification. The calculation for Chlorine just above does not include the denominator of pmult and allows the pmult of .495 to rescale the electron charge in its effect on the fine structure therefore, there is no checkbox in the explorer that makes this particular choice for all ions though it can be entered in the url including for example &fmult=1/pmult

Actually, we *can* ignore the $(1/E)$ as we made an error differentiating Ψ; it is cancelled when we differentiate Ψ with respect to t and a factor of iE appears... perhaps the i also cancels the ratio between the Weyl operator and the restriction of the Legendre operator....but I should really stress that this analysis above is very heuristic, and I have intentionally been uncareful about the order of operations, for instance multiplying $\sum_i 1/r_i$ with $\sum_i 1/r_i^2$ either before or after projecting the action of each term to a single electron configuration; thus the sum of $1/r_i^3$ could be replaced with a sum of $1/r_i^2 r_j$. The absence of a coefficient for the number of terms suggests that it is the perturbation actions that are composed and therefore we see only one term (the dominant diagonal term) from a larger sum of contributions; however the analysis above was really only meant to be a dimensional analysis to explain the order of magnitude of the chosen coefficient. Also we omitted many other terms in the analysis which of course could be continued much further.

Note too that some of the coefficient factors which multiply C_J should be reciprocated and put as a leading coefficient of $-C_L$ if we want to continue to think rigorously of correcting for the failure of the Laplacian to act on derivatives in the classical interpretation.

Something that is not right about this analysis is that I pretended that there is one 'r' which serves the needed purpose with respect to both notions of angle.

In the second place, the actual eigenfunction is not going to be at all a $\mathbb{Q}$ linear combination, or even a $\mathbb{C}$-linear combination, of the basis functions we've chosen. Ignoring the radial part, these functions were taken to be a basis of the homogeneous harmonic polynomials.

I mentioned before that a mistake people make is to assume there is a chosen basis. Well, here it becomes quite obvious that this mistake is prevalent in all understandings of quantum mechanics, not only in the teaching of quantum mechanics, and it arises from the relation between two interpretations, one by Legendre, and one by Weyl.

Recall too, the notion that representation theory should be relevant at all is one the weakness of which Weyl himself was aware of, commenting that molecules really typically do not have any symmetry at all.

The basis of homogeneous harmonic polynomials of degree l which we chose, which is due to Legendre, can be produced starting with

$$(r^2 - z^2)^l.$$

One admits the relation in three space with coordinates x, y, z and a radial coordinate r that $r^2 = x^2 + y^2 + z^2$, but one considers the operator $\frac{\partial}{\partial z}$ which does not preserve that relation. For a number l, beginning with the function

$$(z^2 - r^2)^l$$

one chooses a number $a = 0, 1, 2, ..., l$ and constructs a basis of the homogenous harmonic polynomials in x, y, z consisting of the real and imaginary parts of

$$(x + iy)^a \; \frac{\partial}{\partial z}^{l+a} \; (z^2 - r^2)^l.$$

If we complexify, thinking of x, y, z, r as complex variables, then we may write

$$z^2 - r^2 = x^2 + y^2 = (x - iy)(x + iy)$$

and the expression above is

$$(x + iy)^a \frac{\partial}{\partial z}^{l+a} ((x + iy)^l (x - iy)^l).$$

Since $\frac{\partial}{\partial z}$ commutes with multiplication by $x + iy$ this is just

$$\begin{aligned} &((x + iy)\frac{\partial}{\partial z})^{l+a})(x - iy)^l \\ &= \delta^{l+a}(x - iy)^l \end{aligned}$$

where

$$\delta = (x + iy)\frac{\partial}{\partial z}.$$

It follows that we can combine l and a into a single value m, that is, for any numbers m and l whatsoever we have

$$\delta^m(x-iy)^l$$

has harmonic real and imaginary parts. This is true because the real and imaginary parts of the anti-holomorphic function $(x-iy)^l$ are harmonic, and δ commutes with the Laplacian (its real and imaginary parts are in the rotation Lie algebra as we'll see in a few lines).

This derivation δ satisfies

$$(x+iy)(x-iy) = r - z^2 \mapsto -2(x+iy)z$$

and so

$$\begin{aligned}
&\delta(x-iy) = -2z.\\
&\delta(x+iy) = 0\\
&\delta(z) = (x+iy),
\end{aligned}$$

giving

$$\begin{aligned}
&\delta(x) = -z\\
&\delta(y) = -iz\\
&\delta(z) = (x+iy).
\end{aligned}$$

This calculates δ then

$$\delta = (x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x}) + i(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}).$$

We'll later give a geometric explanation of this, but first let's look at Weyl's representation-theoretic point of view. This is to think that $(x+iy)(x-iy) = r^2 - z^2$ for $r = x^2+y^2+z^2$, and to use operators which act trivially on r. If we restrict to the subvariety defined by the rule $r = 0$, we have $(x+iy)(x-iy) = (iz)^2$. This is the equation of a projective line that can be parametrized as $[u : v]$ with $x+iy = u^2,\ \ x-iy = v^2$, $iz = uv$, and the representation-theoretic lowering operator, $u\partial/\partial v$, considered modulo the Euler derivation as a vector field on the Riemann sphere, acts now on sections of $\mathcal{O}(2)$ by

$$v^2 \mapsto 2uv \mapsto 2u \mapsto 0.$$

Thus by Weyl

$$\begin{gathered}(x-iy) \mapsto 2iz \\ z \mapsto \frac{1}{i}(x-iy) \\ (x+iy) \mapsto 0\end{gathered}$$

so the Weyl operator is $-i\delta$. If we do not restrict to the variety $r = 0$ then the operator $u\partial/\partial v$ sends $x-iy = v^2$ to $2uv = 2\sqrt{x^2+y^2} = 2\sqrt{r^2-z^2}$ and this is no longer equal to $2iz$, in place of i there is a multiplicative factor of

$$-(\frac{r}{z})\sqrt{1-(z/r)^2}.$$

This coefficient does have a multipole, or Taylor series expansion as

$$-\frac{r}{z} + \sum_{i=1}^{\infty} \frac{(2i-3)!}{2^{2i+2}i!(i-2)!}(\frac{z}{r})^{2i-1}$$

and it is an interesting question whether a Borel summation can prevail here to begin to globalize the Schroedinger solutions which by this analysis are very local.

Thus unless we can make sense of this multipole expansion we cannot really make our second correction. Before we discuss the third corrections to the fine structure, it makes sense to describe the way that it can be calculated. For a configuration of k electrons, within the vector space which is the solution space for Hydrogen but with the proton charge suitably adjusted, we choose the vector space which corresponds to an 'electron configuration. By subtracting a suitable integer from each of the three Casimirs (the space rotation Casimir, the 'spin' Casimir, and the diagonal Casimir), and also by subtracting an integer from the matrix which multiplies each basis element by its m_J number, we obtain four endomorphisms of an integer lattice. The rank of the sublattice which is the intersection of the four lattices is the multiplicity of the corresponding term symbol, usually equal to one.

It should be true on general principles that the operator which is the sum of the perturbation coming from the electrostatic effect and the perturbation coming from the Casimir difference times $\frac{1}{r^3}$ should preserve this sublattice. In fact, it turns out, that even the classical perturbation operator needn't commute with the classical rotational Casimir, and therefore our attempt at correcting to match a hypothetical correct Schroedinger differential equation is not exactly right. Nevertheless we *project* the total perturbation operator including the classical electrostatic term plus the correction term as an operator on the sublattice, and this is how we determine the fine structure.

There are two further worries now. One is that the integer vectors which arise as the intersection of four sublattices of a lattice, have been constructed without careful regard to the change of basis between the standard basis of harmonic homogeneous polynomials times analytic radial functions which is created by iterating the Legendre operator to create basic homogeneous harmonic polynomials, versus the basis created by Weyl's lowering operator. The fact that the radial coordinate has actually be set to zero is worrying. A calculation which we'll show later gives that the Legendre lowering operator, once it is restricted to the Severi-Brauer variety agrees with the Weyl operator if one is willing to multiply just by the imaginary number i. Perhaps as the raising operator is multiplied by $-i$ the effect on the Casimir cancels out, as if one replaces f by if and e by $-ie$ in the formula for the Casimir

$$2ef + 2fe + (ef - fe)^2$$

each term ef or fe is unaffected.

Regarding the fact that the sublattice is not actually preserved, and a projection operator must be interposed, a bit later I'll describe how in the javascript, we use a contrivance, which is our third correction to the fine structure : first removing the correction term in the Schroedinger operator, this determines a false fine structure. Then repeating the calculation with the correction term in place, and subtracting the 'false fine structure' which was there, but should not have been there, when the correction term had been removed.

This does not affect the calculation for magnesium, but gives a slight adjustment of fine levels, for carbon, for instance.

This does not address the deeper issue that in place of integer vectors, one is talking about wave functions which are not actually linear combinations of homogeneous harmonic polynomials times analytic functions of r.

An attempt to use perturbation theory with this existing space of functions fails due to the fact that whenever one of the Legendre basis elements is multiplied by any term in the multipole correction expansion, as a coefficient function, it actually becomes completely orthogonal, in the Hilbert space sense, to all the conventionally used basis wave functions.

The use of a basis consisting of homogeneous harmonic polynomials times radial functions fits well with Schroedinger's and Legendre's approach, but the multipole correction needed to make this compatible with Weyl's representation-theory approach, where he lets r tend to zero while allowing x, y, z to remain finite, would require a different function space. I mentioned that the particular choice of Hilbert space structure has no effect on first-order perturbations, except in choice of orthogonal complement. In this case things become orthogonal in the Hilbert space sense anytime after time zero of the perturbation.

A discussion of perturbation theory

Considering the actual sum of the Schroedinger operator plus a constant t times the electrostatic term, we can define a function $e(t)$ for each energy level. That is, once we choose an initial value of each solution for $t = 0$, then by continuity as a function of t we can say which solution is which. That is we can lift a path in t to an appropriate covering space, and we have then that each energy level e is not a function of t. So by path lifting we get functions $e(t)$. These become undefined when two values coincide, and can be extended however complex analytically, in the way that is familiar for maps of Riemann surfaces.

We want to know $e(1)$, and we only can know $\frac{d}{dt}e(t)$ at $t = 0$ independently of the Hilbert space structure. That is, perturbation theory is independent of the Hilbert space structure, only depending on the decomposition of a larger space of functions into the space one is considering direct sum an orthogonal complement, but the inner product structure on that orthogonal complement does not need to be specified at all.

The value $e(1)$ is

$$e(t) + \frac{d}{dt}e(t) + \frac{1}{2!}\frac{d}{dt}^2 e(t) + ...$$

when $t = 0$, and what makes sense is to use an intermediate value of t (a value less than 1). In fact this can be viewed as the 'Taylor theorem with remainder,' whereby the *entire infinite tail* of a Taylor series can be evaluated precisely by changing just the point at which one evaluates the derivative at the last term of the Taylor polynomial.

Thus we are trying to find a number c so that when $t = 0$

$$e(t) + c\frac{d}{dt}e(t) = e(t) + \frac{d}{dt}e(t) + \frac{1}{2!}\frac{d}{dt}^2 e(t) + ...$$

That is, we are trying to find the number

$$c = 1 + \frac{\frac{1}{2!}\frac{d}{dt}^2 e(t) + \frac{1}{3!}\frac{d}{dt}^3 e(t) + ...}{\frac{d}{dt}e(t)}$$

when $t = 0$, although each term of the numerator is unknown. The left side describes an eigenvalue of the Schroedinger operator plus c times the perturbation matrix, meaning the projection of the electrostatic term onto the $e(0)$ eigenspace.

When one looks at the effect of changing the number c on all the predicted energy levels for an electron configuration, it makes them move around like a swarm of flies.

The video `http://spectrograph.uk/fullscreen.html?file=quantumvideo.mp4` shows what happens. The number c which is the coefficient of the perturbation matrix ranges over time from 0 to 1, and one sees initially when it is near zero, the predicted energy levels which are red dots, are near the reciprocal sums of squares, the blue dots.

As time goes on (as c increases) these segments of the step function assemble themselves together. One sees that there is apparently a critical value of the discriminant of the sum of the Schroedinger operator plus electrostatic repulsion, at a point when all the segments of the curve join together and agree with the green dots (actual levels resolved from the observed spectrum).

After this, the green dots appear to move chaotically. What is being shown is this: the red dots are indexed uniquely, each by a pair consisting of an electron configuration (there is only one here) and term symbol. This is because the element here, Beryllium, has multiplicity-free electron configurations. The green dots are assigned also term symbols by convention, although what matters more here is that they have a total ordering by real value.

The numbers are arranged as one would graph a sequence, so that the horizontal coordinate is the unique indexer of these levels. This is done according to the real value of the predicted values. After the c value exceeds its critical value, the ordering of the term symbols changes in order that the real values remain in increasing order. If one thinks about it, it is preferable to think this way, as we rely on no prejudice about which term symbol should actually be assigned to which actual value. This means that the actual values, the green dots, see a permutation in their horizontal position, and the *observed* graph breaks apart into a swarm of separate values.

The graphs are shown with the horizontal coordinate chosen so that the rightmost red dot (highest predicted value) agrees with the highest observed value resolved from the spectrum. In fact the distance vertically from either graph and the blue sums of reciprocal squares graph is very much larger than shown.

Choosing the value of c which is a critical value for the discriminant should make the predicted and actual graphs correspond, but note this is only true near the ionization limit (the right side of the graphs), if we take that as a meaningful and well-defined reference. This would make sense from considerations of notions of absolute energy as this would be the energy when all electrons are separated from protons and each other.

Since we are trying to find the spectrum, and the lines near the ionization limit have vanishingly small values, it makes sense not to use any notion of absolute energy, but rather to focus nearer the ground level.

Unfortunately, the levels are compressed near the ground level, for reasons which certainly should have to do with the unexplained Aufbau, which actually forbids what should be some low levels by the existing theories, and pushes them past the ionization limit.

Ignoring this, there is also the issue that the value of c which has the right permutation for the actual levels, has the wrong slope altogether.

It makes sense instead to do the following: to disallow changes in c from making this permutation, or indeed from affecting the fine lines, coarse lines, or even term symbols or even electron configurations relative to each other whenever they have the same sum of recirpocal squares.

Thus, what we do is to multiply the variable representing proton charge by $1/c$ where it occurs in the exponent of the exponential integrating factor in the formula for the radial Schroedinger solutions, and also in the polynomial part, and also where it occurs as a coefficient of the sum of reciprocal squares, but not in the radial corrrection term of the Laplacian which is the coefficient of our difference of Casimirs $C_J - C_L$.

This has the effect that now the relevant power series as far as their relative effect, only affect spectral lines which are between two levels of differing sums of reciprocal squares.

As for how to choose a value of c, a first attempt which did not work is to consider the energy levels as roots of a polynomial, and seek a critical value of the discriminant as a function of c. Rather than explain why this didn't work, it makes sense to explain what does seem to work to some extent. This is, to notice that the actual ordering of energy levels in nature seems to be a refinement of the lexicographical ordering where sums of reciprocal squares are given highest priority, but that unlike in the video where the effect of sums of reciprocal squares causes discontinuities, rather, the division of the energy calculation into one part coming from sums of reciprocal squares and another part coming from an electrostatic perturbation seems artificial and contrived.

And so that what one sees is that if levels are arranged in lexicographic order, the value of c that is chosen should be the one which minimizes the second successive difference of energy levels in the least squares sense for each subsequence where the l quantum numbers are constant. Choosing this value c (we call the multiplier 'emult' in the javascript) does seem to give very good agreement with experimental data, although this does not fix the compression of levels near the ground.

The actual perturbation coefficient we call pmult. The ab initio energy level is then just a linear combination of two parts, with the coefficients in the linear combination being emult and pmult, and we have an ab initio statistical method of finding emult, while we just set pmult=1.

Using both of these numbers it is possible to closely match many atomic spectra, using the spectrograph at `http://spectrograph.uk`, if you press 'new electron' a few times, and then press 'next config' until it stops flashing and then press 'compare external.'

Since we have removed the unexplained Casimir term, it is no longer true, using this spectrograph, that when both coarse and fine calculations are done, that the coarse value (result of the character calculation) describes what spectrographers call the 'center of mass' of the fine lines.

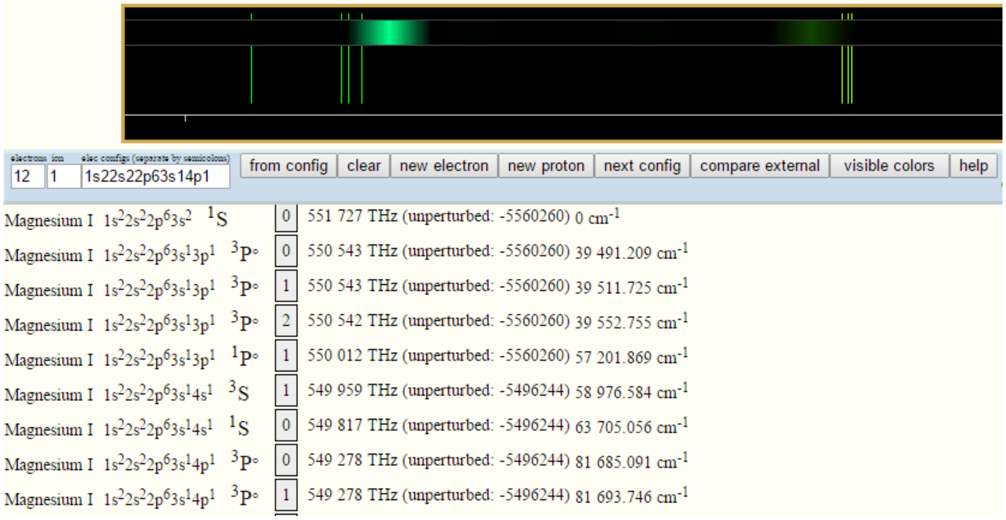
However, there was no reason for thinking that this should have been so. The 'center of mass' is an adjunct calculation with no experimental basis, and had perhaps historical basis because of the very type of character calculation which we're doing now. Yet there is no reason for thinking that the 'center of mass' should correspond to anything in nature.

A reason for allowing a difference between the ‘center of mass’ of the actual fine lines, and the character value calculation, is that any relation between them should rest on the fact that one calculation (the character calculation) uses Weyl’s raising and lowering operators, while the perturbation calculation uses the harmonic functions whose exterior products correspond to the type of tableau which Chemists use (where an orbital of type p is described as a box in which one might put six eggs, and so-on).

But the actual raising and lowering operator which preserves the basis of harmonic functions is the Legendre operator, and it differs from the Weyl operator by a function coefficient. This is not well adapted to perturbation theory as it multiplies the vector space associated to an electron configuration totally into its orthogonal, and perturbation theory cannot apply.

The comparison between the projective geometry and representation theory taking place on the exceptional divisor, versus the harmonic function theory when the square root of r is considered to be a smooth real function, is the domain where things like the McKay correspondence and other open problems in Maths reside.

Here is the spectrum of Magnesium when we perform an ab initio calculation which increases the effect of proton attraction only in its effect on sums of reciprocal squares, to minimize discontinuities (second successive differences) between those successive levels of constant l where the sum of reciprocal squares would change, if this effect were assumed larger than the electrostatic perturbation so that the levels had been lexicographically ordered (though during the calculation no assumption that they actually are lexicographically ordered is needed). The value (called emult in the javascript) calculates to a multiplier of 4.5, We see that the famous $4s^1\ {}^3S_1 - 3p^1\ {}^3P^\circ_{0,1,2}$ triplet which is seen in stars appears in nearly in the right position once three electron configurations are included. Since there is only one discontinuity, this chooses the value of proton charge in that calculation which eliminates the gap between $4s^1\ {}^3S$ and ${}^3p^1\ {}^1P^\circ$, setting both levels to 57 201.869. Nevertheless which is good for neighouring values.



electrons: 12 ion: 1 elec configs (separate by semicolons): 1s22s22p63s14p1

Magnesium I	$1s^2 2s^2 2p^6 3s^2$	${}^1S$	0	551 727 THz (unperturbed: -5560260) 0 cm^{-1}
Magnesium I	$1s^2 2s^2 2p^6 3s^1 3p^1$	${}^3P^\circ$	0	550 543 THz (unperturbed: -5560260) 39 491.209 cm^{-1}
Magnesium I	$1s^2 2s^2 2p^6 3s^1 3p^1$	${}^3P^\circ$	1	550 543 THz (unperturbed: -5560260) 39 511.725 cm^{-1}
Magnesium I	$1s^2 2s^2 2p^6 3s^1 3p^1$	${}^3P^\circ$	2	550 542 THz (unperturbed: -5560260) 39 552.755 cm^{-1}
Magnesium I	$1s^2 2s^2 2p^6 3s^1 3p^1$	${}^1P^\circ$	1	550 012 THz (unperturbed: -5560260) 57 201.869 cm^{-1}
Magnesium I	$1s^2 2s^2 2p^6 3s^1 4s^1$	${}^3S$	1	549 959 THz (unperturbed: -5496244) 58 976.584 cm^{-1}
Magnesium I	$1s^2 2s^2 2p^6 3s^1 4s^1$	${}^1S$	0	549 817 THz (unperturbed: -5496244) 63 705.056 cm^{-1}
Magnesium I	$1s^2 2s^2 2p^6 3s^1 4p^1$	${}^3P^\circ$	0	549 278 THz (unperturbed: -5496244) 81 685.091 cm^{-1}
Magnesium I	$1s^2 2s^2 2p^6 3s^1 4p^1$	${}^3P^\circ$	1	549 278 THz (unperturbed: -5496244) 81 693.746 cm^{-1}

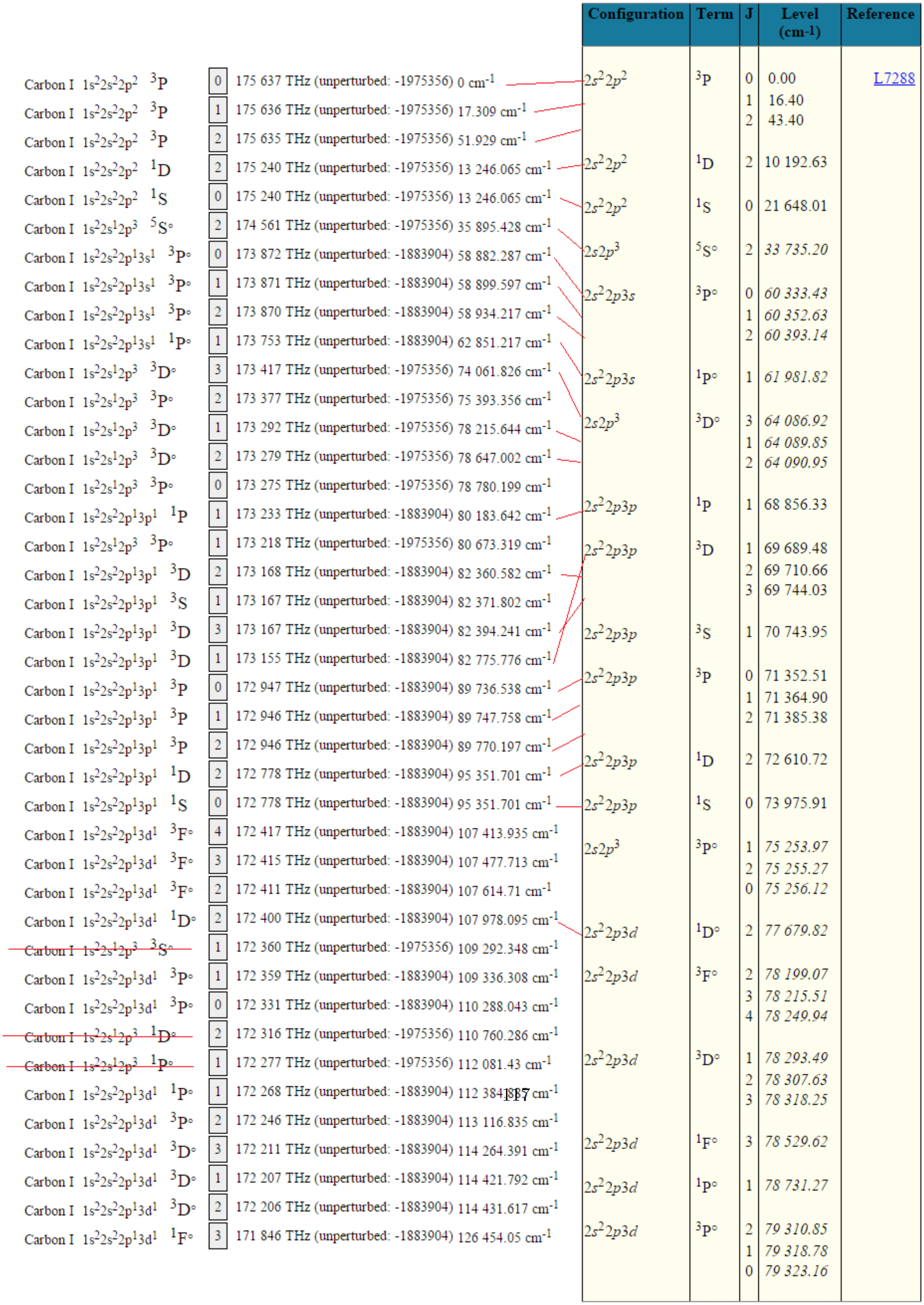
And when this is done the neighbouring yellow triplet also appears.

This calculation can be seen at

`http://spectrograph.uk/index.html?emult=4.5;fmult=2;autocorrect.checked=false&finecorrect.checked=fa`

and then pressing ‘next config’ twice to make the yellow triplet appear beside the green triplet, you will need to zoom in with the arrow keys to see them.

An equivalent calculation, easier to remember but not as well motivated conceptually, is to say that we are artificially changing the electron charge and proton charge, but leaving the perturbation coefficient equal to 1. Here is the ab initio spectrum of Carbon (or rather the ‘energy levels’ whose differences give the spectral frequencies) when we artificially multiply the proton charge by 4 while multiplying the electron charge by 2. We see that except for one misplacement in a fine energy level the first 22 levels including both coarse and fine are in same order as in the NIST database and roughly have the same values. Here we are multipying the electron charge by 2 in the term that relates to the fine structure as well as the coarse structure. Note that the ab initio calculation begines to become incorrect after the first 22 levels and even during the first 22 levels the fine structure becomes too pronounced. Howver the coarse structure is mainly repaired.



Carbon I	$1s^22s^22p^2$	^3P	0	175 637 THz (unperturbed: -1975356) 0 cm^{-1}
Carbon I	$1s^22s^22p^2$	^3P	1	175 636 THz (unperturbed: -1975356) 17.309 cm^{-1}
Carbon I	$1s^22s^22p^2$	^3P	2	175 635 THz (unperturbed: -1975356) 51.929 cm^{-1}
Carbon I	$1s^22s^22p^2$	^1D	2	175 240 THz (unperturbed: -1975356) 13 246.065 cm^{-1}
Carbon I	$1s^22s^22p^2$	^1S	0	175 240 THz (unperturbed: -1975356) 13 246.065 cm^{-1}
Carbon I	$1s^22s^12p^3$	$^5S^\circ$	2	174 561 THz (unperturbed: -1975356) 35 895.428 cm^{-1}
Carbon I	$1s^22s^22p^13s^1$	$^3P^\circ$	0	173 872 THz (unperturbed: -1883904) 58 882.287 cm^{-1}
Carbon I	$1s^22s^22p^13s^1$	$^3P^\circ$	1	173 871 THz (unperturbed: -1883904) 58 899.597 cm^{-1}
Carbon I	$1s^22s^22p^13s^1$	$^3P^\circ$	2	173 870 THz (unperturbed: -1883904) 58 934.217 cm^{-1}
Carbon I	$1s^22s^22p^13s^1$	$^1P^\circ$	1	173 753 THz (unperturbed: -1883904) 62 851.217 cm^{-1}
Carbon I	$1s^22s^12p^3$	$^3D^\circ$	3	173 417 THz (unperturbed: -1975356) 74 061.826 cm^{-1}
Carbon I	$1s^22s^12p^3$	$^3P^\circ$	2	173 377 THz (unperturbed: -1975356) 75 393.356 cm^{-1}
Carbon I	$1s^22s^12p^3$	$^3D^\circ$	1	173 292 THz (unperturbed: -1975356) 78 215.644 cm^{-1}
Carbon I	$1s^22s^12p^3$	$^3D^\circ$	2	173 279 THz (unperturbed: -1975356) 78 647.002 cm^{-1}
Carbon I	$1s^22s^12p^3$	$^3P^\circ$	0	173 275 THz (unperturbed: -1975356) 78 780.199 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^1P	1	173 233 THz (unperturbed: -1883904) 80 183.642 cm^{-1}
Carbon I	$1s^22s^12p^3$	$^3P^\circ$	1	173 218 THz (unperturbed: -1975356) 80 673.319 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^3D	2	173 168 THz (unperturbed: -1883904) 82 360.582 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^3S	1	173 167 THz (unperturbed: -1883904) 82 371.802 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^3D	3	173 167 THz (unperturbed: -1883904) 82 394.241 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^3D	1	173 155 THz (unperturbed: -1883904) 82 775.776 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^3P	0	172 947 THz (unperturbed: -1883904) 89 736.538 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^3P	1	172 946 THz (unperturbed: -1883904) 89 747.758 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^3P	2	172 946 THz (unperturbed: -1883904) 89 770.197 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^1D	2	172 778 THz (unperturbed: -1883904) 95 351.701 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$	^1S	0	172 778 THz (unperturbed: -1883904) 95 351.701 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^3F^\circ$	4	172 417 THz (unperturbed: -1883904) 107 413.935 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^3F^\circ$	3	172 415 THz (unperturbed: -1883904) 107 477.713 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^3F^\circ$	2	172 411 THz (unperturbed: -1883904) 107 614.71 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^1D^\circ$	2	172 400 THz (unperturbed: -1883904) 107 978.095 cm^{-1}
~~Carbon I~~	~~$1s^22s^12p^3$~~	~~$^3S^\circ$~~	1	172 360 THz (unperturbed: -1975356) 109 292.348 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^3P^\circ$	1	172 359 THz (unperturbed: -1883904) 109 336.308 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^3P^\circ$	0	172 331 THz (unperturbed: -1883904) 110 288.043 cm^{-1}
~~Carbon I~~	~~$1s^22s^12p^3$~~	~~$^1D^\circ$~~	2	172 316 THz (unperturbed: -1975356) 110 760.286 cm^{-1}
~~Carbon I~~	~~$1s^22s^12p^3$~~	~~$^1P^\circ$~~	1	172 277 THz (unperturbed: -1975356) 112 081.43 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^1P^\circ$	1	172 268 THz (unperturbed: -1883904) 112 384[illegible] cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^3P^\circ$	2	172 246 THz (unperturbed: -1883904) 113 116.835 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^3D^\circ$	3	172 211 THz (unperturbed: -1883904) 114 264.391 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^3D^\circ$	1	172 207 THz (unperturbed: -1883904) 114 421.792 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^3D^\circ$	2	172 206 THz (unperturbed: -1883904) 114 431.617 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$	$^1F^\circ$	3	171 846 THz (unperturbed: -1883904) 126 454.05 cm^{-1}

Configuration	Term	J	Level (cm^{-1})	Reference
$2s^22p^2$	^3P	0 1 2	0.00 16.40 43.40	L7288
$2s^22p^2$	^1D	2	10 192.63	
$2s^22p^2$	^1S	0	21 648.01	
$2s2p^3$	$^5S^\circ$	2	*33 735.20*	
$2s^22p3s$	$^3P^\circ$	0 1 2	*60 333.43* *60 352.63* *60 393.14*	
$2s^22p3s$	$^1P^\circ$	1	*61 981.82*	
$2s2p^3$	$^3D^\circ$	3 1 2	*64 086.92* *64 089.85* *64 090.95*	
$2s^22p3p$	^1P	1	68 856.33	
$2s^22p3p$	^3D	1 2 3	69 689.48 69 710.66 69 744.03	
$2s^22p3p$	^3S	1	70 743.95	
$2s^22p3p$	^3P	0 1 2	71 352.51 71 364.90 71 385.38	
$2s^22p3p$	^1D	2	72 610.72	
$2s^22p3p$	^1S	0	73 975.91	
$2s2p^3$	$^3P^\circ$	1 2 0	*75 253.97* *75 255.27* *75 256.12*	
$2s^22p3d$	$^1D^\circ$	2	*77 679.82*	
$2s^22p3d$	$^3F^\circ$	2 3 4	*78 199.07* *78 215.51* *78 249.94*	
$2s^22p3d$	$^3D^\circ$	1 2 3	*78 293.49* *78 307.63* *78 318.25*	
$2s^22p3d$	$^1F^\circ$	3	*78 529.62*	
$2s^22p3d$	$^1P^\circ$	1	*78 731.27*	
$2s^22p3d$	$^3P^\circ$	2 1 0	*79 310.85* *79 318.78* *79 323.16*	

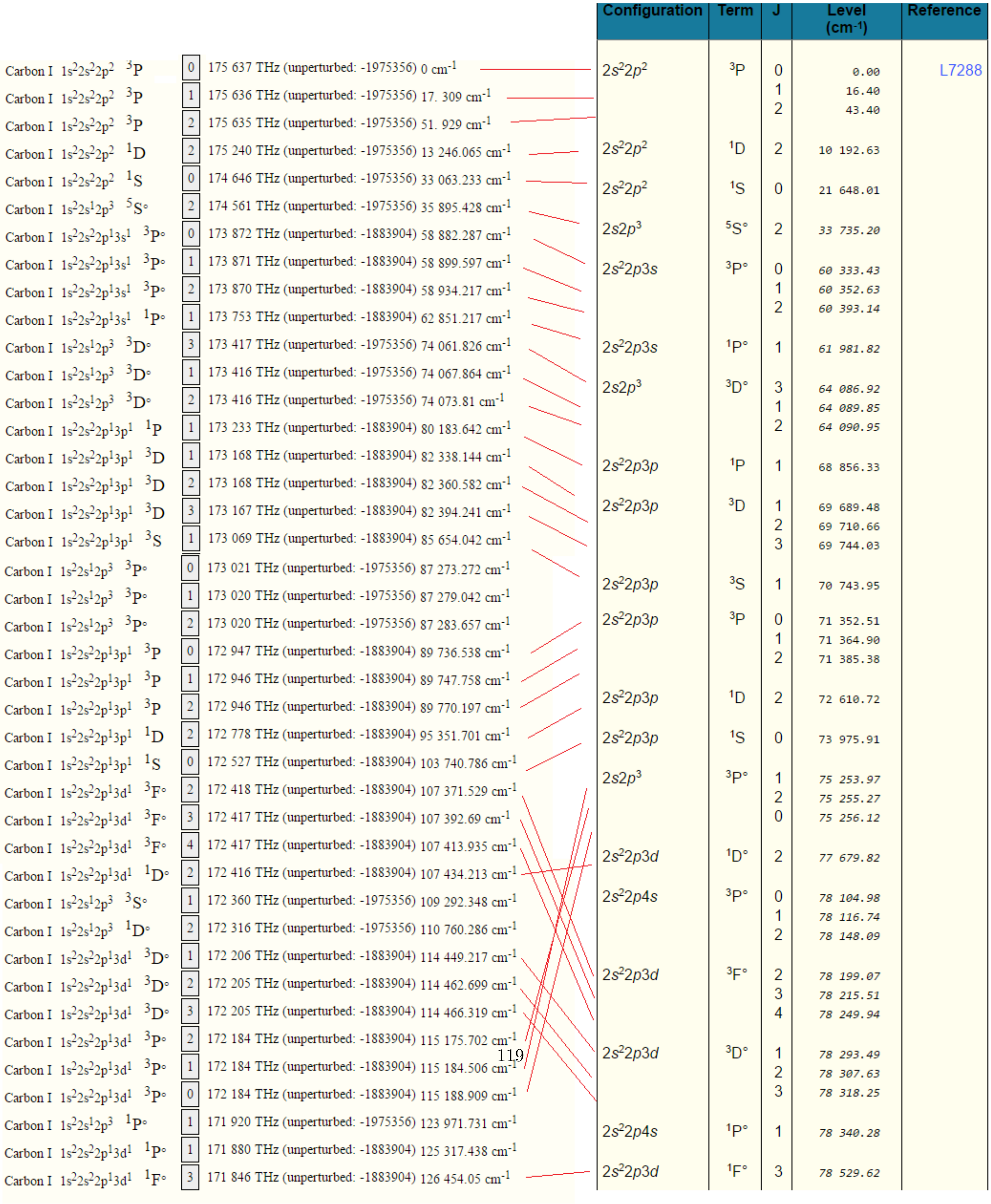
You can generate the data by going to the spectrograph with this link

http://spectrograph.uk/index.html?emult=4&pmult=2&fmult=2&autocorrect.checked=false&dofine.checked=tr

and repeatedly pressing the button labelled ‘next config’, and press ‘compare external’ to compare with the NIST data. I cannot explain why a larger value of $fmult$ is needed than $2/pmult$ although the value of 2 is too large.

If you put &nostop=true after the index.html in the url, the coarse structure will be repaired in the analagous way for each atom or ion which you may choose.

Regarding the fine structure, if you press ‘clear’ and then press ‘fine correct’ (in the current version ‘clear’ reloads the whole page, so instead edit the url to replace ‘finecorrect.checked=false’ with ‘finecorrect.checked=true’) and repeat the calculation, you will see this result



Carbon I	$1s^22s^22p^2$ ^3P	0	175 637 THz (unperturbed: -1975356) 0 cm^{-1}
Carbon I	$1s^22s^22p^2$ ^3P	1	175 636 THz (unperturbed: -1975356) 17. 309 cm^{-1}
Carbon I	$1s^22s^22p^2$ ^3P	2	175 635 THz (unperturbed: -1975356) 51. 929 cm^{-1}
Carbon I	$1s^22s^22p^2$ ^1D	2	175 240 THz (unperturbed: -1975356) 13 246.065 cm^{-1}
Carbon I	$1s^22s^22p^2$ ^1S	0	174 646 THz (unperturbed: -1975356) 33 063.233 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^5S^\circ$	2	174 561 THz (unperturbed: -1975356) 35 895.428 cm^{-1}
Carbon I	$1s^22s^22p^13s^1$ $^3P^\circ$	0	173 872 THz (unperturbed: -1883904) 58 882.287 cm^{-1}
Carbon I	$1s^22s^22p^13s^1$ $^3P^\circ$	1	173 871 THz (unperturbed: -1883904) 58 899.597 cm^{-1}
Carbon I	$1s^22s^22p^13s^1$ $^3P^\circ$	2	173 870 THz (unperturbed: -1883904) 58 934.217 cm^{-1}
Carbon I	$1s^22s^22p^13s^1$ $^1P^\circ$	1	173 753 THz (unperturbed: -1883904) 62 851.217 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^3D^\circ$	3	173 417 THz (unperturbed: -1975356) 74 061.826 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^3D^\circ$	1	173 416 THz (unperturbed: -1975356) 74 067.864 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^3D^\circ$	2	173 416 THz (unperturbed: -1975356) 74 073.81 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^1P	1	173 233 THz (unperturbed: -1883904) 80 183.642 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^3D	1	173 168 THz (unperturbed: -1883904) 82 338.144 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^3D	2	173 168 THz (unperturbed: -1883904) 82 360.582 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^3D	3	173 167 THz (unperturbed: -1883904) 82 394.241 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^3S	1	173 069 THz (unperturbed: -1883904) 85 654.042 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^3P^\circ$	0	173 021 THz (unperturbed: -1975356) 87 273.272 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^3P^\circ$	1	173 020 THz (unperturbed: -1975356) 87 279.042 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^3P^\circ$	2	173 020 THz (unperturbed: -1975356) 87 283.657 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^3P	0	172 947 THz (unperturbed: -1883904) 89 736.538 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^3P	1	172 946 THz (unperturbed: -1883904) 89 747.758 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^3P	2	172 946 THz (unperturbed: -1883904) 89 770.197 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^1D	2	172 778 THz (unperturbed: -1883904) 95 351.701 cm^{-1}
Carbon I	$1s^22s^22p^13p^1$ ^1S	0	172 527 THz (unperturbed: -1883904) 103 740.786 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^3F^\circ$	2	172 418 THz (unperturbed: -1883904) 107 371.529 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^3F^\circ$	3	172 417 THz (unperturbed: -1883904) 107 392.69 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^3F^\circ$	4	172 417 THz (unperturbed: -1883904) 107 413.935 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^1D^\circ$	2	172 416 THz (unperturbed: -1883904) 107 434.213 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^3S^\circ$	1	172 360 THz (unperturbed: -1975356) 109 292.348 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^1D^\circ$	2	172 316 THz (unperturbed: -1975356) 110 760.286 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^3D^\circ$	1	172 206 THz (unperturbed: -1883904) 114 449.217 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^3D^\circ$	2	172 205 THz (unperturbed: -1883904) 114 462.699 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^3D^\circ$	3	172 205 THz (unperturbed: -1883904) 114 466.319 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^3P^\circ$	2	172 184 THz (unperturbed: -1883904) 115 175.702 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^3P^\circ$	1	172 184 THz (unperturbed: -1883904) 115 184.506 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^3P^\circ$	0	172 184 THz (unperturbed: -1883904) 115 188.909 cm^{-1}
Carbon I	$1s^22s^12p^3$ $^1P^\circ$	1	171 920 THz (unperturbed: -1975356) 123 971.731 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^1P^\circ$	1	171 880 THz (unperturbed: -1883904) 125 317.438 cm^{-1}
Carbon I	$1s^22s^22p^13d^1$ $^1F^\circ$	3	171 846 THz (unperturbed: -1883904) 126 454.05 cm^{-1}

Configuration	Term	J	Level (cm^{-1})	Reference
$2s^22p^2$	^3P	0	0.00	L7288
		1	16.40	
		2	43.40	
$2s^22p^2$	^1D	2	10 192.63	
$2s^22p^2$	^1S	0	21 648.01	
$2s2p^3$	$^5S^\circ$	2	*33 735.20*	
$2s^22p3s$	$^3P^\circ$	0	*60 333.43*	
		1	*60 352.63*	
		2	*60 393.14*	
$2s^22p3s$	$^1P^\circ$	1	*61 981.82*	
$2s2p^3$	$^3D^\circ$	3	*64 086.92*	
		1	*64 089.85*	
		2	*64 090.95*	
$2s^22p3p$	^1P	1	68 856.33	
$2s^22p3p$	^3D	1	69 689.48	
		2	69 710.66	
		3	69 744.03	
$2s^22p3p$	^3S	1	70 743.95	
$2s^22p3p$	^3P	0	71 352.51	
		1	71 364.90	
		2	71 385.38	
$2s^22p3p$	^1D	2	72 610.72	
$2s^22p3p$	^1S	0	73 975.91	
$2s2p^3$	$^3P^\circ$	1	*75 253.97*	
		2	*75 255.27*	
		0	*75 256.12*	
$2s^22p3d$	$^1D^\circ$	2	*77 679.82*	
$2s^22p4s$	$^3P^\circ$	0	*78 104.98*	
		1	*78 116.74*	
		2	*78 148.09*	
$2s^22p3d$	$^3F^\circ$	2	*78 199.07*	
		3	*78 215.51*	
		4	*78 249.94*	
$2s^22p3d$	$^3D^\circ$	1	*78 293.49*	
		2	*78 307.63*	
		3	*78 318.25*	
$2s^22p4s$	$^1P^\circ$	1	*78 340.28*	
$2s^22p3d$	$^1F^\circ$	3	*78 529.62*	

with the fine structure also mainly repaired.

One issue is that now there is a 'Lamb shift' even for Hydrogen, though the classical Lamb shift is incorrect, and even has the wrong sign. One of the issues is that one of the integrals in the perturbation calculation fails to converge (this is for s orbitals), our calculation involves a negative binomial coefficient which evaluates to zero while the in actual integral evaluates to infinity. So we would not expect the classical Lamb shift to have the right value.

When the javascript spectrograph is allowed to choose a coarse correction, it will adjust in such a way to find the ratio [pmult:emult] independently of which value of pmult is chosen. Changing this ratio changes the ratio of variance between the electrostatic effect versus the sums of reciprocal squares effect, though it changes this variance ratio in a complicated way, the variance ratio which agrees with the ab initio calculation does tend to be the one which occurs in nature. Then the effect of multiplying both emult and pmult by a constant is, on the coarse scale, to scale levels by a constant, though the effect on fine levels is more complicated. By setting fmult=2/pmult at the outset this effect is compensated and the fine structure appears to fall in line (though the fine correction is slightly more complicated than this, involving as it does the notion of a false fine structure).

Half-integer values of l – first explanation

Regarding the issue of half-integer values of l, or the explanation for the mysterious pair of complex variables u and v which seem to arise from the Aufbau principle, one temptation may have been to consider the symmetrical sphere of a nucleus as the result of the Hopf map, that is the projectivication of a complex two-dimensional normal space. That is, in comparing some maths to some experimental data, it isn't really ever clear what is being forced and what is occurring by choice. The half-integer values may have arisen not due to being forced, but some other choices may have led to a preference to considering functions which actually were only well-defined functions on the normal bundle of an embedded Riemanns sphere in a complex surface. In this case the surface would not be part of nature, but an artefact of the way Sommerfeld had wished to think of it.

The ampleness of the conormal bundle of an embedded Riemann sphere would require it to have negative self-intersection; for example the nuclei of atoms might be considered to be the result of blowing up points in a smooth complex surface. This would be one way of extending the very explicit description of wave functions to the case of half-integral values of l, without a need of a gauge adjustment cocycle.

An immediate difficulty with that idea is that it's hard to imagine the nucleus seen from a distance as looking like anything but one point in space and time, hence only existing for an instant, appearing then more like an event than a particle of matter. Another, less serious, difficulty is whether this precludes a anyone's preferred complex analytic 'space-time' being a minimal surface.

A third, now more serious difficulty, is that a choice of coordinatization such as the Hopf map should *never* be deemed necessary to give an explanation of a physical phenomenon. Then one could rightfully answer that the presence of the Hopf map is unexplained.

Generalities about the Hamiltonian formulation

Before discussing Schroedinger's function W, it might be worth explaining the Hamiltonian formulation, what it was intended to do. I'll use notation from 'classical mechanics primer,' especially as these can be simplified if we allow throughout both the deRham differential d of M and the one d' of its tangent bundle N. Recall that ϵ is the Euler derivation, j its contraction operator, and that a vector field δ is *involutive* if $i_\delta \eta = j$, and it is *Lagrangian* for a closed one-form ω on N if $\delta\eta\omega = \omega$.

It is easy to see that the involutive condition just means that when f is a section of $\mathcal{O}_M$ viewed as a function on N constant along fibers, then $\delta(f) = df$, where we view df as a section of $\mathcal{O}_N$.

If one examines various statements that Lagrangian forms make certain integrals critical, they just come down to conditions which are satisfied just for Lie derivatives of one-forms. They are nothing but criteria for recognizing when a one-form happens to be a Lie derivative with respect to a particular vector field, and they do not need to be considered if one is already happy with the concept that one forms have Lie derivatives.

In coordinates, locally, a section of Ω_N can be written

$$\omega = \sum_i p_i d' dq_i + r_i d' q_i$$

with p_i, r_i sections of $\mathcal{O}_N$ but q_i are only sections of $\mathcal{O}_M$.

Then $\eta\omega$ is only

$$\sum_i p_i d' q_i$$

an arbitrary section of the pullback of one forms from M. And as long as δ is involutive, when we write

$$\delta\eta\omega = \sum_i \delta(p_i) d' q_i + p_i d' \delta(q_i)$$

we can rewrite the last term

$$= \sum_i \delta(p_i) d' q_i + p_i d' dq_i.$$

To say that this equals ω again is to say

$$r_i = \delta(p_i).$$

This is just the condition for ω to be the Lie derivative of a one-form pulled back from M. But if ω is exact locally so it is dL for a function L on M, then

$$p_i = \frac{\partial}{\partial(dq_i)} L$$

$$\delta(p_i) = \frac{\partial}{\partial q_i} L$$

giving the familiar Lagrange condition

$$\delta \frac{\partial}{\partial(dq_i)} L = \frac{\partial}{\partial(q_i)} L.$$

Given that δ is assumed to be involutive, this is not expressing anything other than that we are looking at a Lie derivative of a pullback from M.

The right side can be manipulated by both adding and then subtracting the term $\sum_i \delta(q_i) d' p_i$. An organized way of doing that is to use Cartan's equation $\delta = d \circ i_\delta + i_\delta \circ d$. Thus for general $\eta\omega = \sum p_i d' q_i$ we obtain

$$\delta\eta\omega = i_\delta(\sum_i d'p_i \wedge d'q_i) + d' \sum p_i \delta(q_i).$$

The first term is the contraction of an alternating form, of course, and the second term is the differential of a quantity $\sum_i p_d \delta(q_i)$ sometimes interpreted as twice the kinetic energy. The point is that since we assume this is an expression for ω and that ω is closed, so is the first term on the right side. Locally writing this dH, the fact that i_δ is nilpotent of order two forces H to be invariant under δ; it is sometimes interpreted as minus the total energy, and so the whole right side is interpreted as the deRham differential on the tangent bundle N of minus the total energy plus twice the kinetic energy, or the difference between kinetic and potential energy. The identity between the coefficients of dH and the coefficients of

$$i_\delta \sum_i dp_i \wedge dq_i = \sum \delta(p_i) d'q_i - \delta(q_i) d'p_i$$

is the Hamilton equation which is a simple way of writing an ordinary differential equation determining the rate of change of the p_i and q_i. Note that in our current situation considering δ to be involutive, $\delta(q_i)$ is anyway nothing but dq_i viewed as a section of $\mathcal{O}_N$ and the meaningful information in such an attempt would only be that $\frac{\partial}{\partial q_i} H = \delta(p_i)$.

As a practical matter, the Hamiltonian approach to solving physical problems can nicely be summarized like this, then. To choose any one-form of your choice pulled back from M, which we locally write if we wish $\sum_i p_i d'q_i$ and whose Lie derivative ω is closed. Then if one manages to describe the function $\sum p_i\delta(q_i)$, which is ordinarily considered to be twice the kinetic energy, one is done. Because the difference

$$\delta\sum_i p_i d'q_i - d'\sum p_i\delta(q_i)$$

is again closed; locally writing this as dH for a function H on the tangent bundle, one then has

$$\delta(p_i) = \partial/\partial q_i H.$$

That is, the rate of change of the p_i are determined by the spatial gradient of H, regardless of however one has chooses the coordinates. The p_i are functions on N and as long as $dp_1 \wedge ... \wedge dp_n$ is nondegenerate as an n form on the tangent space fibers, the dq_i can be expressed in terms of these and the rates of change of the dq_i obtained by the appropriate Jacobian determinant. [8]

---

[8] Interestingly, in formula (26) generalizing his treatment of the hydrogen atom to a 'wholly general conservative system,' Schroedinger finds himself conjugating $\partial/\partial q_i$ by the square root of such a determinant, integrating over space to find his wave function by the Lagrange multiplier argument, but it is made assuming the p_i actually are the $\partial/\partial q_i$ and that the matrix is the matrix of a symmetric quadratic form expressing the kinetic energy.

This is an appealling approach to physics, due to Hamilton, and of course it does not depend on any notion of energy or of conservation of energy, nor on the interpretation of the function $\sum p_i \delta q_i$ as twice the kinetic energy. The two terms $d'H$ and $d' \sum p_i \delta q_i$ are the two terms of the Cartan equation for $\delta\eta\omega$. In cases when it is possible to identify the tangent and cotangent bundle with each other one sometimes takes for p_i the function $\partial/\partial q_i$ and then $\sum p_i d' q_i$ is the natural one form, though the impossibility of doing this relates to one of the problems that a relativistic approach would need to deal with.

Schroedinger's function W

In the setting of Schroedinger's paper, we cannot sensibly take the function $W(x, y, z, t)$ to be a function of space and time, constant on fibers of $N \to M$. For $\omega = d'dW$ we would just have

$$\eta\omega = d'W$$

and if δ is any involutive vector field $\delta(d'W) = d'dW$ so

$$\delta\eta\omega = \delta d'dW = \omega$$

showing ω is Lagrangian. Yet since $\eta\omega$ itself is a closed form on the tangent bundle, the term $i_\delta\ d'\eta\omega$ is zero; it is explicitly $\delta(1) \wedge d'W - \delta(W) \wedge d'(1)$ and the condition of a hamiltonian function H that this is $-d'H$ requires H to be a constant not only on orbits of δ but on the entirety of N. Then while the rule $\partial H/\partial q_i = p_i = 0$ is true, such an equation does not determine the $\delta(dq_i)$ unless the q_i are well-defined functions of the p_i.

Some of the times Schroedinger says he is merely speaking in analogies must be because he would have wished to have dW really to have been a a general one form on the tangent bundle pulled back from M, rather than a closed form.

A general $\eta\omega$ is locally $\sum p_i d' q_i$, with q_i sections of $\mathcal{O}_M$ and p_i sections of $\mathcal{O}_N$, and it should not be assumed to be closed. The equation (7) in his paper which Schroedinger writes:

> It is well-known that $p_x = m\dot{x} = \partial W/\partial x$

is an attempt to say that the differential of W should be this form $\sum p_i d' q_i$, using the deRham differential d' of the tangent bundle. Here he assumes that p_x is a component of momentum, an application of the notion that the form $\eta\omega = \sum p_i d' q_i$ can be taken to be the canonical form on a cotangent bundle.

More importantly – a sin which is not forgiven by the assumption of a Euclidean metric – Schroedinger assumes that the form $\eta\omega$ is a pullback to the tangent bundle of a single closed one-form on M. If we pretend that this were so, we could deduce most of his formulas, but really instead of equations equivalent to

$$\delta(W) = -H + 2T$$

he should be writing locally

$$\delta\eta\omega = -d'H + 2d'T$$

with

$$-d'H = i_\delta \sum dp_i \wedge dq_i$$

The wave function is the exponential of iW times a function of space, and as we've discussed so far only the case of standing waves (although he goes further in this paper), the action of δ is only through its action on W.

Half-integer values of l – other explanations

If one does not wish to think of nuclei as curves with self-intersection -1, one might instead think that the reason phases of wave functions sometimes do not line up without a gauge adjusting cocycle is because the actual symmetries, actual changes of perspective have a wavelike propogation. This interpretation even in the simplest and most literal manifestation is one which will always work, for example by just thinking of wave functions as having the domain of definition being a group itself.

However, a very down-to-earth approach, an alternative explanation for the difficulties with half-integral values of l, which is a special case of the three other approaches, is suggested by how Schroedinger's formulas really did not work – they degenerate – if his function W really is taken to be a well-defined time-dependent function on M constant on fibers of $N \to M$. That is, when he would speak in analogies about making the Hamiltonian 'homogeneous of degree two' or replacing p_x, p_y, p_z by differential operators, what he probably meant to say is that he really intended to exponentiate not invariant spaces of purely imaginary functions, but, rather, act upon invariant spaces of purely imaginary one-forms.

Later things like the Bohm-Aharanov effect should not really be in any contradiction with a purely classical mechanics interpretation of electromagnetic waves, if one understands that if Schroedinger had been more careful – rather than speaking in analogies as he admits doing – the phases were never intended to be anything except one forms on the tangent bundle which are in the pullback of the sheaf of one forms on the configuration manifold.

In the end this means he is needlessly, I think, requiring that the logarithm of a wave function needs to be a well-defined function.

That is, it is likely that if Schroedinger's thinking is written down rigorously, keeping track of when one is working on a configuration manifold and when one is working on a tangent bundle, then it becomes clear that what is the one-form dW in this paper should not have been assumed to be a closed form unless the relation with the Hamiltonian approach was meant to be a degenerate observation.

A remaining issue is what it would mean to exponentiate 'the function whose deRham differential is $\eta\omega$' in cases when we know that no such function exists. The interpretation of the phase of the wave function, at least, would be path-dependent and for paths in the configuration manifold it is even a question whether phase changes should depend on the speed of motion along the path, as this would alter the lifted path is in the tangent bundle. And the phases themselves could only be sensibly measured relative to a moving point, something by the way reminscent of what happens with magnetic fields.

The discussion above is tentative, but even so it does not approach any attempt to introduce relativity into the atomic equations, or indeed even time dependence of amplitude, and was just a discussion of a classical mechanics interpretation of standing waves.

The atom

The first thing which we wish to look at, having nothing to do with chemistry or physics, is just the symmetries of our coordinate system.

Let's consider $\mathbb{R}^3$ to mean the usual real algebraic variety with points $\mathbb{R}^3$. When one writes $r^2 = x^2 + y^2 + z^2$ in order to have a radial function r, this is correctly a coordinate function on the affine quadric Q which is the pullback

$$\begin{tikzcd} Q \arrow[r] \arrow[d] & \mathbb{R} \arrow[d] \\ \mathbb{R}^3 \arrow[r] & \mathbb{R} \end{tikzcd}$$

$$(x, y, z) \mapsto x^2 + y^2 + z^2$$

where the right vertical map is $r \mapsto r^2$. Then the top horizontal map is the coordinate function r, and the map $Q \to \mathbb{R}^3$ is branched along the subvariety defined by the equation $x^2 + y^2 + z^2 = 0$. The variety Q is the affine variety in coordinates x, y, z, r given by the equation $x^2 + y^2 + z^2 = r^2$.

The symmetry group of the quadratic form $x^2 + y^2 + z^2 - r^2 = 0$ is not going to be relevant, as this depends on a four-dimensional affine space with little physical meaning.

The affine subvariety V of Q defined by the equation $r = 0$ has one point which is real rational, and if we minimally resolve this singular point we get of V, the resulting variety $\widetilde{V}$ has exceptional divisor P with no real rational points at all; it is a Severi-Brauer variety. The whole of $\widetilde{V}$ is isomorphic to the cotangent bundle of the Severi-Brauer variety P.

When we formally use a sphere of angles which is obtained by blowing up, if we wish to work analytically using a square root of the radius, then we thus find that the sphere of angles is only a Severi-Brauer variety, it has no real rational points. But this is not to say that blowing up the point has made it disappear. Rather we may still work with the function sheaf on the cotangent bundle of the Severi-Brauer variety, including its exceptional divosr, just as we may work with complex eigenvalues of a real linear transformation.

The variety P is not just a point, it has symmetries, while having no real rational points. In fact its Lie algebra of vector fields is $so_3(\mathbb{R})$.

In linear algebra, a person often considers a real matrix such as the matrix of a rotation of a plane, and considers that it has as its eigenvalues a natural complex conjugate pair. Here we have a whole real sphere made up of such complex conjugate pairs. The set of ratios $[x : y : z]$ in complex three space which satisfy the rule that $x^2 + y^2 + z^2 = 0$, reduced modulo the fixed point free continuous action of complex conjugation, gives a real projective plane. But it is not necessary to complexify anything to see it.

As a scheme over the reals P is a well-defined object. The moduli of irreduible coherent sheaves on P has a natural classical topology, it is the same real projective plane which, if one had decided to complexify everything, would have occurred once one had reduced the Riemann sphere modulo a continuous antiholomorphic automorphim. The classical topology on the moduli of irreducible coherent sheaves on P gives the same space (a real projective plane) and does not require complexifying anything to see it, it does not require complex numbers or complex conjugation.

If $\widetilde{V}$, when viewed as a line bundle over P, were the tensor square of some other line bundle M, so $M^{\otimes 2} \cong \widetilde{V}$, then as a variety M would be a cyclic branched cover of order two of $\widetilde{V}$.

As a vector bundle over P, its cotangent bundle, which is isomorphic to $\widetilde{V}$ as line bundle, is not a tensor square, and so this cannot take place.

Rather, if we delete P from $\widetilde{V}$, that is the same as deleting $\{0\}$ from V, and we find that that what is left $V\setminus\{0\}$ has a *four* sheeted etale universal cover, with Galois group cyclic of order four.

Because the Galois group is cyclic, the three etale covers of $V\setminus\{0\}$, one being the identity, one being the complexification, and one being the universal cover, are linearly ordered. It is not possible to perform the branched cyclic cover until after complexifying.

Yet the combination, of complexifying and then taking the branched cyclic cover of the complexification of $\widetilde{V}$, and therefore of the two steps separately, are completely natural.

One is passing to the degree four universal cyclic cover of the cotangent bundle of P which is branched along P. Also each step is familiar in a different way; once $\widetilde{V}$ is complexified it becomes a line bundle on the Riemann sphere $\mathbb{P}^1$ with section sheaf $\mathcal{O}(-2)$, and is covered by the line bundle with section sheaf $\mathcal{O}(-1)$.

It is also relevant, what we'll consider later on, that covering spaces are natural for vector fields – vector fields lift naturally to covering spaces, including etale covers – but not for automorphisms. We can apply this principle for the entire degree four etale cover, and we have that for example vector fields on the complement of P in $\widetilde{V}$ lift uniquely through the degree four etale cover, and become holomorphic vector fields on $\mathbb{C}^2 \setminus \{0\}$. We have seen this in coordinates in Chemistry textbooks.[9]

The complexification of V is isomorphic to the ordinary double point $\mathbb{C}^2/\{1, -1\}$ – the result of contracting a -2 curve, and the correspondence between coordinates is

$$x = \frac{u^2 + v^2}{2}$$

$$y = \frac{u^2 - v^2}{2i}$$

$$z = \frac{uv}{i}$$

and correspondingly

$$u^2 = x + iy$$

$$uv = iz$$

$$v^2 = x - iy.$$

---

[9] In retrospect, it was misleading for me to have earlier quoted Weyl referring to a central extension cocycle as a 'gauge,' without commenting that in the same context he introduced the 'infinitesimal rotations' as an *alternative* explanation, giving the reader a choice. I see now, looking again at his book, that he really interprets the action as a differential action on du and dv leaving it unexplained only why there should be such an infinitesimal action, or what du and dv ought to represent.

So far we have only analyzed the variety defined by the equation $r = 0$ within the quadric hypersurface Q defined by the rule $x^2 + y^2 + z^2 = r^2$. If we blow up the origin here to obtain a smooth variety $\widetilde{Q}$, the exceptional divisor $E \subset \widetilde{Q}$ is an algebraic surface containing the Severi-Brauer variety P. If we complexify the inclusion $P \to E$ we obtain a copy of the diagonal inclusion $\mathbb{P}^1 \to \mathbb{P}^1 \times \mathbb{P}^1$, but the identification of a decomposition of the complexification of E as a cartesian product $\mathbb{P}^1 \times \mathbb{P}^1$ is *not* natural, and there is no natural pair of projections to $\mathbb{P}^1$.

An interesting point also is that the real points of the exceptional divisor $E \cong \mathbb{P}^1 \times \mathbb{P}^1$ in the resolution $\widetilde{Q}$ of the ordinary double point three-fold Q comprise a copy of the two-sphere S^2, it is the real projective variety defined by the homogeneous equation $x^2 + y^2 + z^2 = r^2$; and the map to the real projective plane by the coordinates x, y, z is an *unbranched* topological double-cover. This is because the branching locus is exactly the Severi-Brauer variety P with no real-rational points. The real points of the full $\widetilde{Q}$ can be viewed as the disjoint union of all *oriented* real lines through the origin in $\mathbb{R}^3$, and forgetting the orientation gives a map $\widetilde{Q} \to Bl_{\{0\}}\mathbb{R}^3$, the blowup of $\mathbb{R}^3$ at the origin, which is the disjoint union of the real lines through the origin without any orientation being remembered.

While the topological structure on the double covering of the sphere is that of a covering space, with freely-acting covering group, the scheme structure includes a fixed subscheme, this is a scheme theoretic branching divisor, and it is by contracting two-forms along the Euler derivation of the line bundle and then restricting to the Severi-Brauer variety that we will be able to realize the restriction of the Legendre operator on harmonic functions as a Weyl lowering operator.

The normal bundle of P in E is yet another copy of the cotangent bundle of P, and so $\widetilde{Q}$ contains two copies of $\widetilde{V}$ which intersect along P. One of the two is the divisor of poles of the now rational function r.

If we pull-back the line bundle $\mathcal{O}_{\mathbb{P}^2}(-1)$ along the branched double-cover, the result is what is known as $\mathcal{O}_{\mathbb{P}^1 \times \mathbb{P}^1}(-1,-1)$. That is, it is dual of the line bundle with section sheaf which includes one section crossing the zero section $\mathbb{P}^1 \times \mathbb{P}^1$ at the union of two coordinate lines $\mathbb{P}^1 \times \{p\} \cup \{q\} \times \mathbb{P}^1$, for points $p, q \in \mathbb{P}^1$. Note that the projectivication of the space of dual sections is two-dimensional; yet this description is not natural and there is not a natural decomposition of E as a cartesian product $\mathbb{P}^1 \times \mathbb{P}^1$.

The *restriction* of this pulling back to $\mathbb{P}^1 = P \subset E$ where P occurs as the diagonal under any choice of decomposition, naturally, gives the bundle $\mathbb{O}_{\mathbb{P}^1}(-2)$. The pulling back is an isomorphism on the zero section.

The restriction (=pullback) of the threefold branched double covering $\widetilde{Q} \to Bl_{\{0\}}\ \mathbb{C}^3$ along the inclusion of the quadric curve $\mathbb{P}^1 \to \mathbb{P}^2$ is the branch locus of the branched cover.

$$\begin{tikzcd}
Bl_{\{0\}}\,\mathbb{C}^2 \arrow[r, phantom, "="] & \mathcal{O}_{\mathbb{P}^1}(-1) \arrow[d] & & \\
\widetilde{V} \arrow[r, phantom, "\cong"] & \mathcal{O}_{\mathbb{P}^1}(-2) \arrow[r] \arrow[d, "="] & \mathcal{O}_{\mathbb{P}^1\times\mathbb{P}^1}(-1,-1) \arrow[r, phantom, "\cong"] \arrow[d] & \widetilde{Q} \\
 & \mathcal{O}_{\mathbb{P}^1}(-2) \arrow[r] \arrow[d] & \mathcal{O}_{\mathbb{P}^2}(-1) \arrow[r, phantom, "="] \arrow[d] & Bl_{\{0\}}\,\mathbb{C}^3 \\
 & \mathbb{P}^1 \arrow[r] & \mathbb{P}^2 &
\end{tikzcd}$$

We have then made an additional branched cover in the upper left vertical map.

The right vertical map is the bundle map induced by pulling back along the branched double covering $\mathbb{P}^1 \times \mathbb{P}^1 \to \mathbb{P}^2$, and pullback (=restriction) along the inclusion of the diagonal $\mathbb{P}^1$ is the identity.

The main square in this diagram expresses a branched double covering of the three-fold $\widetilde{Q}$ over $Bl_{\{0\}}\,\mathbb{C}^3$ with branch locus $\tilde{V}$.

The vertical maps on the left (of which one can be considered to be the identity when the three fold branched cover is restricted to its own branch locus), are both constant on the base $\mathbb{P}^1$ and the top map shown is the two sheeted line bundle map induced by tensor square on each line fiber.

Thus, the right vertical map is essentially constant on fibers while the left vertical map is constant on the base.

It is interesting that the restriction of the right vertical map to exceptional divisors $\mathbb{P}^1 \times \mathbb{P}^1 \to \mathbb{P}^2 \subset Bl_0\mathbb{C}^3$, in its action on *real* points, is a copy of the topological double covering of the real projective plane, while the constant $\mathbb{P}^1$ in any term of either left vertical map is the Severi-Brauer variety, whose complex points are a second way of finding a double covering of the real projective plane, this time in the map from complex points to irreducible coherent sheaves on the real Severi-Brauer variety.

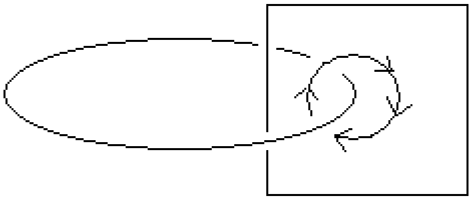
The variety $\widetilde{Q}$ can be constructed in coordinates as follows: if we consider u^2 and v^2 just to be a pair of independent coordinates, complement of the exceptional divisor are the nonzero points of the affine variety defined by the equation $u^2v^2 = (r - z)(r + z)$ while the exceptional divisor is the projective variety given by the same equation, interpreted as being homogeneous in u^2, v^2, z, r. Thus the exceptional divisor in $\widetilde{Q}$ decomposes non-naturally as a cartesian product of two projective lines $\mathbb{P}^1 \times \mathbb{P}^1$ which can be considered to have homogeneous coordinates $[u^2 : z + r]$ and $[u^2 : z - r]$ respectively. The Galois action which negates r induces the action on the exceptional divisor which interchanges these two projective line factors in the cartesian product.

The identifications of $Bl_{\{0\}}\ \mathbb{C}^2$ and $Bl_{\{0\}}\ \mathbb{C}^3$ with line bundles are not natural. The map $Bl_{\{0\}}\ \mathbb{C}^2 \to Bl_{\{0\}}\ \mathbb{C}^3$ does descend to a map $\mathbb{C}^2 \to \mathbb{C}^3$ which is described by the equations a few pages earlier, expressing x, y, z as homogeneous complex polynomials in u, v. But the identifications with line bundles in the diagram just above are not natural. Let us explain this.

Often the symbol $\mathcal{O}(-1)$ is taken to mean the actual bundle of lines through the origin in the plane $\mathbb{C}^2$. Associated to $U \subset \mathbb{P}^2$ the set $\Gamma(U, \mathcal{O}(-1))$ is the ways of analytically choosing a point in each line $L \in U$. And if one actually chooses a point $p \in \mathbb{P}^1$, then $\mathcal{O}(-p)$ is isomorphic to $\mathcal{O}(-1)$.

The abuse of notation is substantial. If point p is replaced by a different point q, there is no natural way to choose an isomorphism $\mathcal{O}(-p) \to \mathcal{O}(-q)$, and there is no such functor as $\mathcal{O}_{(-)}(-1)$ from copies of the Riemann sphere to coherent sheaves.

It is indeed correct to think of the Riemann sphere as the sphere of angles in three dimensional space, indpendently of any choice of Riemannian geometry. But if we want to make the description of the Riemann sphere as a bundle of lines become natural, we must reduce each line in the line bundle modulo the action of a rotation by π radians



The reduction map is the identity on the Riemann sphere, and is a branched cover of order two, which branches along the Riemann sphere. The map is the natural map from a line bundle to its tensor product square, and on the fiber vector spaces V, which are one dimensional vector spaces, the map is the natural map $V \to V \otimes V$ under which a tensor (all are indecomposable) v is sent to $v \otimes v$. The Galois group of the branched covering is just the action of -1 on the line fibers.

If we really think that the Riemann sphere is meant to be the sphere of angles at a point of three dimensional space, then each point naturally has an opposite, and the map sending each point to its opposite is anti-holomorphic, rather than holomorphic. Rather than trying to extend this anti-holomorphic map to the line bundle $O(-1)$ – or what would be more correctly called $\mathcal{O}(-p)$ for some point of the Riemann sphere, it makes more sense to recognize that $\mathcal{O}(-2)$ does make sense, that the connected conformal group of automorphisms of the sphere does act upon it in a natural way, and also that this has a natural two-sheeted branched cover. The group which acts naturally on the branched cover arises naturally too, But there is no natural vector space around which we might call $\mathbb{C}^2$.

Just as the Riemann sphere inside any $\mathcal{O}(-p)$ can be contracted to a point, resulting in a copy of $\mathbb{C}^2$, the Riemann sphere inside the natural surface $\mathcal{O}(-2)$ can be contracted to a point, resulting a surface with an ordinary double point. The coordinate ring of this affine surface can be represented as the subring of the polynomial algebra $\mathbb{C}[u, v]$ in two variables u, v which consists of polynomials whose degree is even (the invariants of the cyclic group of order two which negates u and v). Recall that the defining equation of the affine variety Q is $u^2v^2 = r^2 - z^2$ where we have written $u^2 = x + iy,\ v^2 = x - iy$. The equations we already have seen

$$x = \frac{u^2 + v^2}{2}$$
$$y = \frac{u^2 - v^2}{2i}$$
$$z = \frac{1}{i}uv.$$

can then be deduced by setting $r = 0$.

Here x, y look like the real and imaginary parts of a complex number $x + iy$, but at this time that is not what they are, all of u, v, x, y, z are complex coordinates. This gives a presentation of the subring generated by u^2, uv, v^2 as the algebra

$$\mathbb{C}[x, y, z]/(x^2 + y^2 + z^2).$$

Now it is time to discuss the principal parts bundle. In the development of the theory of things like the deRham differentials, it was a nice simplification to be able to write dx separate from an expression like dx/dt for the differential of a variable x, say, in terms of time t. Sheaf theoretically, if S is a complex manifold, then the first deRham differential has a rigorous definition, for example as a derivation $\mathcal{O}_S \to \Omega_S$ from the structure sheaf to the Kahler differentials. Instead of needing to talk about derivations $\mathcal{O}_S \to \mathcal{F}$ for another coherent sheaf $\mathcal{F}$ we can just talk about linear maps $\Omega_S \to \mathcal{F}$. When $\mathcal{F} = \mathcal{O}_S$ then any vector field δ has its contracting map $i_\delta : \Omega_S \to \mathcal{O}_S$ so that $\delta = i_\delta \circ d$, and the correspondence is bi-unique.

Really, when a person writes dx, they almost always really mean $x + dx$, thinking that a quantity x is already there, and will be changed slightly. So that one could have made a map

$$\mathcal{O}_S \to \mathcal{O}_S \oplus \Omega_S$$

which on local sections is given $x \mapsto x + dx$. There was no need to do this because we knew what x is already, and so understanding dx already implies understanding $x + dx$. But when we use dx we usually think of it as an initial part of an indeterminate or universal power series

$$x + dx + ...$$

of which we've only written the first two terms.

When x is a function defined on say an open subset of S, there is no problem. This is because *the* structure sheaf of S has a natural connection. But if I only know that x is a section of *some* trivial line bundle, then it no longer is true that I can separate out the two parts in the sum $x + dx$.

Just like the deRham differential is something universal, which can be converted into the value of a derivative, once a linear map $\Omega_S \to \mathcal{F}$ of coherent sheaves is given, there is also a very nice coherent sheaf which actually represents connections. So our writing ∇x for the first principal part of x does not contradict the use of the symbol ∇x to mean that we've applied a connection ∇ to a section x of a vector bundle. Here we have applied what might be called the 'universal connection.'

If x is a section of a coherent sheaf $\mathcal{F}$ on an open set U then ∇x is a section of what is called $\mathcal{P}(\mathcal{F})$ on the same open set. There is the universal connection

$$\nabla : \mathcal{F} \to \mathcal{P}(\mathcal{F})$$

and just as in the case of differentials, there is a bijection between actual connections

$$\mathcal{F} \to \Omega_S \otimes \mathcal{F}$$

and coherent sheaf maps

$$\mathcal{P}(\mathcal{F}) \to \Omega_S \otimes \mathcal{F}$$

whose composite with a natural inclusion

$$\Omega_S \otimes \mathcal{F} \to \mathcal{P}(\mathcal{F})$$

happens to be the identity.

In the case of the surface $\mathcal{O}(-1)$, viewed as the total space of a line bundle on the Riemann sphere S, and recall that this is nothing but the disjoint union of the lines through the origin in $\mathbb{C}^2$, although we are now intentionally disregarding the naturality issue which we highlighted in the first section(!), the contracting map $\mathcal{O}(-1) \to \mathbb{C}^2$ merely contracts the Riemann sphere to a point (as it should, if we think that points of the Riemann sphere are really only angles), and if we choose two coordinate functions u, v on $\mathbb{C}^2$ then we can compose with the map $\mathcal{O}(-1) \to \mathbb{C}^2$ to obtain two holomorphic functions on $\mathbb{O}(-1)$ which are zero on the Riemann sphere. However, in this description we've used the vector space $\mathbb{C}^2$ as a sort of crutch, which we should not have done.

The issue is, in understanding physical phenomena, to know what is our actual coordinate system, and what are our prejudices. It is tempting to say that there 'is' a complexified Euclidean plane somewhere, as a starting point. But there is not, except historically. When people learn mathematical manipulations, such as proofs in Euclidean geometry, the reason is not to be able to reproduce those same proofs.

The functions u, v are linear on the fibers, they are global sections of $\mathcal{O}(1)$, and the principal parts $\nabla u, \nabla v$ of u and v when viewed as sections of $\mathcal{O}(1)$ are really no different than the deRham differentials du, dv when u, v are viewed as coordinate functions on the un-projectivized space $\mathbb{C}^2$ whose projectivication is the Riemann sphere. If we write $X = \mathcal{O}(-1)$ it is also the pullback to S of $\Omega_X(log\ S)(-S)$.

What this means is that automorphisms of $\mathcal{O}(-1)$ as a vector bundle do induce automorphisms of the two-dimensional vector space spanned by $\nabla u, \nabla v$.

If we consider just the group SU_2 acting on the line bundle $\mathcal{O}(-1)$ – the action such that the reduction modulo the center of the group is an SO_3 action on the Riemann sphere – then it follows that the group extension

$$1 \to SU_2 \to G \to SU_2 \to 1$$

splits, where G is a group of automorphisms of the rank two principal parts sheaf $\mathcal{P}(\mathcal{O}(1))$ on the Riemann sphere.

It is always true that a self-semidirect product like $SU_2 \rtimes SU_2$ is isomorphic to a cartesian product $SU_2 \times SU_2$, the isomorphism is

$$SU_2 \times SU_2 \to SU_2 \rtimes SU_2$$

$$(g, h) \mapsto (gh, h^{-1}).$$

Then a less mysterious way of describing the sheaf $\tau^*\mathcal{P}(\mathcal{O}(1))$ is as I mentioned before, to think of $\mathcal{P}(\mathcal{O}(1))$ as the pull-back to the zero-section $\mathbb{P}^1$ of the sheaf $\Omega(log\ \mathbb{P}^1)(-\mathbb{P}^1)$ of differentials on the surface $\mathcal{O}(-1)$ with zeroes and logarithmic poles on the zero section. If this were pulled back along the natural projection $\mathcal{O}(-1) \to \mathbb{P}^1$ we would obtain again the whole of $\Omega(log\mathbb{P}^1)(-\mathbb{P}^1)$ and indeed it makes more sense to do this, let's do it. We can think of the Schroedinger solutions for a single electron (including spin) restricted to the sphere $r = 1$, as simply a subspace of the space of global differential one-forms on the line bundle whose section sheaf is $\mathcal{O}(-1)$, and it is those which are invariant under the covering map $\mathcal{O}(-1) \to \mathcal{O}(-2)$ and restrict to zero as one-forms on the zero section.

This latter condition can also be removed since every one form on $\mathcal{O}(-1)$ which is global restricts to zero on the zero section $\mathbb{P}^1$.

And so we can embed the Shchroedinger solutions for the case $k = 1$ of one electron, restricted to $r = 1$, as the space of global one-forms on the surface $\mathcal{O}(-1)$ which are invariant under the cyclic Galois action of order two.

Here is a very easy interpretation.

The space of schroedinger solutions for 1 electron, without 'spin' is just like a subring of $C[x, y, z, r]/(x^2 + y^2 + z^2 - r^2)$.

It is exactly a subring, if you remove the exponential factors from the radial functions and pass to associated graded object. And, what subring? The whole ring.

If you set $r = 1$ you meaningfully then have the coordinate ring of the real unit sphere.

Now, resolving the ordinary double point gives a different thing, which we know well. One 'coordinate chart' of the resolution has coordinates

$$(r, \frac{x}{r}, \frac{y}{r}, \frac{z}{r})$$

These are just the the radius and the direction cosines of the angles!

The defining equation is now

$$r^2 = r^2((\frac{x}{r})^2 + (\frac{y}{r})^2 + (\frac{z}{r})^2)$$

and obviously this is just saying that when r is nonzero, the direction cosines are constrained to describe a point on the unit sphere.

But when r is zero, they are unconstrained; and this corresponds to the fact that the total transform of the singular point meets our coordinate chart at a union of two irreducible components, an affine three space when r=0, and an acutal sphere of radius r at each value of r which is not zero, if we are over the reals.

It is the sphere of angles for each possible radius, and a three space of unconstrained angles. when the radius is zero.

Now, this seems to be a whole description of everything one can see.

But, what implicitly Weyl does with this whole picture, of the three space of unconstrained angles when $r = 0$, and the disjoint union of concentric spheres for all nonzero values of r, is, to *delete* this.

The complement, in the resolution, of all this familiar stuff, is the divisor defined by $r = 0$.

It *seemed* like we already saw both what happens when $r = 0$ and when r is not zero. But that was talking about whether r is zero or not zero on a scale of magnitudes related to the magnitudes of angles.

We were up in a resolution of the ordinary double point, and never considered yet letting r be zero actually.

Anyway, if we set $r = 0$ viewing r as a function on the original variety, we get the whole exceptional divisor, a ruled surface, and also the proper transform of the variety $x^2+y^2+z^2 = 0$, and these intersect along the exceptional divisor of the resolution of the singular point, that exceptional divisor is the Severi- Brauer variety.

The union of the two is also easy to visualize, it is contained in the line bundle of type $(-1,-1)$ on the ruled surface, and it comprises the zero section together with the restriction of the line bundle itself to the diagonal Riemann sphere. Recall too that the ruled surface is not naturally isomorphic to a cartesian product of two Riemann spheres, but the diagonal Riemann sphere occurs naturally.

If we complexify just the proper transform, what we see is a copy of $\mathcal{O}(-1)$, the total space.

One way to visualize the resolution of the ordinary double point then, is to think of the coordinate chart of the resolution which we described as the complexification of ordinary three-space defined by an analytic radius and three direction cosines.

Then, to make this relatively compact as a complex manifold over the ordinary double point, it is necessary to add a boundary divisor. This divisor could perhaps not be considered to be a divisor 'at infinity' as one sometimes calls it, but an infinitesimally small divisor. It has two irreducible components, and the one which seems detectable by observing frequencies of an atom is the one which is a copy of the total space of the line bundle $\mathcal{O}(-1)$ over the Riemann sphere, and particularly the global holomorphic differential one forms on that complex surface.

That is, if you set all the radial functions to 0 in the Schroedinger equation 'with spin,' what you are seeing, as far as the representation theory can detect, is the global one forms on $\mathcal{O}(-1)$, and there is an action of $SU_2 \times SU_2$ on this space of global one forms, and all the character theory and representation theory supports that the diagonal SU_2 is geometrically meaningful.

That diagonal SU_2 is the one where the action on one forms on the complex surface (real four-manifold) $\mathcal{O}(-1)$ is taken to be the functorial one.

Note that in string theory, sometimes in order to include manifolds of higher dimension, there are questions asked about what very tiny sizes might be unobservable. Here, though, quite literally, there are things occurring of size zero. The notion that everything in existence should have a 'size' according to a Euclidean measure is one which seems to have been correctly disregarded in renormalization theory, and earlier in complex geometry, in theories of residues, in which integer orders of vanishing and integer dimensions both occur.

When people use polar coordinates in two dimensions, it already happens that the new coordinate system is already a resolution of singularities.

In three dimensions, using the square root of r as if it were analytic amounts to choosing to work on a coordinate system which has a singular point. To work analytically one might choose to resolve the singular point in the natural way, as one can when there is a minimal resolution of singularities. One finds after blowing up that the variety where the radius is zero has a four sheeted universal branched cover corresponding to the fact that the variety defined by the equation that the radius is zero, but the coordinates are not simultaneously zero, has a universal etale cover of degree four.

Once one has blown up a point to create a Riemann sphere of angles, it then may be needed to use conormal principal parts in order not to lose differential information. All of these are things which one might do in setting up coordinates, and doing things this way can, as we saw, create a smooth family of configuration spaces, parametrized by the radial coordinate, but now lying on a line which extends in both the positive and negative direction, and such that wave forms which correspond to ground state of an atoms of atomic number k correspond to particular fiberwise differential k forms.

With respect to the natural Lie algebra action and automorphism group action of the Riemann sphere, the decomosition of the space for each k matches the character formulas which were written down earlier, and here one has an explicit basis, and explicitly describes the space of k forms which has that particular character.

In order for things to be consistent with a Hamiltonian formulation, in the case of a single electron, one would need to consider not just closed one forms, but rather, to consider sections of the pullback to the tangent bundle of the configuration space of the sheaf of all such one-forms.

I mentioned that we can consider the k forms we have written down as non fiberwise $k+1$ forms, essentially by appending dr to the ones we have written. If we do that, then all are closed as $f_{k,n,l}dr$ being a one form in one variable is the differential of an appropriate indefinite integral.

If we want the Hamiltonian formulation to apply, one issue is generalizing the Hamiltonian notion to work for forms which are of higher degree than just one-forms. A second issue is that one had needed, in the case of one-forms, to be sure that one considers not just pullbacks of closed forms, but rather linear combinations of such pullbacks with coefficients which were functions on the tangent bundle of the configuration space.

The choice of a smooth trivialization of the normal bundle of the complexification of $\widetilde{V}$ may not have been necessary. It might make sense to consider, instead of a family of vector spaces, the variety $\widetilde{Q}$ itself, or a vector bundle over that.

The fact that the coefficient functions of our forms are constant in the vector space direction means that the differential forms would extend to a compactification.

Schroedinger's choice of solutions

In the next section we'll talk about the general theory of residues, and this will explain some of the foregoing. Let's interpose here a comment about Schroedinger's explanation of the Hydrogen spectrum. Recall that the action of the Laplacian on functions $f(r)s$ for s homogeneous harmonic of degree l in x, y, z agrees with $(\frac{d}{dr})^2 + \frac{2+2l}{r}(\frac{d}{dr})$, and what we called the 'Schroedinger solutions,' eigenfunctions for $\alpha + \beta/r$ were particular functions f which took the form of polynomials times exponential integrating factors.

If we write $f(r) = a_0 + a_1 r + a_2 r^2 ...$ it is easy to see just by considering the radius of convergence that for any choice of α, β whatsoever once a_0, a_1 are chosen there is a unique choice of $a_2, a_3, ...$ which describes an entire analytic function $f(r)$ so that $\Delta(f(r)s) = (\alpha + \beta/r)f(r)s$.

The necessity of the relation $\alpha = \frac{\beta^2}{4n^2}$ which was needed so that the polynomial factor of f exists and does not have terms of negative degree, is not required for an entire analytic solutions; it is rather an artefact of our insistence of being able to factorize f as a product of a polynomial times an exponential integrating factor, so that the real values of f would tend to zero at infinity (so the L^2 norm can be finite, for example).

Without a physical reason such as this why such a factorization is preferred in nature, then the relation involving reciprocal squares would not actually be a consequence of Schroedinger's equation, and in any case the Schroedinger equation would only explain the occurrence of differences of reciprocal squares in the Hydrogen spectrum in conjunction with an appeal to something such as an L^2 structure.

These condsiderations may relate to why it had been possible, elsewhere in this document, for us to find an ab initio statistical method of altering the effect of the the perturbation coefficient for electrostatic repulsion in its effect on all but the sums of reciprocal squares. The direct application of the perturbation method incorrectly decreased the effect of the sums of reciprocal squares; and a linear combination of the two effects which minimizes second differences when all else is kept constant agrees with what is found by experiment. But one should ask why it should. One should seek the reason that the two effects are not independent, but are statistically connected in that way in nature.

Residues

The fact that the global one-forms on $\mathcal{O}(-1)$ come from pulling back principal parts of $\mathcal{O}(1)$ on the Riemann sphere means that the principal parts exact sequence for $\mathcal{O}_{\mathbb{P}^1}(1)$

$$0 \to \mathcal{O}(-1) \to \mathcal{O} \oplus \mathcal{O} \to \mathcal{O}(1) \to 0.$$

has a meaning. The middle term can be interpreted as the abstract coherent sheaf restriction to the zero section of the sheaf of one-forms, on the line bundle whose section sheaf is $\mathcal{O}(-1)$, which restrict to zero as local *one-forms* on $\mathbb{P}^1$.

The concept of residues amounts to understanding a comment in Reid's 'young person's guide to canonical singularities,' about the way that there is more than one way pull back a sheaf. The map of pulling back global sections of the locally free sheaf Ω of one forms on the line bundle to one-forms on the zero section $\mathbb{P}^1$ is the zero map, just because there are no nonzero global one forms on the zero section; but when consider instead the locally free subsheaf $\Omega(log\, \mathbb{P}^1)(-\mathbb{P}^1) \subset \Omega$ it is helpful now to analyze the process of pulling back as one-forms in two steps. We may first pull back the sheaf itself to obtain a locally free sheaf on $\mathbb{P}^1$. If i is the inclusion of the zero section $\mathbb{P}^1$ then we obtain $i^*\Omega(log\ \mathbb{P}^1)(-\mathbb{P}^1)$ which is exactly $\mathcal{P}(\mathcal{O}(1)) \cong \mathcal{O} \oplus \mathcal{O}$.

And the restriction map is exactly the map to $\mathcal{O}(1)$ shown above. We can consider $\mathcal{O}(1)$ to contain $\mathcal{O}$ as a subsheaf, but not naturally; to consider it that way requires choosing a global section of $\mathcal{O}(1)$. But if we were to make such an identification, it would seem perhaps paradoxical that the restriction of a subsheaf of one-forms results in a larger sheaf of restricted one-forms. The paradox would be a result of confusion about functoriality. The restriction is functorial and the passage to a subsheaf is functorial, but as we pass to smaller locally free subhseaves of Ω, their restrictions as locally free sheaves, while increasingly positive, are not naturally nested in the positive direction.

If we twist the sequence here by an integer – it will be best in context to use an even number $2l$ for l an arbitrary natural number – then our exact sequence $0 \to \mathcal{O}(2l-1) \to \mathcal{O}(2l) \oplus \mathcal{O}(2l) \to \mathcal{O}(2l+1) \to 0$ induces a filtration of the global sections of $\mathcal{O}(2l) \oplus \mathcal{O}(2l)$ into two parts. This corresponds to the surjection of $S^{2l}(V) \otimes V \to S^{2l+1}(V)$ and its kernel, with V a two-dimensional abstract vector space, and note that the associated graded space describes exactly the same decomposition which in characters is described by the Clebsch-Gordan formula.

Thus, one reason the calculations above seemed to have matched the periodic table to some extent, and spectra, might be because these things could be detected by a residue calculation.

The canonical divisor and the j quantum number.

The exact sequence above, and its positive twists, give a geometric representation explanation of the same Clebsch-Gordan rule which said for characters upon setting $S = L = J$ in the character $e_1(S)e_{2l}(L)$ to get

$$e_1(J)e_{2l}(J) = e_{2l-1}(J) + e_{2l+1}(J).$$

The left side of that rule is the character of the global sections of the middle term of the exact sequence

$$0 \to \mathcal{O}(2l-1) \to \mathcal{O}(2l) \oplus \mathcal{O}(2l) \to \mathcal{O}(2l+1) \to 0.$$

and the two terms on the right side are the characters of the leftmost and rightmost terms, all for the action of SU_2 by line bundle isomorphisms.

The direct sum of the twisted sheaves of the middle term comprise the pushforwards to the exceptional $\mathbb{P}^1$ of

$$\Omega_{\widetilde{V}}(log\ \mathbb{P}^1)(-\mathbb{P}^1).$$

That is, of the one-forms on $\widetilde{V}$ which restrict as one-forms to zero on the zero section $\mathbb{P}^1$.

That direct sum is the middle term of what would result if we twisted this exact sequence by $-\mathbb{P}^1$ and in fact this sequence twisted by $-\mathbb{P}^1$ and pushed down to $\mathbb{P}^1$ is exactly the same as the direct sum of all the sequences we've just described.

$$0 \to \Lambda^2\Omega_{\tilde{V}}(log\ \mathbb{P}^1) \to \Lambda^1\Omega_{\tilde{V}}(log\ \mathbb{P}^1) \to \mathcal{O}_{\mathbb{P}^1} \to 0.$$

Note that the difference between the quantum numbers $(l+1/2)-(l-1/2)$ which are usually associated to the two terms of the filtration can be understood naturally as exactly half the degree of the canonical divisor.

All of this occurs after we've restricted forms on $\tilde{Q}$ to $\tilde{V}$. Forms on $\tilde{Q}$ which are zero as forms on the exceptional $\mathbb{P}^1 \times \mathbb{P}^1$ can be interpreted as forms on $\mathbb{C}^3$. Starting from a volume form $w(x,y,z)dxdydz$ we might apply the adjoint $d*$ of the deRham operator to obtain $\frac{\partial w}{\partial x}dydz - \frac{\partial w}{\partial y}dxdz + \frac{\partial w}{\partial z}dxdy$. The Euler contraction along the radial vector field then restricts to a one-form on our subvariety defined by $x^2+y^2+z^2=0$. This restricted one form has components in the various global sections spaces we've just considered.

The issue is that the differential of our two-form on $\tilde{V}$ is the Laplacian of w times the volume form $dxdydz$. If w is homogeneous of degree l and we write it as $w(x, y, z) = r^l w(\frac{x}{r}, \frac{y}{r}, \frac{z}{r})$ then the action of the Laplacian on the product has as eigenfunctions the sum of the eigenfunctions of its action on the factors. The action on r^l is by $\frac{l(l+1)}{r^2}$ and our correction to the equation to cause the fine structure in the spectrum, which we have only ever so far carried after restricting, was to replace the eigenfunction for the action on the radial component to $\frac{(l+1/2)(l+3/2)}{r^2}$ on the image term in the exact sequence, and to $\frac{(l-1/2)(l+1/2)}{r^2}$ on the kernel term.

Note that this is different than saying “Fermions are anticommutative,” and I’d like to comment on that too.

When one looks at something like the Riemann spere, if one fixes any point, then the complement of that point has a natural structure of affine space, with the automorphisms of the Riemann sphere inducing the affine group. This includes addition and multiplication, or, what we consider to be addition and multiplication. But a person choosing a different point would find a very different notion of addition or multiplication.

The notion that wave functions of Fermions ‘are’ anticommutative seems to presume that instead of us all living in some geometry, or something we might think of as a geometry, or a topological space, or another mathematical object like that, we are living inside an algebra, with a deified calculus of addition and multiplication somehow.

The reason this is at least for me hard to visualize is that things like algebra were introduced as operations, not as ‘things.’ There is no reason not to think that we live in a universe comprised of inherent ‘operations’ like addition and multiplication.

But, the place these operations arose in quantum theory was something nicer, it had to do with only recognizing that certain things, the way we defined them, necessarily are indistinguishable. The notion that there is an operation, and it just happens to be noncommutative, is hard to understand as an observation, and easier to understand as a postulate only.

The purpose of this section is to bring a closer convergence between the global analysis of harmonic functions by Legendre using real analysis versus the local analysis of the azimuthal parts using complex representation theory by Weyl.

We will see that the concept of the canonical divisor of an ordinary double point singularity enters the picture, and is related to the classical notion of a dyadic ‘angular momentum operator.’

The goal is a single equation generalizing the combination of the Schroedinger equation with the extra term that is supposed to explain spin-momentum coupling into a single local equation with a sensible global generalization.

I have already mentioned that the approach requires a slight change to the 'spin-momentum' term, and the conceptual setting requires also a different constant coefficient also. The first has the effect of shifting the spectrum in the coarse structure an amount commensurable with the fine structure, and could be neither supported nor contradicted by any existing experiments that I know of, and the second in a few examples does seem supported by experimental evidence.

Let's again review with the construction of homogeneous harmonic polynomials by Legendre. There one admits the relation in three space with coordinates x, y, z and a radial coordinate r that $r^2 = x^2 + y^2 + z^2$, but one considers the operator $\frac{\partial}{\partial z}$ which does not preserve that relation. For a number l, beginning with the function

$$(z^2 - r^2)^l$$

one chooses a number $a = 0, 1, 2, ..., l$ and constructs a basis of the homogenous harmonic polynomials in x, y, z consisting of the real and imaginary parts of

$$(x + iy)^a \, \frac{\partial}{\partial z}^{l+a} \, (z^2 - r^2)^l.$$

If we complexify, thinking of x, y, z, r as complex variables, then we may write

$$z^2 - r^2 = x^2 + y^2 = (x - iy)(x + iy)$$

and the expression above is

$$(x + iy)^a \frac{\partial}{\partial z}^{l+a} ((x + iy)^l (x - iy)^l).$$

Since $\frac{\partial}{\partial z}$ commutes with multiplication by $x + iy$ this is just

$$\begin{aligned} &((x + iy)\frac{\partial}{\partial z})^{l+a})(x - iy)^l \\ &= \delta^{l+a}(x - iy)^l \end{aligned}$$

where

$$\delta = (x + iy)\frac{\partial}{\partial z}.$$

It follows that we can combine l and a into a single value m, that is, for any numbers m and l whatsoever we have

$$\delta^m (x - iy)^l$$

has harmonic real and imaginary parts. This is true because the real and imaginary parts of the anti-holomorphic function $(x - iy)^l$ are harmonic, and δ commutes with the Laplacian (its real and imaginary parts are in the rotation Lie algebra as we'll see in a few lines).

As we mentioned earlier, derivation δ satisfies

$$(x+iy)(x-iy) = r^2 - z^2 \mapsto -2(x+iy)z$$

and so

$\delta(x-iy) = -2z.$
$\delta(x+iy) = 0$
$\delta(z) = (x+iy),$
giving

$\delta(x) = -z$
$\delta(y) = -iz$
$\delta(z) = (x+iy).$

This calculates δ then

$$\delta = (x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x}) + i(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}).$$

The real and imaginary parts happen to belong to the Lie algebra of rotations of Euclidean (x, y, z)-space.

Let's factorize this operator into three parts, in order to clarify the relation between the canonical reflexive sheaf of a singular point and the classical dyadic angular momentum operator.

We saw already that if we use the finite map given by

$$u^2 = x + iy,\ uv = iz,\ v^2 = x - iy$$

then the purely imaginary operator $-i\delta$ agrees with the lowering operator $u\partial/\partial v$ in its action on on homogeneous complex polynomials of even degree in (u, v)

$$v^2 \mapsto 2uv \mapsto 2u^2 \mapsto 0.$$

The polynomials of even degree in u, v can be considered the affine coordinate algebra of an ordinary double point singularity, and this is the subvariety of the complexification of the affine quadric defined by the equation $x^2 + y^2 + z^2 = r^2$ defined by the equation $r = 0$.

The operator δ preserves the whole affine quadric; it is a lifting of the Legendre operator $(x+iy)\frac{\partial}{\partial z}$ to the quadric.

We can verify that it acts by zero on r because of how it was constructed, or directly, as

$$\begin{aligned} 2r\delta(r)\delta(r^2) &= \delta(x^2 + y^2 + z^2) \\ &= 2x\delta(x) + 2y\delta(y) + 2z\delta(z) \\ &= 2x(-z) + 2y(-iz) + 2z(x + iy) = 0. \end{aligned}$$

and r is a non-zero-divisor in the coordinate ring.

We can relate δ both with the so-called ‘dyadic’ angular momentum operator of earlier quantum physics, and with the euler derivation in (x, y, z) space, and also with the canonical sheaf of the Severi-Brauer variety defined by $x^2 + y^2 + z^2 = 0$.

Denote by ϵ the Euler derivation

$$\epsilon = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z}.$$

The contracting operator i_ϵ gives an exact sequence

$$0 \to \Lambda^3\Omega_{\mathbb{R}^3} \to \Lambda^2\Omega_{\mathbb{R}^3} \to \Omega_{\mathbb{R}^3} \to \mathcal{O}_{\mathbb{R}^3} \to 0.$$

The map from two-forms to one-forms acting on the general two-form $fdydz - gdxdz + hdxdy$ gives

$$\begin{aligned} i_\epsilon(fdydz - gdxdz + hdxdy) &= f(ydz - zdy) - g(xdz - zdx) + h(xdy - ydx) \\ &= (zg - yh)dx + (xh - zf)dy + (yf - xg)dz. \end{aligned}$$

In the special case when there is one function u with

$$f = \frac{\partial}{\partial x}u$$

$$g = \frac{\partial}{\partial y}u$$

$$h = \frac{\partial}{\partial z}u$$

we have

$$i_\epsilon(fdydz - gdxdz + hdxdy) =$$

$$(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z})(u)dx - (z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z})(u)dy + (y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y})(u)dz$$

The coefficients of dx, dy, dz are exactly the three components of the so-called 'dyadic' angular momentum operator applied to u, and so we see that contracting the two-form dual to a vector field along the Euler derivation corresponds to applying the older angular momentum operator to a function whose gradient is that vector field, if there is such a function. In that sense, contracting along the Euler derivation is a generalization of the older 'dyadic' operator.

The differential one-form shown above is a pullback from a one-form on a two sphere of any desired radius, along the projection of three space with the origin deleted to a sphere.

If we let $\tau = \partial/\partial y - i\partial/\partial x$ then it follows that

$$\begin{aligned}\delta(u) &= i_\epsilon\ i_\tau(fdydz - gdxdz + hdxdy)\\ &= i_\delta\ i_\tau\ \nabla(u)\end{aligned},$$

that is, the operator δ which restricts to the Weyl operator is the composite of three parts: the gradient operator ∇ sending u to a two-form, then contracting along τ and finally contracting along the generalized angular momentum operator ϵ.

The Weyl lowering operator, as I've mentioned too many times, is the restriction of $-i\delta$ in its action on the complixivication to the level $r = 0$. That is, it is the action of δ on the Severei-Brauer variety defined by the equation $x^2 + y^2 + z^2 = 0$.

Varying r from the level $r = 1$ to the level $r = 0$ we could find a deformation between the unit sphere and the Severi-Brauer variety, but it is not this deformation which will relate the Legendre operator and the Weyl operator conceptually, as there is no special significance which we can give to the radial value of 1.

While most of this analysis makes sense if we use only real numbers, the Severi-Brauer variety although it has no real rational points, it occurs within the exceptional divisor of the minimal resolution of the afffine quadric threefold hypersurface defined by $x^2+y^2+z^2 = r^2$, where the whole exceptional divisor is the projective variety defined by the same equation. The inverse image of the affine threefold in the transform of (x, y, z, r) space has one affine open set with coordinates $(r, x/r, y/r, z/r)$ and defining equation

$$r^2 = r^2(\frac{x}{r}^2 + \frac{y}{r}^2 + \frac{z}{r}^2)$$

and so is a union of two irreducible parts, defined in these coordinates by the equations

$$r^2 = 0$$

$$1 = \frac{x}{r}^2 + \frac{y}{r}^2 + \frac{z}{r}^2 .$$

The first equation defines a linear space of dimension three, where we consider that the ratios $\frac{x}{r}, \frac{y}{r}, \frac{z}{r}$ are unconstrained when $r = 0$, and the second defines what is in the real points a cartesian product of a two dimensional sphere with a line of unconstrained values of r. This cartesian factor of the unit sphere does not depend on choosing a finite radius of 1 in the Euclidean space, it is a very nice occurrence of a sphere of angles in the exceptional divisor. The two affine varieties intersect at a copy of the unit sphere.

This unit sphere is the intersection of the exceptional divisor in the four dimensional transform of real (r, x, y, z) space with an open affine subset of the proper transform of the threefold quadric. That is, the copy of the unit sphere the exceptional part of an open affine subset of the minimal resolution of the threefold quadric. And this open affine subset has as its real points the cartesian product of a two dimensional sphere with a line.

Note that the complexification of this unit two-sphere is a copy of $\mathbb{P}^2 \times \mathbb{P}^2$ with the diagonal subvariety deleted.

The whole of the minimal resolution of the affine quadric three-fold is compact, and it results by adjoining at the boundary of the affine open subset we are looking at a copy of the Severi-Brauer variety described as a projective variety by the equation $x^2 + y^2 + z^2 = 0$ or equivalently if we want to use coordinates $(x/r, y/r, z/r)$ projectively, we could write it $(x/r)^2 + (y/r)^2 + (z/r)^2 = 0$.

One sometimes visualizes a boundary in a compactification as being ‘at infinity,’ but it makes more sense intuitively to think of this Severi-Brauer subvariety of the minimal resolution as occurring ‘at zero,’ because it is the intersection of the exceptional divisor in the minimal resolution of the affine threefold quadric with the proper transform proper transform of the subvariety defined algebraically by the equation $r = 0$ in the unresolved threefold quadric. That is, it is the exceptional divisor in the minimal resolution of a twofold quadric.

Then, rather than comparing the restriction of $i\delta$ to the subvarieties of the affine quadric defined by the equations $r = 1$ and $r = 0$, we should consider instead lifting $i\delta$ to the minimal resolution. This preserves the exceptional divisor by naturality, and it must preserve the proper transform of the variety defined by $r = 0$, and so it must act on the Riemann sphere which is the complexification of the Severi-Brauer variety.

In coordinates $\frac{x}{r}, \frac{y}{r}, \frac{z}{r}$ we have the action on the unprojectivized vector space

$$\delta(\frac{x}{r}) = -\frac{z}{r}$$

$$\delta(\frac{y}{r}) = -i\frac{z}{r}$$

$$\delta(\frac{z}{r}) = \frac{x}{r} + i\frac{y}{r}.$$

Or, switching coordinates, and taking account of the relation $x^2+y^2+z^2=0$, we can say that $u\frac{\partial}{\partial v}$ acts on $\mathbb{C}^2$ and the three-dimensional vector space of global vector fields on the Riemann sphere is spanned by $u\frac{\partial}{\partial u}, u\frac{\partial}{\partial v}, v\frac{\partial}{\partial u}, v\frac{\partial}{\partial v}$ with the relattion that $0 = u\partial/\partial u + v\partial/\partial v$.

Thus δ induces a 'parabolic flow' fixing one point of the Riemann sphere; and if we think of this as a point at infinity, we can identify $i\delta$ with a translation of the Euclidean plane.

The variety defined by the equation $x^2+y^2+z^2=r^2$ is a branched double cover of three-space (obtained by adjoining a square root of $x^2+y^2+z^2$) and when we are away from the region where $r=0$ we can work instead on ordinary three-space.

Then a smooth function u is harmonic if and only if the corresponding two-form form τ is closed, and in this way we see that the smooth harmonic (=exact and co-exact) two-forms on $\mathbb{R}^3$ are bijective with the smooth harmonic functions.

This is true locally, and therefore remains true, away from the locus where $r=0$, on the two-sheeted branched cover (which is an ordinary two sheeted cover away from $r=0$), in the sense that the sheaf of co-exact smooth two-forms is isomorphic to the sheaf of smooth functions, and the sheaf of harmonic two-forms corresponds to the sheaf of harmonic functions.

The one-forms dx, dy, dz restrict not to one-forms on the Rieman sphere which is the projective variety defined by the equation $\frac{x}{r}^2+\frac{y}{r}^2+\frac{z}{r}^2 = 0$. Rather they restrict to first principal parts of the conormal sheaf, so global sections of $\mathcal{P}(\mathcal{O}(2))$ on the Riemann sphere.

The whole proper transform of the variety defined by $r = 0$ is a copy of the cotangent bundle of the Riemann sphere, and the pullback of the first principal parts sheaf along the cotangent bundle projection is a subsheaf of the cotangent sheaf of that line bundle. (That is, a subsheaf of the cotangent sheaf of the cotangent bundle of the Riemann sphere). It is the sheaf of one-forms on the cotangent bundle which map to zero in the push forwards of the cotangent sheaf of the zero section.

Therefore it is simpler to think of dx, dy, dz as global one forms on the cotangent bundle of the Riemann sphere. The map which contracts the zero section of that cotangent bundle to one point is the map to the variety whose coordinate ring is the even total degree polynomials in $\mathbb{C}[u, v]$, and dx, dy, dz are pullbacks of one forms on affine space in coordinates u, v, we can find these one-forms by remembering the relation we wrote earlier expressing x, y, z in terms of u, v. This gives

Note though that the relation between the Legendre and Weyl operators cannot be considered to result from merely restricting the one-forms dx, dy, dz to the Riemann sphere, as, although that restriction is well-defined, it is zero.

Rather, the meaningul relation will require considering meromorphic forms with nontrivial poles, and it is a matter of comparing the action of the Legendre operator on forms with the Weyl operator on the residues of those forms.

Of the affine variety $x^2 + y^2 + z^2 = 0$, even if we do not pass to its minimal resolution, we may describe the 'canoncacal sheaf' or what is in this case the 'canonical module' to be the free module over the coordinate ring spanned by the element

$$\omega = \frac{1}{x}dydz = -\frac{1}{y}dxdz = \frac{1}{z}dxdy.$$

This is a basis element for the reflexivication of the module of two-forms, and an interesting property that this has is that if we restrict a co-exact two-form

$$\tau = adydz - bdxdz + cdxdy$$

on $\mathbb{R}^3$ to this subvariety, the co-exactness together with the formula for ω implies that the result is

$$2\epsilon(\psi)\omega$$

where ψ is the smooth function corresponding to τ, and ϵ is the Euler derivation $x\partial/\partial x + y\partial/\partial y + z\partial/\partial z$.

Intuitive description of polarization

If you think about defining ocean waves by differential equations, you can say perhaps there is *some* solution and just keep in mind the equation itself, which has all this symmetry.

Or you can say, I want to see what the actual waves look like *now*

Now, an obvious group theory lemma is this: if you define a 'polarization' to be a choice of a maximal torus and a fundamental system of positive roots, then this can actually corresponds to something physical in the Schroedinger equation solution space.

Recall that there actually is a finite-dimensional vector space of solutions associated to what is labelled an 'electron configuration,' and these are actually full solutions of the correct Schroedinger equation – there is not technology in PDE's or numerical analysis to write these down, but they are there.

These are alternating forms, and up to isomorphism as a vector space it is just, if the 'electron configuration' is a configuration of k electrons, it is as a vector space the k'th exterior power of the space of solutions for a single electron

Such a thing actually corresponds to a solution space of the Schroedinger equation, and this remains true regardless of whether we include electron-to-electron repulsion, or whether we include the little operators near the identity as coefficients of the potential terms $k_p e^2/r_i$. Because there is the perturbation which we can apply to move this solution uniquely into place, and we can even know its first derivative, so we know *which* schroedinger equation it is a solution to, in the sense that the constant term E of the eigenvalue, we know the constant and linear terms of it in terms of a perturbation or deformation parameter.

Although there is not one wavefunction for each polarization, once you index things by 'electron configurations,' and choose an electron configuration (also in the rare cases when one term symbol can occur with multiplicities, choose just one term symbol) then up to amguities only of a complex phase and magnitude, there is exactly one wave function that 'has' each polarization.

For these wave functions there is a possibility to have one's cake and eat it too. To have a fixed image of a standing wave, which has a variable complex coefficient. And choosing that coefficient really does describe what the field is 'now' at each point of space. That is, it determines a particular complex alternating form, up to an undefined coefficient.

Among general wave functions, they are just a special type, and while they cannot represent every energy level that can occur, and we might think of them as analagous to when planets go in planar orbits separately.

A polarization can be interpreted in a very easy way. For instance if one thinks of one atom as being just a set of electrons, and includes both ordinary and infinitesimal components of wave functions. For an atom with,say, three electrons, one can visualize three ordinary spheres, like three globes, and each having a very tiny sphere inside it.

Then a polarization just means marking each large sphere by one point, and marking each small sphere by one point. One can do this by placing a large 'vector' and a small 'vector' whose tail is at each electron, not caring exactly how large or small they are.

Then the space of wave functions does decompose into Fourier components, for the action of the subgroup which has a copy of $SO_3 \times SU_2$ for each orbital. The components are indexed by a choice a sequence assigning one term symbol for each orbital – these are the same term symbols one would assign to the ground state of an atom itself if it had only that orbital as its last unfilled orbital – and each irreducible component so indexed has a wave function that 'has' that polarization, unique up to a choice of complex phase (including magnitude and angle). But these components are large-dimensional components are not related to energy levels.

If one begins to think the electrons are more coalesced together, then one uses this smaller symmetry group. When they are all considered coalesced, now it is just a single large sphere and a single small sphere. Or, choosing just one large vector and one small vector. The space of polarizations is now a cartesian product of two spheres. And again there is a unique wave function, up to complex phase and magnitude, which 'has' each polarization, within each Fourier component. And now, what was not true before is true, at least coarsely. All the wave functions in each Fourier component have the same, what is known as, coarse, energy level, and this means that for a polarization in this sense, there really is a wave function that 'has' the chosen polarization and, at least coarsely, represents each energy level.

Up until cases like an excited configuration of Nitrogen or Fluorine the coarse energy level determines the Fourier component, but this is not true generally, each Fourier component is allowed to occur more than once, with more than one coarse energy level, but usually it only occurs once.

An issue about 'spin' is that the symmetry group that is relevant for the small sphere is not just rotations of space, but this is because there is no reason for it to be that, it is symmetries of the residue of the wave function which is not a wave function in space. But it does not affect what one means by a polarization, and this detail can be ignored.

Now, if we are *even more* accurate, we realize that the two spheres, the large sphere and the small sphere, are actually not different after all. But, the symmetry group is not just the spatial symmetry group, if you care about what you mean by a wave function, including the infinitesimal part. It is a symmetry group of a bundle of lines, and there are two symmetries that correspond to each one rotation of ordinary space. But it is a double cover of the ordinary rotation group.

When one realizes that the two spheres are not different after all, then all a polarization means is a point of a sphere, or an actual direction in space, as if you are looking at the atom itself, and the vision determines one direction into it.

And each Fourier component that corresponded to one coarse energy level (though more than one coarse energy level could correspond to a Fourier component) now splits into parts in a way that is easily understood in terms of Clebsch Gordan theory.

Again, there is a unique wave function in each of these smaller Fourier components which 'has' each polarization. And now, because the rotation group (or more correctly its double cover) really is the actual symmetry group of the atom, it really is true that there is a polarized wave function representing every possible energy level.

The reason these are useful is that if one wanted to find all the energy levels, and did not care about anything else, at any point of this analysis one can ignore all but the special wave functions that 'have' one chosen polarization.

And then, thinking of distinct Fourier component subspaces as being different, there is a bijection between the fine energy levels and the special wave functions, defined up to complex phase and magnitude, which 'have' any one fixed polarization.

So that once a polarization (single point or point of view) is fixed, each fine energy level really does determine exactly one wave function (up to phase and magnitude) and vice-versa.

Now, it is *not* true that every wave function 'has' a polarization. That would be like saying every solution of the n body problem consists of planets in separate planes.

But it is true, once we are down to the smallest relevant symmetry group, that in the multiplicity free case a polarization and energy level determine a unique wave function up to a coefficient determining a complex phase and agnitude.

I think that Feynman was wrong to think that such coefficients are just intrinsically undefined, but it has to do with making a choice about what you want to see.

Now, For a general type of wave function, even if it is isotypical in the multiplicity free case, it is not true that it admits any polarization.

And this is just the assertion that Dirac was tranfixed by, when he would talk about how operators are generalizations of numbers.

That is, we can visualize it representation-theoretically, and we can say there simply isn't one element or line that has been specified. That was perhaps a mysterious phenomenon in Dirac's day, but the notion of 'operator' has been replaced by the notion of the rational representation theory of Lie groups.

To reiterate, I am not asserting that an electron actually *has* such a polarization as this, defined by choosing a maximal torus and a system of positive weights, or even that one electron is separate from others in an atom.

Rather, what people say seems to happen is that the electron seems to actually orbit the nucleus just as the earth orbits the sun.

Then there might be an argument for adopting as an analogy, what happens in the n body problem, in the case of a solar system like the one we happen to live in, where each planet has an elliptical orbit, and the orbits are actually in planes, and tilted at various angles.

The sense in which it is an analogy is one which is a bit subtle perhaps, it is that we have insisted on global analytic solutions, but these were analytic on a resolution of singularities only.

About why a polarization in the sense of choosing a long and short arrow for each electron does not correspond to 'energy levels,' this too is sort of obvious. The attempt to make a mixture of frequencies to describe an atom is just an analogy to trying to look at something to see what it is, the eye only perceives frequencies (not differences of light polarization etc etc), and so one is trying to take a three dimensional phenomenon and convert it into a two dimensional phenomenon (or one dimensional depending on how one thinks of ordinary Fourier series). The eye (vision) loses a lot of information if one is able to think of waves more generally, and so, oddly, the wish to find what energy levels are there is just a wish to filter out the same information that gets filtered out if you look at anything else, and only see colors, not anything more interesting, unless you are looking say on a hot day and seeing mirages and things.

Relation between the smooth and holomorphic Laplacian operators

Let's start with one simple observation about the surface $\mathcal{O}_{\mathbb{P}^1}(-1)$ which is the disjoint union of the lines in the plane, over the complex numbers.

That if you have a flow on that surface, a holomorphic flow, or better, if you look at the sheaf of holomorphic flows, which are allowed a pole on the exceptional $\mathbb{P}^1$, then you find that the sheaf generated by global sections is smaller, and only consists of flows which are holomorphic on the exceptional $\mathbb{P}^1$.

This is obvious because you can think of the complement of $\mathbb{P}^1$ as the complement of the origin in a 2 dimensional vector space, and there is no such thing as a flow on a smooth surface which has a pole at one point.

But there is a second way of seeing the same thing, using Cramer's rule.

For smooth manifolds, one way of using Cramer's rule is this.

That a flow gives an action by Lie derivatives, acting on differential forms of every degree, and preserving that degree.

But if you represent it by linear maps, then the linear map of coherent sheaves which represents a flow is one which decreases degree by one. And it sends the natural canonical sheaf into the $n-1$ forms, hence giving a section of $n-1$ forms twisted by the anticanonical divisor. Thus, on any complex surface, whether compact or not, the one-forms can be naturally identified with flows tensored with the anticanonical sheaf.

For (compact) projective varieties, with each choice of canonical divisor these are in turn naturally identified up to a scalar multiple with the sheaf of flows which have a simple pole on the canonical divisor. When there is a natural choice of a canonical divisor, then there is a natural identification. The question whether there is a natural canonical divisor is one of the types of things that eventually gets analyzed in minimal model theory.

The canonical divisor of $\mathcal{O}(-1)$ is the exceptional $\mathbb{P}^1$, counted with the ordinary multiplicity $+1$. Because the quasiprojective variety $\mathcal{O}(-1)$ is not compact, the divisor does not naturally determine the canonical sheaf; we could choose a volume form such as $du \wedge dv$ which has a simple zero on the exceptional $\mathbb{P}^1$ of course; then contraction against this two-form maps the sheaf of vector fields with a simple pole on $\mathbb{P}^1$ isomorphically to the sheaf of holomorphic 1 forms on the surface $\mathcal{O}(-1)$.

All the global one-forms restrict to zero on the exceptional $\mathbb{P}^1$ because $\mathbb{P}^1$ supports no global one-forms.

So the fact that no global vector fields on $\mathcal{O}(-1)$ have even a simple pole on the exceptional $\mathbb{P}^1$, is the same statement as that global one forms on $\mathcal{O}(-1)$ always restrict to zero on the exceptional $\mathbb{P}^1$.

This notion of vector fields allowed to become infinitely large on the exceptional $\mathbb{P}^1$, and this sheaf having no global sections when restricted to $\mathbb{P}^1$, is reminiscent of the difficulty about the two interpretations of raising and lowering operators.

Here, for a single electron, we know that the representation theoretic classification of spectral lines is very consistent with a notion that they do relate to one forms on the surface $\mathcal{O}(-1)$. We can think of these as being vector fields, flows, which are allowed a simple pole on the exceptional $\mathbb{P}^1$ if we like, and as far as global sections the allowed pole is inessential.

If one really wants to go all the way to a Hamiltonian interpretation, one is required at some time to think of flows on the tangent bundle; and if I am thinking of flows on the tangent bundle of the surface $\mathcal{O}(-1)$, these are sections of a four dimensional vector bundle on a four dimensional manifold, and suddenly we are in complex dimension 8, real dimension 16.

So let's not do that, at least not now, probably not ever, it might have been the wrong interpretation.

In the case of Helium for instance we have the four manifold which is $\mathcal{O}(-1,-1)$ on $\mathbb{P}^1 \times \mathbb{P}^1$, and if we think now of 2 dimensional flows, these correspond to maps from the canonical sheaf into 2 forms, or we could just then say that they are twisted 2 forms, and again the twisting is inessential, does not affect global forms.

If you look at what actually happens when you apply the Laplacian to real functions, you see that it does not behave well with respect to internal products, but it does with respect to external tensor products and exterior products.

That is, for functions $f(x, y, z)$ of the three real variables, if I have two such functions f, g, then

$$\Delta(fg) = f\Delta(g) + g\Delta(f) + 2\ grad(f) \cdot grad(g)$$

and this gradient dot product term depends on our metric, as does the definition of the Laplacian in the first place. But note that if I have functions of variables $(x_1, y_1, z_1, x_2, y_2, z_2)$ and if I have functions $f(x_1, y_1, z_1)$ and $g(x_2, y_2, g_2)$ then

$$\Delta(fg) = f\Delta(g) + g\Delta(f)$$

with no gradient dot product term (or, the gradients are perpendicular).

And if I want to restrict to the diagonal, taking $x_1 = x_2, y_2 = y_2, z_1 = z_2$, then what happens? Clearly the term $grad(f) \cdot grad(g)$ will not matter anyway if I use an antisymmetric product, and we knew anyway that the Laplacian will behave well with respect to exterior products since we already know that it can be interpreted as being the deRham differential.

Now we have to be a bit careful, as to interpret the Laplacian as the DeRham differential we need to be in a situation where we have, in the three dimensional ordinary interpretation, interpreted each function as representing its gradient flow, and even more than that, we need to think of this as being a codimension one differential form on three space. There is absolutely no difficulty doing this, representing a function f as meaning

$$\frac{\partial f}{\partial x}dydz - \frac{\partial f}{\partial y}dxdz + \frac{\partial f}{\partial z}dxdy$$

When we apply the deRham differential d to such a thing, we are applying the Laplacian to f, we get the Laplacian of f in the usual three dimensional sense, times the basis form $dxdydz$, which we just can interpret as a fixed trivialization of the canonical sheaf of ordinary three space.

Note that the two-forms of the type above are exactly the co-closed two-forms.

If we are a little more rigorous and say we are working on the variety defined by $x^2+y^2+z^2=r^2$ then this same expression represents a two form on that variety too, and also because we can pull back two forms, it represents a two form on the smooth variety which resolves that ordinary three fold double point.

If I talk about tensor or exterior alternating products, then there are k sets of variables (x_i, y_i, z_i) for $i=1,2,...,k$, and then there are codimension k forms on a smooth manifold, which could also be viewed as a resolution of singularities, now of a variety with more than isolated singularities.

This is a manifold of dimension $3k$.

When $k=1$, the manifold is the total space of the line bundle isomorphic to $\mathcal{O}(-1,-1)$ on the ruled surface $\mathbb{P}^1 \times \mathbb{P}^1$.

And so we have in that case we can interpret the classical Laplacian as the deRham differential on two forms of this smooth threefold.

It is very tempting to apply the Euler contraction and arrive at one forms on the ruled surface, but the issue is that the full automorphism group of $\mathbb{P}^1 \times \mathbb{P}^1$ would act and there is no evidence for this.

I am rather sure that the manifold we want to restrict to is really the restriction of the $\mathcal{O}(-1,-1)$ bundle to the diagonal $\mathbb{P}^1$ which is natural here, and the restriction becomes $\mathcal{O}(-2)$ and for some reason we then take the two sheeted branched cover.

The issue is that in order to restrict, we really need a transverse vector field.

So here is the real issue where the lowering and raising operators disconnect, between the Legendre and Weyl interpretations.

We have got global 2 forms on the total space of $\mathcal{O}(-1,-1)$ on $\mathbb{P}^1 \times \mathbb{P}^1$, and we want to restrict to global 1 forms on the diagonal $\mathcal{O}(-2)$ on $\mathbb{P}^1$, and, even better if possible to the double cover.

Now, the normal bundle of the zero section $\mathbb{P}^1$ in the zero section $\mathbb{P}^1 \times \mathbb{P}^1$ is $\mathcal{O}(-2)$ which has no global sections, but actually this is totally fine, as we are allowing forms to be identically zero on the zero section $\mathbb{P}^1$ inside the surface $\mathcal{O}(-2)$.

It is notationally confusing as there are two copies of $\mathcal{O}(-2)$ here. One is the manifold we're trying to restrict to, and the other is the normal bundle of just the exeptional submanifold $\mathbb{P}^1$ into the larger exceptional submanifold $\mathbb{P}^1 \times \mathbb{P}^1$.

Anyway, what we're looking for at the moment – which would lead to a way of restricting global 2 forms on the total space of $\mathcal{O}(-1,-1)$ to become global one forms on the total space of $\mathcal{O}(-2)$ – is a transverse vector field to that surface even if it is zero along the whole $\mathbb{P}^1$ inside the surface.

Clearly though the normal bundle of the total space of $\mathcal{O}(-2)$ in the total space of $\mathcal{O}(-1,-1)$ is nothing but the pullback of the normal bundle of the exceptional $\mathbb{P}^1$ inside the exceptional $\mathbb{P}^1 \times \mathbb{P}^1$ along the bundle projection $\mathcal{O}(-2) \to \mathbb{P}^1$.

The global sections are then the global sections of

$$\mathcal{O}(-2) \oplus \mathcal{O}(0) \oplus \mathcal{O}(2) \oplus O(4) \oplus +.....$$

on $\mathbb{P}^1$. Now there is a natural one dimensional space of global sections there, it is the second term.

This means, mod mistakes, that up to a complex scalar there is in fact a unique vector field which is transverse to the submanifold $\mathcal{O}(-1)$ inside $\mathcal{O}(-1,-1)$ everywhere away from the exceptional $\mathbb{P}^1$.

So we can apply this contracting vector field, and all the classical harmonic functions etc, once represented as holomorphic $2k$ forms, in the case of k electrons, become holomorphic k forms, as needed.

Now, how is the complex holomorphic Laplacian related to the real one?

The ‘real’ Laplacian is the deRham differential of the larger manifold, the ‘complex’ one is the deRham differential of the submanifold.

If we were somehow allowed now to restrict attention to those differential 2 forms which are invariant for our transverse flow, then the Cartan equation

$$i_\delta d + d i_\delta = \delta$$

where the right side is the Lie derivative, being zero, would imply that the contraction operator anticommutes with d, meaning that up to sign we can identify the real and complex Laplacians, when applied to such functions.

The subvaritety is defined by $r = 0$, if we let r be the fourth coordinate on our smooth threefold, and surely what is happening here is that when we are on the exceptional divisor we have to worry about the whole proper transform of the variety defined by $r = 0$ in the singular ordinary threefold double point, but away from the exceptional divisor we have that the flow $\partial/\partial r$ is the one to use, and so the differential forms that behave so nicely here, the ones where, if we restrict to those we can identify the complex Laplacian as only the negation of the real one, once working on the submanifold, are those which are invariant under the Lie derivative of the operation $\partial/\partial r$.

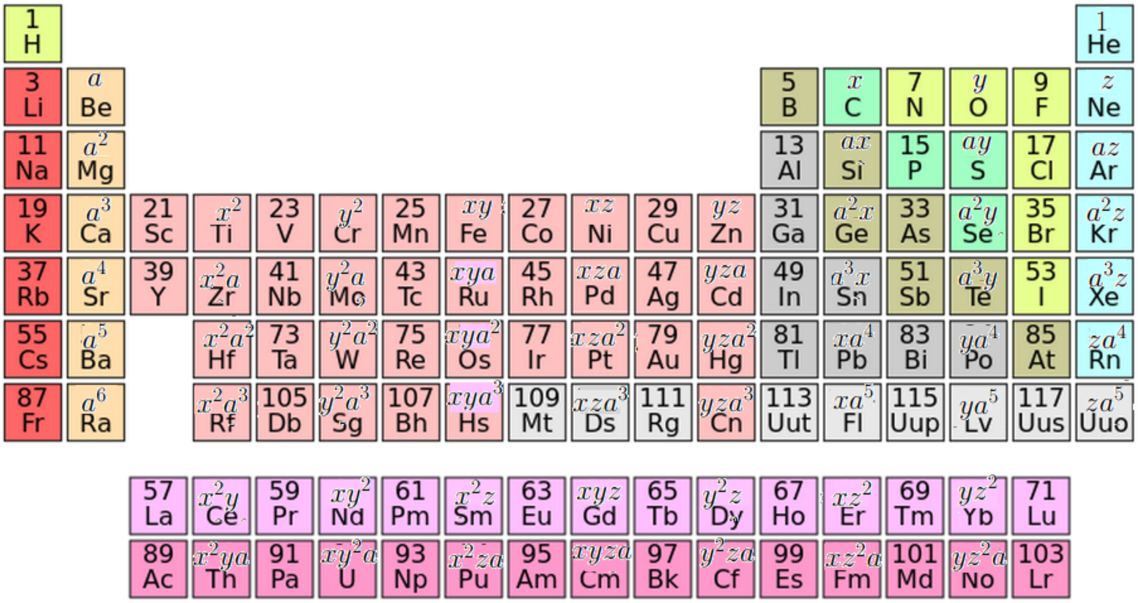
For forms which are not Lie invariant under that operator, then the relation between the real and complex Laplacian is more complicated than saying that one is the negation of the other.

A coincidence about the periodic table

This section and the next are a little light-hearted, and may be skipped, as it concerns the Aufbau only.

If we make a small change in the varieties we we looked at earlier, that is, if we consider adjoining not a square root, but a fourth root of $x^2 + y^2 + z^2$, so we have a homogeneous coordinate ring of a singular variety in weighted projective space, then a Riemann Roch theorem could relate vanishing of Plucker coordinates (dimensions of spaces of wave functions) to dimensions of global sections of $\mathcal{O}(i)$, and the global sections are nothing but a basis of monomials in x, y, z, a where we give a half the degree of x, y, z, and include the relation $a^4 = x^2 + y^2 + z^2$.

Empirically these basis elements happen to match the even numbered elements in the periodic table, I have just contrived this coincidence by taking the square root of what would be the radius, here a^2. For example, for Iron, Fe, I have omitted writing z^2 because it can be rewritten as linear combination of x^2 and y^2 and the later a^4.



1 H																	1 He
3 Li	a Be											5 B	x C	7 N	y O	9 F	z Ne
11 Na	a^2 Mg											13 Al	ax Si	15 P	ay S	17 Cl	az Ar
19 K	a^3 Ca	21 Sc	x^2 Ti	23 V	y^2 Cr	25 Mn	xy Fe	27 Co	xz Ni	29 Cu	yz Zn	31 Ga	a^2x Ge	33 As	a^2y Se	35 Br	a^2z Kr
37 Rb	a^4 Sr	39 Y	x^2a Zr	41 Nb	y^2a Mo	43 Tc	xya Ru	45 Rh	xza Pd	47 Ag	yza Cd	49 In	a^3x Sn	51 Sb	a^3y Te	53 I	a^3z Xe
55 Cs	a^5 Ba		x^2a^2 Hf	73 Ta	y^2a^2 W	75 Re	xya^2 Os	77 Ir	xza^2 Pt	79 Au	yza^2 Hg	81 Tl	xa^4 Pb	83 Bi	ya^4 Po	85 At	za^4 Rn
87 Fr	a^6 Ra		x^2a^3 Rf	105 Db	y^2a^3 Sg	107 Bh	xya^3 Hs	109 Mt	xza^3 Ds	111 Rg	yza^3 Cn	113 Uut	xa^5 Fl	115 Uup	ya^5 Lv	117 Uus	za^5 Uuo
		57 La	x^2y Ce	59 Pr	xy^2 Nd	61 Pm	x^2z Sm	63 Eu	xyz Gd	65 Tb	y^2z Dy	67 Ho	xz^2 Er	69 Tm	yz^2 Yb	71 Lu	
		89 Ac	x^2ya Th	91 Pa	xy^2a U	93 Np	x^2za Pu	95 Am	$xyza$ Cm	97 Bk	y^2za Cf	99 Es	xz^2a Fm	101 Md	yz^2a No	103 Lr	

The same monomials in x, y, z as they can be considered modulo $x^2 + y^2 + z^2$, correspond to a basis of all the homogeneous harmonic polynomials of all degrees.

Previous sections implicitly gave some justification for considering the variety $a^2 = x^2 + y^2 + z^2$, rather than the one which produces these monomials pictured above. While introducing a square root of $x^2 + y^2 + z^2$ had been necessary even to consider analytic solutions of the Schroedinger equation, it seems hard to thin of any reason why a further square root would be appropriate.

We will not discuss this further. A construction which might have a similar effect would be a second type of phenomenon like the one which is considered to be electron spin; there might be an effect from a second conormal sheaf which might explain the doubling of rows in a different way, more like the way that 'electron spin' works.

Note that atomic number of the m'th Alkaline Earth Metal could have been stated more simply, that for m even it is the binomial coefficient $\begin{pmatrix} m+3 \\ 3 \end{pmatrix}$ and for m odd, it is the average of the values for the two surrounding even values of m.

Although we won't explain this repetition of periods in the periodic table (it does also seem to be explained by the Aufbau, though that is not explained), in the next section we'll begin explaining this pattern in a way that does not require characters, and and attempts nevertheless to decode the exterior products that have empirically seemed to be needed (Pauli exclusion).

Linear systems of wave forms

When we consider the case of Nitrogen, the space of wave forms specified by the Aufbau is a 20 dimensional space of alternating forms, containing for the ground state a four dimensional irreducible subspace specified by Hund's rule.

It is amusing to try to work with less reliance on Pauli exclusion, the Aufbau, the Hund rules or exterior powers, and it is possible to convert the space of alternating wave forms simply into a 20 dimensional linear system.

What we would ordinarily do is to consider the seventh exterior power of a representation with character

$$f_{7,1,0}e_1(S) + f_{7,2,0}e_1(S) + f_{7,2,1}e_1(S)e_2(L).$$

The summand with largest sum of reciprocal squares in the second subscript of the f's – or more relevant the one determined by the Aufbau – is just the fourth exterior power of the sum of the first two terms times the third exterior power of the last term. So the ground state character will correspond to an irreducible component of

$$f_{7,1,0}^2 f_{7,2,0}^2 f_{7,2,1}^3 \Lambda^3(e_1(S)e_2(L)).$$

When we turn to calculating the third exterior power of the representation with character $e_1(S)e_2(L)$, a chemist might notice that it is the third elementary symmetric polynomial in the set of values

$$\begin{array}{ccc} SL^{-2}, & S, & SL^2 \\ S^{-1}L^{-2}, & S^{-1}, & S^{-1}L^2 \end{array}$$

and would consider that each basic way of choosing three of these monomials constitutes 'an electron,' or 'an electron configuration.' If all the monomials are chosen from the top row, then one would say there are 'three electrons which are all spin up,' and so-on.

Here is finally an example where the character which the Aufbau produces is reducible, and we would need the Hund rule to which part represents the ground state. We have

$$\begin{aligned} \Lambda^3(e_1(S)e_2(L)) &= \Lambda^3((S+S^{-2})e_2(L)) \\ &= \Lambda^3(Se_2(L)+S^{-1}e_2(L)) \\ &= S^3\Lambda^3e_2(L)+(S+S^{-1})e_2(L)^2+S^{-3}\Lambda^3e_2(L)) \end{aligned} .$$

Here we have used

$$\Lambda^2e_2(L) = \Lambda^1e_2(L) = e_2(L).$$

Since $\Lambda^3e_2(L) = 1$ and $e_2(L)^2 = e_4(L) + e_2(L) + 1$ this simplifies to

$$\begin{aligned} S^{-3}+S^{-1}+S+S^3+e_1(S)(e_2(L)+e_4(L)) \\ = e_3(S)+e_1(S)(e_2(L)+e_4(L)) \end{aligned} .$$

Thus now the Hund rule would say to choose $e_3(S)$ as representing the ground state.

What is amusing is to think of $e_3(S)$ is the character of the span of

$$\alpha^3,\ \alpha^2\beta,\ \alpha\beta^2,\ \beta^3$$

all times the 'determinant.'

What do I mean by 'determinant?' I mean

$$(xy - yz) \otimes z + (yz - zy) \otimes x + (zx - xz) \otimes y$$

but this $\otimes$ is symmetric, and we can use the Lie algebra identity to replace each of

$$(xy - yz), (yz - zy), (zx - xz)$$

by

$$rx, ry, rz.$$

Since $x^2 + y^2 + z^2 = r^2$, the determinant is the *third power* of the radius r^3, and we get the four monomials

$$\alpha^3 r^3, \alpha^2\beta r^3, \alpha\beta^2 r^3, \beta^3 r^3$$

Next, for $e_4(L) + e_2(L)$ we think of this as the character of all possible tensors of

$$xy - yx, yz - zy, zx - xz$$

with just

$$x, y, z.$$

Again we replace $xy - yx$ by rz etcetera, and again there is a relation, $x^2 + y^2 + z^2$ is the radius squared and we aren't going to count it again. So there are $9 - 1 = 8$ new basis elements, and this agrees with $(4+1)+(2+1)$ the value at $L = 1$ of $e_4(L) + e_2(L)$.

We again use the PBW relations, and write this as the six symmetric ones (with r^3 not counted so there are five) and these become just

$$x^2r, y^2r, xyr, xzr, yzr$$

and the others are commutators, which arise because we have the PBW relations, so that when we combine for instance $xy - yx$ and y, after writing $xy - yx = z$ and taking the tensor product $rz \otimes y$ we also have $r[z, y] = r^2x$. And we get the new monomials r^2x, r^2y, r^2z.

So in all the $e_4(L) + e_2(L)$ just gives us

$$x^2r, y^2r, xyr, xzr, yzr, xr^2, yr^2, zr^2$$

All of this is times

$$\alpha^2\beta \text{ and } \alpha\beta^2.$$

So in all, we get

$$r^3(\alpha^3, \alpha^2\beta, \alpha\beta^2, \beta^3),$$

$$r(\alpha^2\beta, \alpha\beta^2)(x^2, y^2, xy, xz, yz, rx, ry, rz)$$

So what had been a $\binom{6}{3} = 20$ dimensional space of alternating forms has been converted into a 20 dimensional space of commuting monomials, homogeneous of degree three in α, β and of degree three in x, y, z, r. Each of these is a slightly generalized wave form; if we include the coefficients (power series in r which are polynomials in the $f_{k,n,l}$ and r) we will have expressions where the radial part is a product of radial parts of solutions of the central charge equations while the azimuthal parts are now merely homogeneous harmonic polynomials.

Because of the labelling by monomials in α, β, the expressions are differential forms, but not just exterior ones, in this case just symmetric ones (like dr^2 is used to evaluate arc length). These evaluate things in the conormal direction.

Here is a general version of the same construction which does not require changing the multiplication in the universal enveloping algebra. The Schroedinger equation (with central charge assumption) describes subspaces of

$$\mathbb{C}[[r]] \otimes_{\mathbb{C}[r]} \mathbb{C}[x, y, z, r]/(x^2 + y^2 + z^2 - r^2)$$

It is quite simply that, the left factor is the power series giving a radial function, and the right factor viewed as a module over $\mathbb{C}[r]$ is graded and each part free of odd ranks, $1, 3, 5, 7$, copies of the space of homogeneous harmonic polynomials of degrees, $0, 1, 2, 3$ now tensored over the reals with $\mathbb{C}[r]$, and with the grading matching the periodic table very well.

And conormal principal parts are just a direct sum of two copies of this, replacing $\mathbb{C}[[r]]$ by $\mathbb{C}[[r]]^2$ to the left of the tensor sign, with a basis α, β.

Now, a space of such solutions (various values of n, k, l) is usually dealt with by taking an exterior power. But the right tensor factor is the associated graded of

$$U(so_3)[r]/(x^2 + y^2 + z^2 - r^2) = U(so_3)[\sqrt{x^2 + y^2 + z^2}].$$

Let's pass to a subalgebra of $U(so_3)[\sqrt{x^2+y^2+z^2}]$. Calling r a square root of $x^2+y^2+z^2$, let's pass to the subalgebra generated by r, xr, yr, zr. If we rename the new generators x, y, z again, the subalgebra now has presentation

$$\begin{cases} xy - yx = rz \\ yz - zy = rx \\ xz - zx = ry \\ x^2+y^2+z^2 = r^4 \\ rx = xr \\ ry = yr \\ rz = zr \end{cases} .$$

The associated graded ring is the commutative algebra which, in the earlier section, by coincidence matches the even numbered spaces in the periodic table, with coincidences about periods, energy levels, and the Aufbau.

With x, y, z thus redefined, we have the map

$$\Lambda^*(\mathbb{C}[[r]]^2 \otimes_{C[r]} U(so_3)[\sqrt{C}]\ ) \\ \to T^*(\mathbb{C}[[r]]^2)\ \otimes_{C[r]} U(so_3)[\sqrt{C}].$$

with C the Casimir element. Each of x, y, z is interpreted as a generator of the Lie algebra times (the same) square root of the Casimir element. The map is the one which writes exterior products as alternating tensors and interpret the rightmost component of the tensors as elements of $U(so_3)[\sqrt{C}]$. We consider the same square root as being the radial function r and we complete polynomials in r to include the radial component of solutions of the Schroedinger equation and therefore their products.

It would be interesting to see whether an interesting part of the exterior algebra survives this map.

Assuming one has chosen an isomorphism between the algebra and its associated graded, one can identify the images of the exterior powers of subspaces of the associated graded ring as being subspaces of

$$T^*(C[[r]]^2) \otimes_{\mathbb{C}[r]} \mathbb{C}[x, y, z, r]/(x^2 + y^2 + z^2 - r^2),$$

now our having renamed x, y, z to their original names. The image is not quite converted into a space of solutions of Schroedinger's equation for the radial charge, even in the coefficients of basic tensors in α, β, because the coefficients are products. That is, the coefficients in the base ring $\mathbb{C}[[r]]$, are products of radial functions of solutions rather than solutions themselves. Also there is some adjustment in powers of r which I still find confusing.

Abstractly the ring is very much like a tensor product of a tensor algebra over power series in r with just the direct sum $\oplus\mathcal{H}_j$ of the odd-dimensional spaces of homogeneous harmonic polynomials; but there is a slight difference in the way r is involved in the tensor product.

In cases when only the second tensor power is considered, the left factor, it is a direct sum of two parts (symmetric and exterior) and the decomposition still agrees with what is called the 'singlet' and 'triplet' configuration. Radial functions with different values of n (not only l) are linearly independent; one typically will fix k to be the atomic number. Then the part of each odd dimensional rank in the right side of the tensor factor can occur as many times as pairs n, l. That is, the actual dimension of the space of functions which arises is a sum of odd numbers times the various n, l and it is a question whether these spaces may be more directly related to the periodic table than the characters coming from exterior powers (elementary symmetric polynomials).

The point is that a character formula can be interpreted as saying that a particular space of antisymmetric tensors is *isomorphic* to a space of commuting polynomials, and yet some multilinear algebra can actually replace the alternating products with commuting products in the coefficients of tensors in α, β in various ways. Though the calculations here are probably degenerate and not correctly related to more essential ideas about vector bundles which we'll discuss later.

I don't know to what extent these can be nonambiguously interpreted as commuting polynomials in x, y, z, r times basic tensors (words) in α, β, and times radial functions. This depends on deciding whether there is any natural identification between $U(so_3)[\sqrt{C}]$ and its associated graded.

One thing that is appealling about the notion of converting the antisymmetric tensors into symmetric coefficients of tensors in α, β is that eigenvalues of the Casimir element, which we know are related to energy level changes, are mixed in with the structure constants of the universal enveloping algebra.

I know that Dirac was transfixed with how commutators are a special case of Poisson brackets. But that did require postulating a Hamiltonian.

Lie algebra actions are there more naturally, and although they are they are well known and historically prior explanation, they are the one used by chemists.

But chemists sometimes go no further than looking at character diagrams. The disjunction of the wave functions of hypothetical electrons didn't really match anything, so exterior products were needed.

Here I've just interpreted them as having more to do with lie bracket, and one can wonder whether converting the exterior products into Lie brackets is a better simplification than considering only characters. Transparently, such a calculation is closely related to the Aufbau, which wasn't explained by what is in general the much larger spaces of wave forms that are usually used. However it is the vector bundle approach which is good at matching the fine and coarse structure, on the other hand.

As a final comment, as Weyl and others authors point out, a general molecule has no symmetry. The usefulness of understanding atoms should be that it gives some understanding of electromagnetic waves, and chemical interactions may be understood as something along the lines of a fluid mechanical phenomenon, rather than as a combinatorial phenomenon related to quantum numbers of atoms.

In fact, if you think about it, it is because in the theory of sound phases do not matter much, that it was considered to focus on the decomposition of wave functions into components in representation spaces. But in higher dimensional harmonic theory, what needs to play the role of phase in Fourier theory is the actual representation components.

There is something to say about generalizing the calculations in this paper to molecules, but let us leave that for now.

Hodge theory

I think rather than endlessly editing the foregoing, it makes sense to point out inherent weaknesses in the criticism above. One issue is, the point upon which I am nit-picking Schroedinger's analysis is in the issue that if $\pi : N \to M$ is the structural map of the tangent bundle, then it is not the case that a section of $\pi^*\Omega_M$ on a subset of N is necessarily a pullback of any section of Ω_M. That is, one should not confuse the notion of 'a section of a pullback' and ' a pullback of a section.' The notion of a section and pullback do not commute with each other.

And if you look at even my own analysis, I ungrammatically and incorrectly confuse the notions, assuming the reader will take care of the syntax on my behalf.

But I do want to return to Schroedinger's statement that it is 'well-known' that

$$p_x = m\dot{x} = \partial W/\partial x.$$

On the general issue of deception, I would like to say this. That, some days ago, I encountered in the news what, it occurred to me, is a really good example of a long-term, insidious and intentional deception of the public. This is genuintely not connected with academics or universities, and I think, though, that I somehow forgot to make any mental note of what the story was about. I remember that it genuinely was painful to think about, and maybe the fact I honestly cannot even bring to mind this example, or any serious example – while knowing that if I even wait a few hours I'll see yet another and yet another – might be an example of what Streissand had sung, in a song which I do not like but in this context, at least, comes to mind in place of what I'm trying to reover, "What's too painful to remember, we simply choose to forget."

I know of many examples when deception is done at universities, always in a way that in the final analysis, in understanding that the means justify the ends, is seen as truly compassionate towards the public, towards each individual who is involved.

Perhaps one sees this when a student has failed an examination. Even in closest friends, when one has made a mistake of thought, if he is capable of understanding his error, others will not hide this from him, will not humour him as though he is insane and unable to see truth.

And I do not wish to dishonour Schroedinger nor his forebears. The fact that it seems, from understanding his paper, that he has, in my opinion, found the legitimate explanation for the spectrum of hydrogen by finding assumptions about waves and geometries which I believe more than any other, should console them if I should dishonour his memory by what I am about to say.

But, really, is it not a serious unintentional deception to say that it is 'well-known' that $p_x = \partial W / \partial x$?

Now, I have to also point out an omission in what I wrote above. Even in summarizing his argument, I initially stated that the gradient of W is $(p_x, p_y, p_z, -E)$, and I did not give any but the first variable any name.

The reason why I did this is that in physics writing, there is a convention that it is in some sense illegal to factorize this

$$p_x = m \frac{d}{dt} q_x.$$

And this is done because, the ease with which it *could* be done, combined with reluctance to do it, is something that the reader understands must have taken place for some intentional reason. The reason is that one has two copies of $\frac{d}{dt} q_x$, one interpreted as a section of the tangent bundle, and another interpreted as the rate of change of a coordinate of point in the base.

It absolutely does not matter whether one does the actual factorization or not. In the formula for what I called the spatial gradient of W the occurrence of $\sqrt{m}$ in the denominator takes care of this. If I had not explicitly said that p_x is the x component of momentum, and likewise for y and z, this would have become clear when the factor of $\sqrt{m}$ occurred, and when the value was given of $9.1 * 10^{-31}$ this would have become abundantly clear.

But even if we understand that the m was implicitly there, and if we understand correctly that there are two different ways the symbol $\frac{d}{dt}q_x$ might be used, and analogously for y and for z, one really should be startled by the notion that it is 'well-known' that $\frac{\partial}{\partial x}W = p_x$.

It is, for example, well-known that the frequency of 0.76 petahertz was observed to occur, near infrared range. It would have looked like glowing embers in a fire look, the same colour.

It might also be well known that the chain rule holds for derivatives. Here, when I say 'well-known,' I mean, in a mathematical sense, it is known that particular agreed axioms for what the symbols mean and how they are agreed to behave, means that they are agreed to behave in such a way that it is agreed that one expression can be substituted for the other without changing the meaning of what is said.

The statement that it is 'well-known' that $\frac{\partial}{\partial x}W = p_x$ is of neither type. To say that it was well-known, speaking to physicists, was either to state something false, or to unintentionally credit mathematicians for intuition which exceeds any intuition which an honest mathematician could ever have.

Now, I have mentioned in the past that the nilpotent operator η on the cotangent sheaf of the tangent bundle if it is to be made scalar equivariant by a tensor product with a tensor power of the natural representatino of the scalars, needs the -1 tensor power, the one in which multiplication is reversed. It may be best to only worry about invariance for the group $U(1)$ within the multiplicative group of scalars, and so when I write $\overline{\mathbb{C}}$ I mean the inverse of the natural representation of the unitary group. Then η and j are $U(1)$ equivariant

$$\eta : \Omega_N \otimes \overline{\mathbb{C}} \to \Omega_N.$$

$$j : \Omega_N \to \mathcal{O}_N$$

$$i_\delta : \Omega_N \otimes \overline{\mathbb{C}} \to \mathcal{O}_N.$$

So if δ is any vector field on N then $i_\delta \eta$ has the same domain and codomain as $j \otimes \overline{\mathbb{C}}$ and we can if we wish define the notion of δ being equivariant as the condition that i_δ commutes with the scalar action in this sense.

I've avoided here using the symbol $\mathbb{C}$ as it ambiguously might mean either with natural or with trivial scalar action, according to whether one uses conventions of linear algebra or representation theory.

Whenever a vector field δ on N is $U(1)$ equivariant in this sense, or if we extract the equivariant part, then in coordinates $q_1, ..., q_n$ we have

$$\delta(dq_\alpha) = \sum_{\beta,\gamma} a_\alpha^{\beta,\gamma} dq_\beta dq_\gamma.$$

The coefficients $a_\alpha^{\beta,\delta}$ are sections of $\mathcal{O}_M$ and this is a symmetric expression (the product is a product of functions whose domain is the tangent space N); it describes a connection on M. It is a torsion-free connection since $a_\alpha^{\beta,\gamma} = a_\alpha^{\gamma,\beta}$.

On the other hand, if we consider in the expression for each p_i in $\eta\omega = \sum_i p_i d'q_i$, writing the 'degree one' part which transforms as scalars, as

$$p_i = \sum h_{ij} dq_k$$

with now h_{ij} sections of $\mathcal{O}_M$ then

$$\eta\omega = \sum_{ij} h_{ij} dq_j d'q_i$$

This is now a tensor product, and the $U(1)$ action is the natural one on the first factor and the trivial one on the second. The form ω is thus determined by the connection matrix $a_\alpha^{\beta,\delta}$ our general matrix $h_{i,j}$ and it is, assuming δ to be involutive,

$$\omega = \delta\eta\omega = i_\delta \; d'\eta\omega + d' \; i_\delta\eta\omega$$

$$i_\delta \sum_{ij} h_{ij} d'dq_j \wedge d'q_i + d' \sum_{ij} h_{ij} dq_j \delta(q_i)$$

$$= i_\delta \sum_{ij} h_{ij} d'dq_j \wedge d'q_i + d' \sum_{ij\beta\gamma} h_{ij} a_j^{\beta,\gamma} dq_j dq_\beta dq_\gamma$$

In the first part of the expression, one has the contraction of a two form in which each monomial is a tensor product of one which is in the $\overline{\mathbb{C}}$ isotypical subsheaf with one which is in the invariant subsheaf and indeed is a pullback of an individual form from M. Thus the antisymmetric form which underlies the Hamiltonian is compatible with the isotypical decomposition of Ω_N.

The second part of the expression is the deRham differential, on the tangent bundle, of a cubic symmetric form now.

If we wished to consider whether first part may or may not be considered to be a Hermitian form, we might from the outset replace $\overline{\mathbb{C}}$ with its tensor square, so that here the action on the first tensor factor is through the squaring map and on the second is the identity. Then tensoring with one copy of the unmodified $\mathbb{C}$ gives the same tensor product which occurs in Hodge theory as far as the $U(1)$ action, and there results a sensible involution whose invariant part is a Hermitian form if M has a complex structure and the sheaves we are talking about such as $\mathcal{O}_M$ are considered to be the sheaf of maps of real manifolds to the complex numbers as a two dimensional manifold; and if we then take the $U(1)$ action is the one induced from the action of the unit circle on the complex valued real smooth cotangent sheaf.

Whenever relativistic considerations provide a notion that the tangent bundle and cotangent bundle can be identified with each other in various ways then such a matrix always arises. If it is taken to be positive definite Hermitian then it corresponds to a Riemannian metric on the underlying real manifold of M which is invariant for the $U(1)$ action on the real smooth complex valued cotangent sheaf. It need not be taken to be positive definite. When it is nondegenerate the vector field is determined by that matrix as we have seen, and locally if $-dH$ is the contraction of the form then indeed the $\frac{\partial}{\partial q_i}H$ will be the rates of change of the dq_i viewed as functions on the tangent bundle, and deterine the vector field.

Therefore, in particular, whenever the matrix h_{ij} is nondegenerate it determines the connection matrix $a_{\alpha}^{\beta,\delta}$.

That is,

$$\frac{\partial}{\partial q_i}H = \sum_{i,j,\alpha,\beta} h_{ij} a_{\alpha}^{\beta,\gamma} dq_{\beta} dq_{\alpha}$$

as section of $\mathcal{O}_N$, and when h_{ij} is an invertible matrix this determines the matrix $a_{\alpha}^{\beta,\gamma}$ because it determines the section $a_{\alpha}^{\beta,\gamma} = a_{\alpha}^{\gamma,\beta}$ because the monomials $dq_{\beta} dq_{\alpha}$ for $\alpha \leq \beta$ are linearly independent over $\mathcal{O}_M$.

If $\eta\omega$ is interpreted as being electromagnetic field, it must be a field which exists and is not actually ever zero at all points of configuration space M, in such a case.

The type of wave functions which Schroedinger considers, or as we've considered them, wave forms, all become holomorphic once we resolve singularities in the coordinate system. What concerned me in the classical primer was the impossibility of extending any such involutive δ to the tangent bundle of a Kahler compactification of M if the Chern numbers of even the uncompatified M are not all trivial.

A much more serious objection is that one should not impose a complex structure on a manifold that does not arise naturally without a complete analysis of the deformations of complex structures, of the choices that have been made.

A final objection in this section: we have not considered as yet what general considerations might render $\delta\eta\omega$ a closed form. This is the Lagrangian condition, a necessary condition for $\eta\omega$ to be the type of non-closed wave form we're considering. Let's abandon any consideration of Hermitian structures and consider what is both the the easier and more general real Riemannian case in the next section.

The Levi Civita action is not Lagrangian for its Riemann metric

Turning for a moment just to the case of a real Riemannian manifold M, where we know that there is an involutive vector field, it is the relevant question what is the condition for a particular natural involutive vector field to be Lagrangian with respect to a natural one-form. The first port of call is to see whether the involutive vector field actually coming from the (torsion-free) Levi Civita connection is actually Lagrangian with respect to the one-form on the tangent bundle N coming from the metric on M.

We will see that in general this is not the case.

So we consider the one form $\eta\omega = \sum_{st} g_{st} dq_s d'q_t$, and consider the derivation coming from the Christoffel symbols

$$\Gamma_i^{jk} = \sum_r g^{ir}(\partial_k g_{rj} + \partial_j g_{rk} - \partial_r g_{jk})$$

with superscripts denoting entries of the inverse matrix. To check if $\delta\eta\omega$ is closed it will be enough to check if $i_\delta \sum_{st} d'(g_{st}dq_s) \wedge d'q_t$ is closed; this is

$$\sum_{st} g_{st}\delta(dq_s)d'q_t + dg_{st}dq_s d'q_t - g_{st}dq_t d'dq_s - dq_s dq_t d'g_{st}$$

The only term where the symbol δ occurs is where δ had been applied to a product containing a factor which was d of something.

Note that the g_{st} in that term contracts against the first factor g^{ir} in the Christoffel symbol, and both may be ignored. Then we obtain the second factor of the Christoffel symbol suitably re-indexed, and thus the whole expression becomes

$$\sum_{tjk}(\partial_k g_{tj} + \partial_j g_{tk} - \partial_t g_{jk}) dq_j dq_k d'q_t$$

$$+\sum_{st} dg_{st} dq_s d'q_t - g_{st} dq_t d'dq_s - dq_s dq_t d'g_{st}$$

The reason only one term has a function that is not a differential of either type is because of the differential $d'(g_{st}dq_s)$ in an earlier formula.

The first part simplifies now and this becomes

$$\sum_{jt} dg_{tj} dq_j d'q_t + \sum_{tk} dg_{tk} dq_k d'q_t - \sum_{tjk} \partial_t g_{jk} dq_j dq_k d'q_t$$

$$+\sum_{st} dg_{st} dq_s d'q_t - g_{st} dq_t d'dq_s - dq_s dq_t d'g_{st}$$

Three of the terms are equal with the same sign So we obtain, it appears, modulo errors,

$$3\sum_{st} dg_{st} dq_s d'q_t - \sum_{ijt} \partial_t g_{ij} dq_i dq_j d'q_t - \sum_{st} dq_s dq_t d'g_{st} - \sum_{st} g_{st} dq_t d'dq_s.$$

And we can simplify further recognizing something is a d' and we get

$$3\sum_{st} dg_{st} dq_s d'q_t - 2\sum_{st} dq_s dq_t d'g_{st} - \sum_{st} g_{st} dq_t d'dq_s.$$

The differential of this is not zero in general, and so even for a compact Riemannian manifold, the action coming from the Levi-Civita connection is rarely Lagrangian for the corresponding one-form.

The notion of an action (automatic extension of conscious control) is difficult and paradoxical; even when a natural one exists (when there is a natural Riemannian metric for some reason) there is no known natural one form with respect to which it is Lagrangian. Another difficulty with such a notion is that even if one finds that dualities produce Lagrangian actions, yet a duality represents a type of relativity that only relates two points of view, not more than two.

Foundations

Rather than now thinking more about the relation between the term symbols and the finer frequency divisions said to come from spin-momentum interaction, or the relation between W, e^W, and dW, it makes sense to make some general comments about things like the theory of groups, about linear algebra, Galois theory, and set theory.

The first thing to say is that altough things like the special relativity model of space time, are considered to be a set of points, yet, no-one in either Math or Physics, and rightfully so, has ever cared about whether points of space or space time are elements of a set. For example, it contradicts Galilean relativity that if one a person on land has coordinatized a map of the sea as a set of points, while someone travelling on a ship has coordinatized positions on the deck of the ship as another set of points, if one really believes one set should be a subset of the other. What in set theory is sometimes jokingly called a 'universe,' is an idea that is not entertained seriously, and does not play any part of any currently accepted theory of sets.

I remember my constant frustration in classes when a teacher would be speaking in analogies, for example asking us students to imagine five identical objects, and then asking us to interchange two of them. Surely the teacher would never know whether the students had successfully completed that task, nor, indeed, could a student check whether he's successfully done it, or done it twice, or a million times, or never.

If the teacher asked me to describe the difference between the two objects which I was supposed to have interchanged, I should be able to say, this question does not make sense, because that difference cannot be *observable* to you. A teacher should not tell the class that every equilateral triangle has three vertices, known as the nip, the nap, and the nup; and then give an examination with rows and rows of pictures of equilateral triangles, upon each of which the student is charged with labelling the vertices nip, nap, and nup. In subtler ways, though, this type of thing *does* happen.

If a student is given a linear transformation f of a finite dimensional vector space, and asked to find an eigenvalue, which is a number λ so $f(v) = \lambda v$ for some vector v, if he cannot find such a number anywhere in his field, then within the space of linear transformations of the vector space, a set to which f already belongs, there is a larger field. There is more than one such field, all containing copies of f under projections. These are ways we might have considered that f is a number after all. A familiar case, when we have a real two-dimensional vector space, is when the span of 1 and f is a copy of the complex numbers. One might say, there are two eigenvalues, one is f and the other is the complex conjugate of f. When the matrix of f is diagonalized over the complex numbers, these two entries occur in the diagonal.

But, really, when you go through the details, there is not 'f and also the complex conjugate of f.' Rather, f has ramified into a pair of indistinguishable elements.

The axioms of set theory don't happen to include anything like the functor which applied to any set, gives a disjoint union of two indistinguishable copies of that set. When things are formalized there is the operation of taking the cartesian product with a two element set, but there is no two element set whose two elements are indistinguishable.

This is a mild detail, only.

By the way, when I said that f 'is' an eigenvalue, I did not mean to say λ equals f and so that $fv = \lambda v$ for all v. Rather, now there are two copies of the vector space V, and we might take their tensor product $V \otimes V$. Then what I am calling f is $1 \otimes f$ while the eigenvalue, belonging to the endomorphism ring of the leftmost tensor factor, which we interpret as our extension of scalars, is $f \otimes 1$. Then one must prove that for any linear transformation f there is always a $v \in V \otimes V$ such that $(f \otimes 1)(v) = (1 \otimes f)(v)$. Or, if f is invertible, that the invertible linear transformation $f \otimes f^{-1}$ always fixes a point of $V \otimes V$.

There is a symmetry of the situation, so that just as $1 \otimes f$ is an eigenvalue of $f \otimes 1$, so is $f \otimes 1$ an eigenvalue of $1 \otimes f$.

The moment one begins to wonder what makes a linear transformation invertible, one encounters things like how you can naturally dualize V by tensoring the (covariant!) space $\Lambda^{n-1}V$ with just the dual of the one-dimensional vector space $\Lambda^n V$, where n is the dimension of V.

Then, a student given list upon list of linear transformations, and asked to find an eigenvalue of each, could just turn the page upside down, and where had been written $1 \otimes f$ is now written $f \otimes 1$.

Such a solution would seem Zen like, but in a bad way. It would seem Zen like in the sense of saying ‘The answer to your question is identical to the question which you asked.’

But, it is sometimes important to do that. What it comes down to is that people who do not know much Maths, think that Maths is about numbers, and that they know where numbers come from, and what they are. So a Maths teacher might give a student a list of linear transformations, thinking ‘these are something I will never understand until they are tabulated and classified numerically.’ Then the student is charged with converting these mysterious objects into something tangible, into numbers as can be written on the paper and handed in as solutions.

Perhaps there are two types of student experiences. There is the type of experience where one learns to subtract λ times the identity from the matrix, leaving λ as a variable; then takes the determinant, sets it equal to zero, solves the polynomial equation to find a list of possible values of λ, then for each of these values calculates the kernel of the matrix minus λ times the identity, and finds in this way the eigenvectors.

And then, perhaps, there is another type of experience, which amounts to getting confused, losing contact with the clear boundaryline between what is accepted to be a number, and what can never be accepted as being a number. Being a student who never again works out which side of the boundaryline he is occupying in any future calculation.

At times there is a phenomenon, which one should be deeply suspicous of, like when a person has been working with complex numbers, and eventually writes down an expression that is invariant under complex conjugation. This would be a notion based on the fact, if f has been ramified into two indistinguishable copies of f, then the permutation group which interchanges them, ought to fix any meaningful expression.

The reason I say one should be suspicious of such a phenomenon is, because, for example, one might say, if you blow up a point in space, then because all the points of the exceptional divisor have sprung into existence all at once, with no conscious act which possibly could have distinguished one point from another, then there should likewise be a group acting transitively, so that any meaningful combination of conormal principal parts should be one which is invariant under not only the symmetries of the sphere, but also this independent group action.

If you believed that, you could conclude when the assumption of a central electrostatic field is violated, the corresponding departures from a set of frequencies of emitted light from just being differences of k fold sums of reciprocal squares should not cause each spectral line, which had previously been found in proportion to a difference of two sums of k reciprocal squares, to split into any more parts than can be accounted for by the spectrographic terms $e_{2l}(L)e_s(S)$. That, for example, the decomposition of each such term into a linear combination of $e_j(L)$ upon setting $S = L$, as though only the symmetries should have been allowed arise by exponentiating infinitesimal rotations of three space to the diagonal subgroup, should be invisible in the spectrum.

Yet, the finer structure is not invisible, and so it cannot be true that when the origin is blown up, within $\widetilde{V}$, the divisor of poles of the potential function which had become analytic on $\widetilde{Q}$, that we may correctly interpret the set of points that are created as new and indistinguishable points.

It was definitely true about the degree four etale cover, that points in the fibers, if we work over the complex numbers these become reduced to two-element fibers – are mathematically indistinguishable. But this is rare. Blowing up is a functor. Just the fact that it is a functor, just the fact that I can even speak of natural transformations, means that there must exist physical models in which the appropriate automorphism group is just the trivial group.

The conormal principal parts are conormal in the variety where we have set r to zero, and the Severi Brauer variety P is the locus where x, y, z are all zero. So the conormal principal parts of P within a variety where r is zero do seem intuitively like something very fictional. But we could give a precise mathematical definition to the term 'fictional,' to mean in a context similar to this one something like the rule which assigns to any function f and any point y in the codomain, the set $f^{-1}y$.

It is hard to think about this, because one would say that the only important case of this is when Y has one element, and then $f^{-1}y$ is just a set, and the rule assigns to any set its set of elements. Yet, this operation is the identity, hardly fictional, and I admit being confused upon this point.

Within concrete categories, we want to say that something is fictional if it is one of those things which is a slight generalization of a functor, but misses being functorial because when it returns a value of a set, the elements of that set are indistinguishable. The failure of being a functor may imply an automorphism group of the various sets that are returned, and one would say that a function is not observable if it is not invariant under the group action; if it does not respect orbits.

An example is the tangent bundle of a manifold, one should say that since it depends functorially on the manifold, one cannot apply a vector bundle automorphism of the tangent bundle sight unseen. After the automorphism had been applied everything would be moving in the wrong direction when it moves! Then one should say, arbitrary sections of the tangent bundle are observable; then, if one forgets that it is the tangent bundle, and only thinks that it is a vector bundle, not every section is observable anymore.

Earlier I said that I admired Schroedinger's creation of a differential equation model which explains the earlier formula for the spectral lines of Hydrogen. Something now that I admire is what Quantum Mechnics decides to do at this juncture. When one has chosen the relevant subgroup (either all of $SU_2 \times SU_2$, or the diagonal subgroup SU_2, or just the torus $\mathbb{C}^\times$), one says, spaces of functions which are observable can only be those, under the group action on the set of all subspaces, which are fixed under the group action. These are then representations of the chosen subgroup. But, what is observable is not only the vector space, but the vector space together with the isomorphism type of the representation of the stabilizer subgroup acting on the points of that subspace.

One does not say, 'the points of the exceptional divisor are indistinguishable and so we know no more than if we had never done the blowup.' That is a true statement by the way, though it is not spoken.

One says, once we minimally resolve this point, we obtain a Riemann sphere, which has al its points indistinguishable because any one can be transformed to any other by an element of its autormorphism group. If I allow myself to forget the ambient surface in which the point had been, then no one vector field of the Riemann sphere is observable. Yet, the whole space of vector fields is, and also the isomorphism type of the space of vector fields as a representation of the automorphism group of the Riemann sphere.

I cannot think of any general principle that is a better context for quantum mechanics than just to say it is a nice theory. I am very uneasy if someone says, here is a three element set, and now I am going to start permuting its elements. Maths by itself is, as we know, paradoxical from the start. Yet, the notion of setting up a space and a sheaf of analytic functions, in order to try to explain spectroscopic lines and the periodic table is in some sense the simplest and most obvious choice.

If we were using a circle, or $\mathbb{C}^\times$, to understand something in physics, and using analytic functions, we would be writing down Fourier series which is the same as Laurent series. The indexing set for our functions would have the affine structure of the integers, and no one would say that something about the spacing of the integers is telling us anything about the physical world. The Fourier coefficients have certain geometric positions just because we chose to set up our coordinates in a certain way.

Likewise, the fact that we have Fourier coefficients indexed by numbers s and l is because we chose to work analytically, and, although I do not completely understand the situation mathematically, we are working on a variety which is the divisor of poles of the potential function V when r is made analytic by a two sheeted branched covering, and becomes a variety with an ordinary double point, and one passes to the minimal resolution.

It would not be correct to say that the fact that both s and l are needed has anything to do with a spinning electron. In fact s is clearly needed to explain the periodic table. We would not say that the periodic table has its structure because we chose r to be anaytic, but rather, the transformations we needed to do to make r analytic, so that wave functions or forms can be described analytically, ended up also making it easy to explain the periodic table in at least one way.

And it is also quite possible that measurements of s may indeed have to do with a spinning electron, with relativity and magnetism, with precession. In fact, it is known (see Wikipedia) that the Pierre Curie constant for the degree of paramegnetism of a material is proportional to $j(j+1)$ for j the magnetic quantum number. For example, the ion Gadolinium III, which occurs in Gadolinium triChloride, has ground state with character $e_0(L)e_7(S)$ and $j = 7/2$ is used as an agent in MRI scans because of its ability to react to a magnetic field.

People who work in moduli spaces or stacks think more deeply and correctly about the issues of naturality which I mentioned.

I shouldn't have said that fibers $f^{-1}(y)$ are not functors...I was somehow imagining a case when someone never specified y.

A better example is just universal covers.

If someone has a configuration space M, then does some analysis on the universal cover M', then when they are done, if they haven't worked equivariantly for the fundamental group, their answer could still depend on a choice of basepoint.

So it can make sense to have 'the' universal cover, admitting that it is not a correct functor, and then work equivariantly – which means the only vector spaces considered will be modules and the only maps invariant for the group action, fixed that is.

Then if one finds that spaces of solutions of some differential equations are representations of that group, this is of course not because that group represents something in the real world moving or spinning. That is obvious.

The analagous analysis is not quite true for blowing up, in cases when it is natural, in cases when a minimal surface exists and is unique.

It only would become true in cases when there is not a unique resolution.

Here there is a unique and canonical resolution, and yet part of the spectrum is invariant and part is not.

It is not inconsistent that part is invariant, and the existence of part that is not is proof, if one needed it and believed that the model matches the real world exactly, that minimal resolutions in this case in fact are functorial with respect to automorphisms of the ambient space.

As a final little comment on these topics, the equations which Schroedinger wrote at the beginning, ended up in his considering eigenfunctions of the Laplacian. Yet, if he had written instead of $\psi = A(x, y, z)e^{iW(x,y,z,t)}$, but more simply $\psi = e^W$ then things might simplify using the rule

$$\Delta(e^W) = (\Delta(W) + |gradW|^2)e^W.$$

So the condition that a function f is an eigenfunction is equivalent to the Poisson problem

$$\Delta(W) = (f - |grad\ W|^2).$$

With his conventions, $|grad\ W|^2 = E - V(x, y, z)$ the kinetic energy, which in a more general Hamiltonian formulation is $i_\delta \eta \omega$, the contraction of a one form on the tangent bundle along an action vector field. Since f itself is a constant plus a constant times V then $i_\delta \eta \omega$ is already a constant plus a constant times V. In any case, the potential does have a pole when $r = 0$ and a correct generalization may need consideration of residues.

Unification of the various coupling schemes

In an earlier section, I mentioned a coupling scheme that is different than Russell-Saunders, which is used for example for Neon. This is said to combine various aspects of orbit-orbit and spin-orbit coupling.

It is true that the various orbit-orbit coupling schemes describe in the end the same list of irreducible representations, even as subspaces of one and the same vector space, and so it is worth considering whether there is any reason to use more than one scheme.

From the standpoint of perturbation theory there is not, and it seems likely also that if Hartree-Fock or other approaches are correctly formulated they will not either.

An orbit-orbit coupling scheme describes a hierarchy of representations, and yet only the irreducible representations of the actual rotation group or its double cover have physical significance.

In the case of the perturbation theory approach, for the coarse structure, this is seen in the way that one can ignore all but one eigenspace of the Laplacian plus potential term (including repulsion and attraction), to start with, and the full calculation only depends on linear maps of that eigenspace which come from the action of the operator on Hilbert space, composed with the inclusion and projection to make it become an operator on a finite-dimensional vector space. Since the full potential term is invariant under the cartesian product $SU_2 \times SU_2$ its eigenspaces will also be, and comprise sums of irreducible representations. Except in astoundingly rare cases (which would not occur in reality) they will simply be such irreducible representations, and once term symbols are resolved into multiplicities like $P^\circ, P^{\circ\ bis}, P^{\circ ter}, \ldots$ they will correspond to such term symbols too. This only depends on choosing the decomposition of the isotypical space to be one which is preserved by the operator, that is, according to eigenspaces of the restriction of the operator to the isotypical component, or indeed, what is practically much simpler, to its action on the center of the endomorphism algebra of the isotypical component as a representation of $SU_2 \times SU_2$, which is, in case of multiplicity m, only an m dimensional vector space.

There is no second way of doing the calculation that gives a different result, and no choices have been made. So, for orbit-orbit coupling, all that needs to be done is to reiterate the details of this.

For orbit-spin coupling as I mentioned, this is only a matter of correcting the definition of the Laplacian to be one which acts, as it were, diagonally, and this can be done by adding the correction term, a function multiple of $C_J - C_L$.

Thus, all the various orbit-orbit and spin-orbit schemes can be subsumed, from the standpoint of a perturbation theory approach, and, certainly, from the standpoint of a theoretical understanding, into a single classification scheme.

This calssification scheme, to fill in the obvious details, goes like this: A molecule may have upon it an ion. Firstly, now, once a number of protons k_p is chosen for the ion, the number of electrons is a number k with $0 \leq k \leq k_p$.

Secondly, a 'sum of reciprocal squares' energy number, a rational number c which is a sum of k reciprocal squares, is chosen. There are infinitely many such rational numbers, but they are well-ordered, and finitely many if any bound is chosen.

Thirdly, an actual particular sequence $n_1, ..., n_k$ with

$$\frac{1}{n_1^2} + ... + \frac{1}{{n_k}^2} = c$$

is chosen, the order does not matter so we may as well take it to be an increasing sequence.

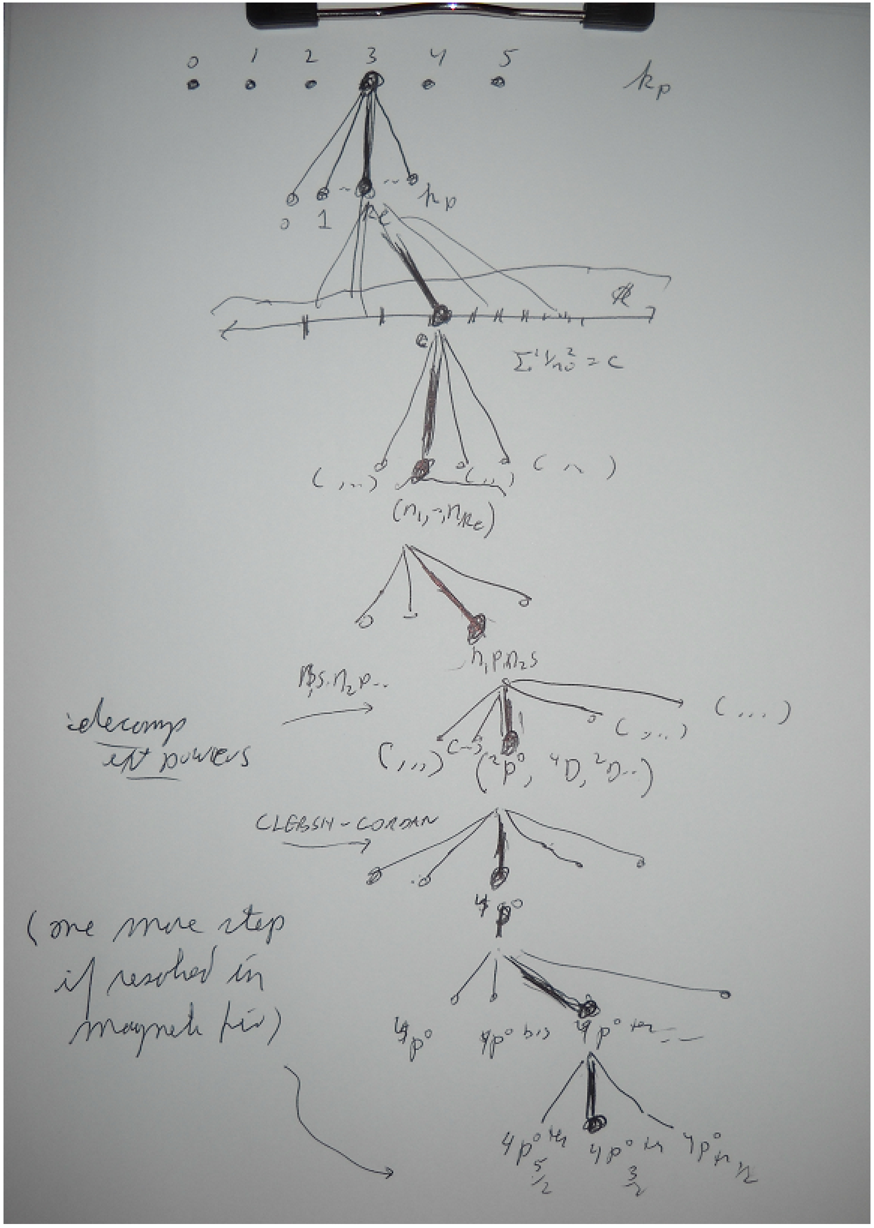
Fourthly, an electron configuration with this sequence of n values in some order is chosen. For instance if the sequence of n values is $2, 3$ we have as possibilities $2s^1 3s^1, 2s^1 3p^1, ...$ These are more familiarly abbreviated $s23s, 2s3p$. There are finitely many possibilities because of the fact that 'l is less than n', and we include here all possibilities, even ridiculous ones like $3s^1 2d^1$ which do not occur in nature. Part of the unexplained Aufbau is essentially the practical limitation on which of these finitely many choices really occur.

Fifthly, an assignment is made of a term symbol to each orbital of the chosen electron configuration.

Sixthly, the restriction to the diagonal $SO_3 \times SU_2$ is done. This means that the tensor product of the irreducible representations assigned to the term symbols in the sequence is decomposed, and one term symbol is chosen. The superscript circle can be included but does not matter as it is determined by the electron configuration, so the next choice is a symbol like ${}^3P^\circ$.

Seventhly, each term symbol has a multiplicity within which it occurs in the electron configuration, I've started just using the latin superscripts, so from ${}^3P^\circ$ we must choose either the undecorated ${}^3P^\circ$, or else ${}^3P^{\circ\ bis}, {}^3 P^{\circ\ ter}, ...$ The list is finite, usually has only one entry, and is totally determined by the electron configuration and term symbol.

Eighthly, the subscript is applied, an integer or half-integer, there are finitely many possibilities depending only on the underling term symbol, so finally we have a symbol like ${}^3P_2^{\circ\ ter}$. Here is a careless sketch of the tree



Starting from the same number of electrons and protons, a different route down a different branch of the tree gives a second such symbol, and a pair of such final symbols (one decorated with a circle and one not) corresonds to a theoretical frequency in the spectrum of a polarized wave that could be received from this ion.

Because we are talking about two ends of a tree, there is a unique path in the tree from one end to the other without retracements, and there are various possibilities for how far up in the classification one has to go to connect one end to the other.

This classification is by a tree with eight levels of branching, of which the only infinite one (for a fixed number of protons) is in a choice of a rational number which is a sum of k reciprocal squares.

For an example which we already discussed, the green triplet for Magnesium involves three paths. These go all the way up to the top of the tree, where nothing has been chosen except the number of electrons and protons, and all the way back down a different branch. At the very end, there are three choices of subscript $0, 1, 2$ for the term symbol, and that is why there are three green spectral lines.

The nearby yellow triplet is totally different, not requiring going up to the root of the tree.

So the green triplet is a phenomenon like seeing one leaf of a tree, very nearby three other leaves. But when you look at the tree, you see that the one leaf is on a totally different branch, and you have to go back and back through branching to get all the way to the base of the tree, before you find the shortest path connecting that one leaf to the three others. The relative positions of the three leaves would be fixed, but the positions of the three together relative to the one would depend on deep structural properties of the tree. And this is why the green triplet is sensitive to even small changes in the compensation coefficient, but not the yellow triplet.

The three lines in the triplet are said to be part of the same 'fine structure,' but this is a contrivance and there is no reason that two lines need to be closer if they are close by reason of proximity in the tree, than if they are far. The tree structure is a heuristic, with historical origins in projective geometry and representation theory, and yet it does give a sensible classification which a person might find useful. It is a beautiful algebraic construction, which does also to some extent match the closeness of spectral lines, but it does not describe any physical 'coupling,' and there is no need to adjust spectral lines, or the calculation of spectral lines, to make them match the algebra.

In the case of the ground state, some of the classification is likely to degenerate and become simpler. If you consider in the classification,the step where you have chosen a sequence of term symbols, one for each orbital, because of the Aufbau for the ground state, this is identical to what you would do if you were classifying spectral lines separtely for separate atoms each with one of the unfilled orbitals as its only unfilled orbital.

Then the notion of polarization that is relevant, for the cartesianproduct of one copy of $SU_2 \times SU_2$ for each *orbital,* is the same as wanting to think of wave functions polarized in the way that planets orbiting a star are, but with one sort of plane for each orbital.

And, the important thing is that these do not have a lot of symmetry, but within the space of wave functions we've made no essential choice.

It is like saying, I want to calculate the potential energy of the earth rotating about the sun, then I can choose a coordinate system where the earth is in the(x, y) plane. I have not made an essential choice, but now once that choice is made, then the symmetry is broken and there are restrictions on what *subsequent* choices can be made.

The fact that wave functions which respect such a polarization do not represent every energy level even coarsely now corresponds to the fact that separately polarizing more than one wave function *does* further constrain the symmetry.

But there is an issue here of actual physics, and that is, the classification which I gave just now is very abstract, but I wonder about the practicalities of the step where you assign one term symbol to each orbital, in essence choosing one irreducible component of an exterior power of an irreducible representation, and then tensor all these together and decompose again.

The reason I wonder about this is that in nature, a situation of an atom even having more than one unfilled orbital at the same time is rare. It occurs in excited states, but not in the ground state.

So if we are really talking about ground state waveforms, then nothing goes wrong here. When we look at the term symbols we've really assigned to the orbitals, practically speaking the onlyl energy levels that are going to arise are the ones where we've just assigned type S to all but one of the orbitals. Then the step degenerates where we take a tensor product and decompose.

Then, the term symbol we get at the end is nothing but one of the term symbols we would have had for a different atom with just that same unfilled orbital as its unique unfilled orbital. Or, truth be told it is no longer a different atom, I am saying, our atom must already be one of those basic trivial atoms.

So for the ground state, if I really do choose that very restrictive polarization it actually is not really restrictive at all because all but one of the orbitals are rotationally symmetrical because of being filled.

I had been sort of hoping that a notion of such restricctive polarizations might relate to bond angles, but here we see that there is no relation with bond angles, as in the ground state the polarization even in this restrictive sense does not impose any constraint upon the atom and is an inessential choice like choosing the (x, y) plane for the orbit of the earth.

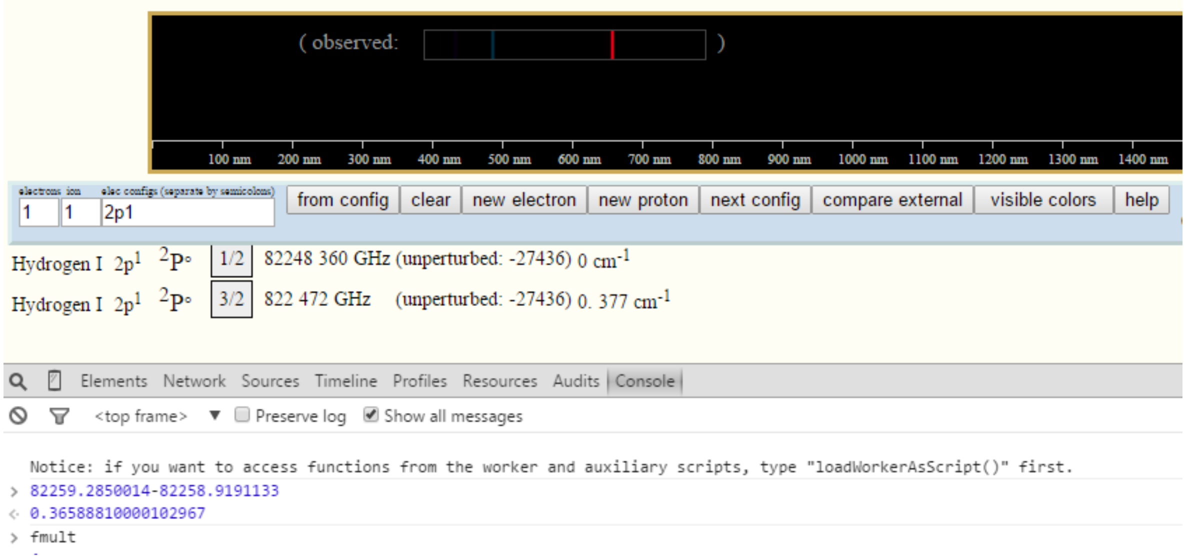
Regarding the spin-orbit coupling, in some sense this already is part of the fact that we used $SU_2 \times SU_2$ and one of them is somehow said to have to do with 'spin.' But, for the fine structure, the strange quantization of angles, or notion of 'angular momentum operator' is not needed for any of the calculations that are said to be explaining 'spin-orbit' coupling, it is just necessary to use the correct Laplace operator in the first place, or correct it by the addition of the function coefficient (which we mentioned already) times $C_J - C_L$. This fails the rule that the position of a coarse line by the character agrees with the 'center of mass' of the fine lines, but there was never any reason for asserting that this should have been true, and it is certainly wrong to add an unexplained term to Schroedinger's equation to make true a rule which could have no experimental verification.

Finally, just to reiterate this in what I hope will be a convincing way, to have a classification sheme for something does not classify it, and there is always more than one classification scheme. We might say that actual trees in nature are classified by binary rooted trees. There is a universal binary rooted tree in which any one can be embedded, and the only choices needed to make is whether each branch goes to the left or the right. In nature, if we decide that a tree branches in a binary way, always deciding that one branching occurs a little above or below another, and if we have a notion of north and south, then this gives a conceptual embedding of a finite rooted binary tree which matches the living tree, into the universal one. The rational ends of the universal one can be considered to be rational numbers with denominator a power of 2, and so then each end of the tree is labelled by such a dyadic rational number.

This is not to say that the dyadic rational numbers have anything to do with trees, only that we have chosen for ourselves a classification scheme which is convenient, which we happen to understand. If I want to describe one leaf of one tree, I have to have a way to say how to climb to find it, whether to go north or south at various times, and these are only my particular instructions. They are useful in classifying the leaves so that when one person describes a leaf, another person can find that same leaf, by following the instructions. The instructions themselves, the way they are formulated, do not matter, and in this way coupling schemes in quantum mechanics should not matter either. They should maybe be considered decoupling schemes, as if a scheme is organized like a tree, then each end has a unique path, and there is no difficulty such as two people given different instructions, finding the same leaf, incorrectly thinking that they have found different leaves.

Discussion of the problem of nonconvergent integrals

The difficulty with the fact that the perturbation action of $(\frac{1}{r^3})$ was described by non-convergent integrals might be because in place of the perturbation action of $\sum_i(\frac{1}{r_i^3})$ we were meant to compose the perturbation action of $\sum_i(\frac{1}{r_i})$ with that of $\sum_i(\frac{1}{r_i^2})$. When this is done, we do obtain the correct sign of the Lamb shift, and if we choose fmult=4, which would be consistent with using a Casimir in which the 'degree' of r is two, we obtain a value of the Lamb shift of 0.377, where the observed value is 0.365 Unfortunately this interpretation fails for almost every other element.



electrons 1 ion 1 elec configs (separate by semicolons) 2p1

Hydrogen I 2p^1 ^{2}P° 1/2 82248 360 GHz (unperturbed: -27436) 0 cm^{-1}

Hydrogen I 2p^1 ^{2}P° 3/2 822 472 GHz (unperturbed: -27436) 0. 377 cm^{-1}

```
  Notice: if you want to access functions from the worker and auxiliary scripts, type "loadWorkerAsScript()" first.
> 82259.2850014-82258.9191133
< 0.36588810000102967
> fmult
```

The ethics of science

I am going to here interject a correction to something which I wrote in my Economics text. I wrote that like

> those scientists who debunk one after another magic trick, for the benefit of those few who are fooled by magicians

a possible role of Maths or Philosophy might be to 'become proficient enough in science to beat the scientists at their own game, to expose how unethical it is.'

I had been referring to the notion of energy, and conservation of energy, for example, the National Academy K-12 education guidelines which advise school curricula to require at great length and detail teaching a lenghty and detailed catechism. A typical quote is

> By the end of grade 12. Conservation of energy means that the total change of energy in any system is always equal to the total energy transferred into or out of the system. Energy cannot be created or destroyed, but it can be transported from one place to another and transferred between systems. Mathematical expressions, which quantify how the stored energy in a system depends on its configuration (e.g., relative positions of charged particles, compression of a spring) and how kinetic energy depends on mass and speed, allow the concept of conservation of energy to be used to predict and describe system behavior.

Just in an ordinary conversation in the common room, A. Braun commented to me about how really fair scientists are in their research practise. When the concept of conservation of energy has needed adjustment, for example relativistic adjustments, or adjustments to include transfer between matter and energy, these have always been consistently done. Any time there has been any exception to a believed rule, the exception has been given full, interested attention by all. No one has been dogmatic about his scientific interpretation about conservation of energy.

Although my chairman has disabled my access to the free library, I can see enough from old textbooks online to see that spectrographers, especially, in understanding energy levels, have been ethical, cautious, and fair. For example, Condon and Shortley's book [4] from 1935, which was reprinted in several editions until 1959, includes work of H. N. Russell, not only on the frequencies of spectral lines related to Russell-Saunders coupling, but actual use of extensions of Maxwell's equations to a new context to explain ratios of intensities of the lines.

There is something, tangentially related to this, which I have not mentioned. Schroedinger's paper, at the point where is is about to give the solutions to his equation, says, after describing what are above the values of α and β such that solutions exist,

> Though I cannot enter here upon the exact and rather tiresome proof of the foregoing statements, it may be interesting to describe in rough feature the solution...

If we just identify the basic solutions,

$$\Psi(x, y, z, t) = f_{1,n,l}\ s$$

$$\Psi(x, y, z, t) = A(x, y, z) sin(\frac{h}{2\pi}(S(x, y, z) - tE)$$

for s homogeneous harmonic of degree l. Even if s depends on t, the $f_{1,n,l}s$ have no spatial oscillating behaviour unless $A(x, y, z)$ has cancelling reciprocal oscillations; and $S(x, y, z)$ in the second equation is bounded. Once tE surpasses $S(x, y, z)$ there are no wavefronts. It just can't happen, what Shroedinger wanted, that the wavefront speed is equal to $E/|grad\ S|$.

A standing wave could have moving wavefronts. Putting aside the tangent bundle or differential forms, just trying to revisualize what Schroedinger wanted to see, one could write L for the gradient flow of S, with divergence $div(L)$, and then the Laplacian is

$$\Delta(A\ sin(\frac{2\pi}{h}(S - tE))$$

$$=(\Delta(A) - \frac{4\pi^2}{h^2}div(L)A)\ sin(\frac{2\pi}{h}(S - tE)) + \frac{2\pi}{h}L(A)\ \ cos(\frac{h}{2\pi}(S - tE)).$$

A corresponding and slightly simpler complexified version of the right side is

$$(\Delta(A) - \frac{4\pi^2}{h^2} div(L) + i\frac{2\pi}{h} L(A))Ae^{i\frac{2\pi}{h}(S-tE)}.$$

Schroedinger's equation now generalizes to the notion that the amplitude function alone is an eigenfunction (in the sense of eigenvector) of $\alpha + \beta/r$ (in the sense of eigenvalue) with, α and β as we defined earlier, for the operator

$$\Delta - \frac{4\pi^2}{h^2} div(L) + i\frac{2\pi}{h} L.$$

That is, Schroedinger's equation for the amplitude function A generalizes to

$$(\Delta + i\frac{2\pi}{h} L)A = \frac{4\pi^2}{h^2}(-2mE - 2me^2/r + div(L)) \cdot A.$$

I have called the operator by the name L, as for example it is possible to scale elements of the Lie algebra so_3 by a radial function $g(r)$ to obtain a few examples of such vector fields one might wish to consider. In order to satisfy that the rate of motion of the wavefronts is $E/\sqrt{2m(E-V)}$ since the hypothetical particle speed for just L is wr for some constant w we take $g(r) = \frac{1}{wr}\sqrt{2m(E + e^2/r)}$. This is based on the notion that the hypothetical particle speed times the wavefront speed is equal to E in absolute value.

For type s orbitals, if we take A to be radially symmetrical and L to be such a vector field, then $L(A) = 0$. Also $div(L) = 0$, for example

$$div(gx\frac{\partial}{\partial y} - gy\frac{\partial}{\partial x}) = x\frac{\partial g}{\partial y} - y\frac{\partial g}{\partial x}$$
$$= (\frac{xy}{r} - \frac{yx}{r})dg/dr.$$

Then the equation reduces to the ordinary Schroedinger equation, so for type s orbitals there are cases when there are at least some solutions; those for which the amplitude equation agrees with the one from Schroedinger's unmodified equation; and so there is indeed a type of solution for type s which has the wave front speed which Schroedinger had asked for, although which is not a function.

Such solutions can likely be best viewed as differential forms and the correction to allow moving wavefronts in some cases may make almost no change to how things are calculated. It seems interesting to consider beyond type s orbitals whether the same considerations apply to other orbitals; then, we need not assume that L is an element of so_3 rescaled by a radial function, only.

The existing notion, unlike the explanation of the *intensities* of the Russell-Saunders lines, of the *frequencies* of those lines, does not consider that the wavefronts are moving; it rests on the notion that solutions of Schroedinger's equation include 'inherent angular momentum.'

But, what was the 'inherent angular momentum' supposed to be if the function is, for example, the coordinate function x times the radial function $f_{1,2,1}$ for a type p orbital? How on earth do linear forms on three space have 'intrinsic angular momentum?'

Attempts to explain the known and verified rational ratios among spectral lines, attributed to various coupling schemes, rest not only on a notion of intrinsic spin, but on a notion of intrinsic angular momentum.

I shouldn't have said that science needs to be overseen. It is not here, in the origins of scientific thought, where there is anything unethical. There is weakness, only. Only because things when they are quantified can seem beautiful, and one can wish to capture, for example, the number theoretic structure of the periodic table, or the infinite beauty of atomic spectra.

And it is not at all unethical that, at the very base of all our understanding of such things, are equations which are obviously wrong, which obviously refer to things that can't exist, or for which there is no good evidence that they exist; things which seem to contradict symmetry, contradict good sense; things which will be abandoned the first instant when the next researcher has a believable interpretation.

What is unethical is the marketing of research that sometimes happens, which sounds to me like Churchill's speech – that also well-intentioned – about the 'sunlit uplands.'

I am going to argue a little later that I do regret that there is no natural locally consistent definition of energy. All our understanding of the complexities of these spectra is based on shifting sands, and the early researchers who formulated quantum mechanics wrote that it was their choice to try to build upon a foundation of a consistent notion of something conserved, something which might be called energy.

We do not know, if Physics had been intended differently, whether a notion of such a conserved quantity would have been a part of the theory, whether it would have been an important part.

The fact that in ten minutes someone can look at Schroedinger's equation and see that it does not do what he hoped, and see ways it could have and should have been improved, is not meant to be a startling observation. It is an obvious observation. Every scientist and every researcher knows that the route to an understanding of a scientific phenomenon is a sequence of stepping stones across a stream, where each stone could have been put differently, where what is missing in one aspect of an explanation, needs to be compensated by extra effort in another part.

No scientific researcher has faith in one interpretation, no scientific researcher has more belief in one technique or principle, more than that it is here this moment, a place to try to stand, to peer over that high fence in hopes of catching a glimpse of meaning, a glimpse of understanding of what really is the deserved beauty of scientific observation.

That high fence was built by well-meaning individuals, teachers, parents, and scholars. It too was built with the best intentions. People who hope to enthuse their students, with notions of the wonderful insights which are promised. The higher, brighter, future which they will attain with their newfound understanding.

It should not be surprising that any schoolchild, as soon as he learns a little calcululus, can look at any of the basic equations upon which all his subsequent learning is to be based, and object, 'That does not make sense to me!'

It seems, always, like students are thick, like they are dumb, like they need to be pushed to understand, perhaps.

But, when they are confused, it usually is because they had greater hopes for the amount of insight which the new theories, notations, and practises would be capable of revealing to them. Just as it is said that as a baby grows, the learning which takes place is a neural pruning, as a student learns, much of the learning amounts to learning the ways of thinking which are going to be rejected as being not rigorous, as being too close to superstition, as being low class, and not how things are done.

But never, never does an original researcher like Schroedinger for example ever think that he has answered big questions, with one formulation, with one idea. He is part of a conversation, and it could be a conversation with that student who is discouraged because he does not understand Maths, and truth be told, it probably is exactly that conversation which takes place, with someone not conversant well with the subject, at moments when changes are made to how things are understood. Dirac, for example, claimed that Heisenberg did not know about matrix multiplication in any other way than a method of combining quantum numbers.

Any beginning student, asks himself, but why didn't they ever consider *this* or *this*. And, if a beginning student were ever eloquent enough to pose the question directly to researchers who are trying to formulate a theory, the answer would be 'we *want* to consider that, we only need to know what you were curious about.'

There was nothing unethical about spectrographers wishing to understand spectra; nor were there any harmful consequences either. But this is not to say that a spectrographer is a muse, is someone who can give advice about future policy. Spectrographers still do not understand the first things about the spectrum of Hydrogen. It is as much a mystery as looking at a tree is, and trying to understand the things growing there. Yet, if someone replaces the Hydrogen with another gas, they will see the difference, they will perhaps know what the other gas is, given a list of choices.

Some of the practical consequences of the curiosity of spectrographers is the way their research has flourished over the years, now encompassing nuclear magnetic resonance, and proton spin; making equipment for hospitals, and imaging equipment.

Such research at times has given possibilities not precedented during human evolution, and nuclear research, just like petroleum research, is an area where a person might legitimately understand that if it has not been possible to make particular discoveries, this would have been better and safer.

But, it is not possible to remove the possibility of making some discoveries, only.

My personal belief is that things in medicine like sutures, copy other things in technology like sharpened knives. That there may be a principle to the effect that choices unprecedented during the vast part of human evolution are ones which will lead to disaster if they are chosen. But that this principle has exceptions.

To explain it a way my friend Charles Freeman-Core once explained this to me, attributing his thinking to Kant, once a choice has already been made which transcends what was possible during the vast majority of human evolution, then choosing to disregard that choice is itself another unprecedented choice.

If we already have, for example, waste leaking from a power station, and an incidence of cancer, then it is a mistake to say, let's cut our losses and forego using an NMR to investigate the cancer, in order not to compund the original error.

Then, even a homeopathic principle of medicine could justify things like the use of nmr in diagnosing and locating cancer, and radiotherapy to treat it. The principle that when an action causes disease, sometimes the same type of action, repeated to a different extent, can be used to treat that disease. A very low and safe type of radiation, in the manifestation of an X ray or even a magnetic field, to find the location of cancer; and then a very very high dose of gamma radiation, the same which had caused the cancer, but in a much larger intensity, to cure it.

It is not the researchers who popularize new technologies, who interpret them as a panacea, as is done in every case without exception.

First concepts of the Lamb shift

Currently, with the fine structure corrected as we've done, the universe explorer at `http://spectrograph.uk` gives the wrong value of the Lamb shift for Hydrogen, the wrong sign even for the shift which is the original Lamb shift (though many others seem almost reasonable). Clearly rather than having a correction term in the Schroedinger equation it is better to really find the more natural variant of Schroedinger's equation. That is, rather than abstractly identifying the Weyl operator with the residue of the Legendre operator, we should try to give a holomorphic description of something generalizing harmonic two-forms on Euclidean space which restrict after lifting to the line bundle over real two-dimensional projective space, and Euler contraction to the one-forms on the line bundle over the Severi-Brauer variety.

We are working here with sheaves, not global sections only.

Thus we start with the ordinary projective plane $\mathbb{P}^2$.

Then as in *functorial affinization of Nash's manifold* or elsewhere, there is the exact sequence for any coherent sheaf $\mathcal{F}$

$$\to S^{n-i}\mathcal{F}\otimes\Lambda^i\mathcal{P}(\mathcal{F})/torsion \to S^{n-i+1}\mathcal{F}\otimes\Lambda^{i-1}\mathcal{P}(\mathcal{F})/torsion$$
$$\to ... \to S^n(\mathcal{F})/torsion \to 0$$

which is a resolution of $S^n(\mathcal{F})$. We are going to take the variety to be $\mathbb{P}^2$ and $\mathcal{F} = \mathcal{O}_{\mathbb{P}^2}(1)$.

This gives taking $n = 1$ (and allowing negative exponents as we can since $\mathcal{O}_{\mathbb{P}^2}(1)$ is invertible of course)

$$\begin{aligned} 0 &\to \mathcal{O}_{\mathbb{P}^2}(-2) \otimes \Lambda^3 \mathcal{P}(\mathcal{O}_{\mathbb{P}^2}(1)) \\ &\to \mathcal{O}_{\mathbb{P}^2}(-1) \otimes \Lambda^2 \mathcal{P}(\mathcal{O}_{\mathbb{P}^2}(1)) \\ &\to \mathcal{P}(\mathcal{O}_{\mathbb{P}^2}(1)) \\ &\to \mathcal{O}_{\mathbb{P}^2}(1) \\ &\to 0 \end{aligned}$$

with augmentation kernels in this order,

$$\mathcal{O}_{\mathbb{P}^2}(1) \otimes \Lambda^2 \Omega_{\mathbb{P}^2},\ \mathcal{O}_{\mathbb{P}^2}(1) \otimes \Lambda^1 \Omega_{\mathbb{P}^2},\ \mathcal{O}_{\mathbb{P}^2}(1) \otimes \Lambda^0 \Omega_{\mathbb{P}^2}.$$

Now, what we will do is to let $X \to \mathbb{P}^2$ be the total space of $\mathcal{O}_{\mathbb{P}^2}(-1)$, and let π be the bundle projection, and apply π^*. We get (writing $E \subset X$ for $\mathbb{P}^2$ viewed as the zero section divisor)

$$0 \to \mathcal{O}_X(2E) \otimes \Lambda^3(\Omega_X(logE)(-E)) \to \mathcal{O}_X(E) \otimes \Lambda^2(\Omega_X(logE)(-E))$$

$$\to \Lambda^1 \Omega_X(logE)(-E) \to \mathcal{O}_X(-E) \otimes \Lambda^0(\Omega_X(logE)(-E))) \to 0,$$

and note that the last two terms are only

$$\Omega_X(logE)(-E) \to \mathcal{O}(-E) \to 0.$$

These are subsheaves of the exterior powers of Ω_X, and in fact the maps here are exactly the restrictions of the contraction which we called i_ϵ, the Euler contraction in the direction of the line bundle fibers, the fibers of $X \to P$.

Moreover, the DeRham differential preserves all these subsheaves, and when we write

$$i_\epsilon d + d i_\epsilon = \epsilon - 0$$

now ϵ is invertible, multiplying each term by a nonzero degree, so the maps i_ϵ and d can be viewed as a pair of chain homotopies trivializing the isomorphism ϵ, and proving that the complex is contractible.

Very interestingly, now the sequence of augmentation kernels is

$$\mathcal{O}_X(-E)\otimes\pi^*\Lambda^2\Omega_P,\ \mathcal{O}_X(-E)\otimes\pi^*\Lambda^2\Omega_P,\ \mathcal{O}_X(-E)\otimes\pi^*\Lambda^1\Omega_P,\ \mathcal{O}_X(-E)\otimes\pi^*\Lambda^0\Omega_P.$$

Here these are just the same as the pullbacks of the exterior powers of $\Omega_{\mathbb{P}^2}$, each twisted only by $\mathcal{O}_{\mathbb{P}^2}(1)$ before pulling back.

So we have differential forms of all degrees on the projective plane, all allowed a simple pole on a hyperplane in every coefficient.

Now, an important point is I have nowhere taken any global sections. these are complexes of sheaves, and they are complexes of coherent sheaves except the map d is not a map of coherent sheaves.

But what we have is that $\mathcal{O}_X(E)\otimes\Lambda^2(\Omega_X(logE)(-E))$ which we can also call $\Lambda^2(\Omega_X(logE))(-E)$ is a direct sum according to the decomposition of the isomorphism ϵ into the direct sum

$$di_\epsilon + i_\epsilon d$$

of mutually annihilating operators.

So the local sections of closed forms within that sheaf are all in the image of di_ϵ. And so the local sections of closed forms are deRham differentials of sections of one forms in the image of i_ϵ. So they are deRham differentials of sections of one-forms in the kernel of i_ϵ, that is, in the augmentation kernel, which we already know is

$$\mathcal{O}_X(-E) \otimes \pi^* \Omega_{\mathbb{P}^2}$$

This sheaf (more rigorously its pushdown to $\mathbb{P}^2$) is

$$\Omega_{\mathbb{P}^2}(1) \oplus \Omega_{\mathbb{P}^2}(2) \oplus \Omega_{\mathbb{P}^2}(3) \oplus ......$$

That is, it is $\Omega_{\mathbb{P}^2}$ tensor on $\mathbb{P}^2$ with the direct sum of $\mathcal{O}_{\mathbb{P}^2}(i)$ for $i = 1, 2, 3, 4, ...$

So to get closed 2 forms on X we just apply the deRham differential to these.

So closed 2 forms on X are isomorphic to this sheaf on X modulo its intersection with the kernel of d, which needn't be a coherent kernel.

Now this next part is not done, but I am thinking that this sheaf intersects the kernel of d trivially, just because I haven't been able to find any nonzero sections in the intersection yet.

If that is so, then the closed 2 forms on X which belong to our subsheaf are in fact isomorphic to a coherent holomorphic sheaf after all, it is what I was mentioning before

$$\Omega_{\mathbb{P}^2}(1) \oplus \Omega_{\mathbb{P}^2}(2) \oplus .....$$

When I said that the last 2 terms are only $\Omega_X(logE)(-E) \to \mathcal{O}_X(-E) \to 0$, now it is the global sections of the kernel of this that we are considering, and this is exactly the kernel of the map $\mathcal{O}_X \oplus \mathcal{O}_X \oplus \mathcal{O}_X \to \mathcal{O}_X(-E)$ coming from the fact that three global sections generate the ideal sheaf $\mathcal{O}_X(-E)$.

In fact

$$\pi_*\mathcal{O}_X = \mathcal{O}_{\mathbb{P}^2} \oplus \mathcal{O}_{\mathbb{P}^2}(1) \oplus \mathcal{O}_{\mathbb{P}^2}(2).....$$

and the map is induced by

$$\mathcal{O}_{\mathbb{P}^2} \oplus \mathcal{O}_{\mathbb{P}^2} \oplus \mathcal{O}_{\mathbb{P}^2} \to \mathcal{O}_{\mathbb{P}^2}(1)$$

So on global sections this is exactly the end of the Koszul complex of the ideal $(x, y, z) \subset \mathbb{C}[x, y, z]$, and the 2 forms upon which ϵ acts by $i + 1$ will correspond to polynomials of homogeneous degree i. The dimension of the global sections of the kernel is

$$\begin{aligned} &3\binom{i+2}{2} - \binom{i+3}{2} \\ &= \frac{3}{2}(i^2 + 3i + 2) - \frac{1}{2}(i^2 + 5i + 6) \\ &= i^2 + 2i. \end{aligned}$$

A question about Pauli exclusion

One thing that the detailed tree-like classification does is it clarifies a question whether or not Pauli Exclusion probably should be strengthened a bit, from the standpoint of understanding it in terms of differentials.

For instance, for Magnesium, theoretically there is an electron configuration

$$1s\ 2s\ 2p^4\ 2d\ 3d\ 6p^4$$

although one would never find 'unfilled orbitals' low down like that in nature. But the spectral lines if such a thing existed, according to combinatorial Pauli Exclusion, would consider it to be a tensor product (I hope that the meaning of this abbreviated notation is clear)

$$(1s\ 6p^4\ 2d) \otimes (2s\ 2p^4\ 3d)$$

The issue that would make it be a tensor product is an issue about differentials and rational function fields.

That is, the radial part of the first factor has exponential integrating factor (using units so $\beta = 1$) $e^{-r-4r/36-r/4}$ and the radial part of the second factor has integrating factor $e^{-r/4-4r/4-r/9}$.

Even though the sequences $1, 6, 6, 6, 6, 2$ and $2, 2, 2, 2, 2, 3$ are different,they have the same number of terms, and the sum of reciprocal squares is the same and that means that if I wedge product the radial functions, in a case when the azimuthal functions are the same, I will get zero.

That is, the wedge product of differentials when, it is nonzero this is the usual thing about how different powers of the exponential function are linearly independent over the rational function field in r. Their differentials over r are linearly independent only because the different powers of e^{-r} are.

Pauli exclusion does not rule out spectral lines coming from representations which are summands of the tensor power modulo the exterior power.

But if the explanation of Pauli exclusion is this simple fact about differentials, then the exclusion rule should apply higher up in the tree, and more lines should be pruned away.

This example in the case of Magnesium, of course the javascript will show that the extra lines *are* there.

The actual data will not have them for reasons that the energy level is far above the ionization limit.

I wonder if it is possible to find examples of lines which should be ruled out by the differential forms formulation depending on independence of radial functions, but not by classical Pauli exclusion OR by being above the ionization limit, and which interpretation will be supported by the experimental evidence.

The notion of probability

There is a sense in which I should correct what I said in 'unification of the various coupling schemes.' I had been implicitly understanding things in terms of the decomposition of the solution space, which derives from the decomposition of the Hydrogen solution space with central charge only, as what I think is a basis of $L^2(\mathbb{R}^3)$.

That is to say, there is a type of 'spectral theorem' which is still true when one speaks of eigenfunctions rather than eigenvalues; this gives a natural direct sum decomposition of the vector space span of the basic Hydrogen solutions, into parts indexed indeed by the quantum numbers l and n.

For example, for the case of the radial functions of type s, we might argue like this: the Laplacian in the action on analytic functions of the radius r, is just the conjugate

$$r^{-1} \circ (\frac{d}{dr})^2 \circ r$$

with some adjustment for what we mean by r^{-1} applied to a constant function. Thus the Schroedinger equation for constants α, β

$$\Delta\ f(r) = (\alpha + \beta/r) f(r)$$

can be written if we take $h(r) = rf(r)$ as

$$(\frac{d}{dr})^2 h(r) = (\alpha + \beta/r) h(r).$$

Now, amusingly, the L^2 integral of $f(r)$ as a function on three dimensional space is the integral with respect to the differential form $4\pi r^2 dr$ on the positive real line, and thus under our conjugation the L^2 integral of the differential form coming from a product of two solutions $4\pi r^2 f_1(r) f_2(r) dr$ is just $4\pi h_1(r) h_2(r) dr$. That is, as well as converting the Laplacian into the ordinary second derivative, the conjugation by r converts the L^2 integral on three dimensional space to the L^2 integral on the line times the constant 4π.

Finally one can replace d/dr by a sum $d/dr + \lambda$ by making one further substitution, considering $h(r) = g(r)e^{-\lambda r}$

In this way, the vector space span of the basic Hydrogen solutions for type s is isomorphic to the polynomial solutions of the ordinary differential equation $(d/dr + \lambda)^2 g(r) = (\alpha + \beta/r)g(r)$. This notion leads immediately to the constraints

$$\alpha = \lambda^2$$

$$\beta = 2n\lambda$$

with n the polynomial degree, and whence $\alpha = \frac{\beta^2}{4n^2}$.

The issue now is, why should eigenfunctions for different choices of α, β be orthogonal? Let's just argue roughly here and omit careful checkign. For the functions $h(r)$ this is orthogonality in $L^2(R)$, and one way of understanding this is to write, taking primes to mean the derivative with respect to r

$$0 = \int_0^\infty (h_1'(r)h_2(r))'dr$$

$$= \int_0^\infty h_1''(r)h_2(r)dr + \int_0^\infty h_1'(r)h_2'(r)dr.$$

Subtracting the same equation with h_1 and h_2 interchanged gives

$$\int_0^\infty h_1''(r)h_2(r)dr = \int_0^\infty h_1(r)h_2''(r)dr.$$

Now, using the Schroedinger equation, transformed so that the operator is just the second derivative, if we have

$$h_1''(r) = (\alpha_1 + \beta/r)h_1(r)$$

and

$$h_2''(r) = (\alpha_2 + \beta/r)h_2(r)$$

(note the β should be the same for both h_1 and h_2) then each integral is a sum of two terms, the one involving β equal for both and may be removed, and we have just as for the spectral theorem that the integral is zero unless $\alpha_1 = \alpha_2$.

For the azimuthal parts the argument is easier but rather than describing a Hilbert space basis of $L^2(\mathbb{R}^3)$ one should think that what is being determined is exactly the orthogonal complements of sums of the wave function spaces by orbitals, which are used in the perturbation analysis for the electrostatic effect. In other words, that there was no artificial choice of basis that needed to be made, and no artificial choice of Hilbert space structure that needed to be made.

I have not checked any of these calculations carefully, for instance whether the functions described above really are zero at $r = 0$, nor is this the important point here. Nor whether what we are describing is a Hilbert space structure on $L^2(\mathbb{R}^3)$. It really does seem like it should be possible using the description of each homogeneous polynomial as a sum of homogeneous harmonics times even powers of r, together with the fact that functions of r are in the L^2 closure of the analytic L^2 functions in x, y, z, that any choice of orthonormal bases of the homogeneous harmonic polynomials times all the radial functions indexed by n which can be attached to those of degree l, provide a Hilbert space basis of $L^2(\mathbb{R}^3)$.

The point is, if one relies on such a notion, or relies on the L^2 inner product of such functions, then one can justify what I said in dispensing with any notion that different orbit-orbit coupling schemes should give rise to different calculations of spectra.

Because the orthogonal complements are determined when the electrostatic term is present only with coefficient zero, and that is all that is needed for the perturbation analysis.

But, here is a rather important point: even in cases when there are no repeated term symbols (as is true in every ground state I've seen), and so the space of wave functions in each electron configuration has a direct sum decomposition first by term symbols and then by the fine levels, the *overall* decomposition is of course far from multiplicity-free. The tree-like structure of the coupling scheme can serve to hide this fact.

If one did not think that the L^2 inner product were sacrosanct, then there might well be only a filtration, detrmined by the Aufbau (as arbitrary as *that* is), and no natural splitting of this filtration.

This is precedented in easy algebra for example in Serre's book about representations of finite groups, where he mentions that the *characters* of a finite group comprise a Hilbert space. But the characters only determine an *isotypical* decomposition, and one must think more deeply to obtain an irreducible decomposition.

It seems, in the way that the Clebsch-Gordan rule or its generalizations to other algebraic groups arises, that it arises in cases when one first considers a tensor product of line bundles over a cartesian product (each pulled back via a different projection) and then to get the tensor product of the global sections, one cannot merely restrict the resulting tensor product line bundle to the diagonal, but one must use an infinitesimal neighbourhood of the diagonal. And what is natural then is the *filtration* by infinitesimal neighbourhoods.

If one chooses different coupling schemes, as a way of indexing isomorphism types, in the absence of any sacrosanct choice of any Hilbert space structure, then legitimately they might describe other subspaces than the ones which can be obtained by combining the Aufbau filtration with the result of repeated orthogonal complements. And in that case, it is not true that the coupling schemes are unified.

Now, people often interpret the meaning of an absolute L^2 norm as related to probability.

In familiar games, one can speak of absolute probability. If I tell you that at a carnival, there are three gambling machines, each with a fixed rate of payoff, say each of which may or may not produce a 100 pound prize, and if I tell you the rate of payoff of the possible machines, but not which is which, then each time you pull a lever and record whether you have won or lost, the probability of winning for each machine changes.

There is a very clear uniformity to the information which I've given to you, and the information which I've withheld. You can imagine a different possible world for each permutation of the gambling machines, and rightfully assign each possible world equal probability with the others at the outset, and with each new result, a win or failure to win, you can adjust the probabilities of the possible worlds, so that the sum over all permutations adds to one.

But the person who has set up this set of possible worlds is me, the carnival organizer, if I've (truthfully and known truthfully etc) told you about the probabilities but withheld telling you which machine is which.

When you are dealing not with a carnival organizer, but with nature itself, there is a question whether it ever made sense to speak of 'absolute' probabilites. If it is the case that different coupling schemes really need to be understood as giving rise to different calculations of spectral lines, we have to begin to question whether there will ever be an absolute notion of probability in nature.

Concluding remark

To end on a somewhat more optimistic note, having understood Schroedinger's paper, at least the first part of it, I really am enthusiastic for the interpretation he has taken for wave functions. Yet also, now understanding this too for the first time, the Hamiltonian approach to physics seems deeply insightful. Yet it is not connected with Schroedinger's idea; although he said it is known it is not.

Without an understanding of relativity it may be impossible to connect Schroedinger's wave idea with Hamilton's idea. But there are inklings that if they can be connected, paradoxes like electron spin, half-integral azimuthal quantum numbers, the Bohm-Aharanov effect, and indeed the difference between elelectricity and magnetism, will all be simply explained together.

What would be needed is that the form $\eta\omega$ should not be closed – in cases when it is closed the Hamiltonian theory degenerates – but it would be closed along paths and since it is a form on the tangent bundle these are paths in the tangent bundle – it is a section of the pullback of forms from M but should not be a pullback of one form. And by contrast, its Lie derivative which is not anything like a pullback of a one form from M does need to be closed. Schroedinger imagined that $\eta\omega$ is closed, and the fact its Lie derivative is closed would have followed from that. To say that it should be closed when the right form $\eta\omega$ is found is to say that one has some faith that Hamiltonian functions should exist somewhere.

The necessary hypotheses of such a hope, of a natural torsion free connection, on the configuration space M, whose associated involutive vector field sends a natural appropriately nondegenerate – and therefore non-closed – section of the pullback of one-forms on M to a closed one-form on the tangent bundle, may not be understood together any other way except relativistically.

The false fine structure

Here is the issue: let's go back for a moment to the more classical understanding of 'spin' in which we just replicate our space of wave functions; so we consider the artificially excited configuration $2p2$ for Helium as a fifteen dimensional space of wave functions which we consider to be merely the exterior square of a direct sum of two three dimensional representations.

Now, the electrostatic perturbation has a multipole expansion in which, not surprisingly, the dipole term is dominant, other terms insignificant. And it is surely rotationally symmetric. Yet it is not actually true that the Casimir for space rotations commutes with this perturbation matrix, as we have calculated it explicitly above.

The problem can be seen if we focus on the nine dimensional space of wave functions which would be called those for which the electrons have 'opposite spin;' it is the tensor product of the two basic representations within the exterior algebra on the direct sum.

In this section we are not considering the action on ‘spin’ coordinates so there is no harm going ahead and considering the basic one forms, and writing our nine dimensional space as a space of one-forms on the Severi-Brauer variety; and in the complexification the basis is

$$f_{2,2,1}v^2du\wedge f_{2,2,1}v^2dv,\ f_{2,2,1}v^2du\wedge f_{2,2,1}uvdv,\ f_{2,2,1}v^2du\wedge f_{2,2,1}u^2dv$$

$$f_{2,2,1}uvdu\wedge f_{2,2,1}v^2dv,\ f_{2,2,1}uvdu\wedge f_{2,2,1}uvdv,\ f_{2,2,1}uvdu\wedge f_{2,2,1}u^2dv$$

$$f_{2,2,1}u^2du\wedge f_{2,2,1}v^2dv,\ f_{2,2,1}u^2du\wedge f_{2,2,1}uvdv,\ f_{2,2,1}u^2du\wedge f_{2,2,1}u^2dv$$

with the wedge product considered not to commute with u or v (eventually to be viewed as differentials themselves).

The operator $v\partial/\partial u$ annihilates the left factor of each of the first three terms, so the action on the first three terms is caused by the second factor; the third goes to twice the second, the second to the first.

The inner product here is no different than for the tensor product (there is no ‘exchange’ term since du and dv are unequal), and when one integrates the multipole expansion one sees that the dipole perturbation of each of the first three terms projects by zero to the other two, while the self-projections act in the number-theoretic ratio [158 : 149 : 158].

The lowering operator simply does not commute with the dominant dipole term in the electrostatic perturbation action.

If it does not commute with even one lowering operator, it is not going to commute with the rotational Casimir, and it is not rotationally symmetric.

What can cause this apparent paradox, whereby a rotationally symmetric Hilbert space structure has a symmetry which can be broken by just taking a tensor square?

The answer is that there are as we mentioned two different notions of angle in ordinary Euclidean space. One is that we resolve the ordinary double point singularity in the hypersurface $x^2 + y^2 + z^2 = r^2$, and then choose a real rational point of the exceptional divisor.

And a second totally different concept of angle is that we look within the complex exceptional divisor, abstractly isomorphic to $\mathbb{P}^1 \times \mathbb{P}^1$ at the branching locus, a Severi-Brauer variety whose moduli of irreducible coherent sheaves form a real projective plane, topologically, whose universal (double) cover is a Riemann sphere which is the diagonal complex variety within $\mathbb{P}^1 \times \mathbb{P}^1$.

We have drawn diagrams containing both spheres, both concepts of angle simultaneously. But the point is, the failure of rotational symmetry in the Hilbert space structure is not related to the fact that we are considering perturbations – it is not related to a notion that rotational symmetry fails to imply differential rotational symmetry. Rather, it is caused because there is a sense in which the Hilbert space structure never was rotationally symmetric from the start.

When I have said that it was, I was speaking only approximately, and the result is that even before we make any change which should have created the fine structure, there has been a false fine structure, and the actual spectrum (in the sense of eigenvalues) is affected by this. So really what we calculate is “fine+error,” and also we can calculate “error” by using the classical calculation (and without any Casimir term either), and when we use fine correction in the Explorer, what we really calculate is (fine+error) - error. But the two notions of error are not really the same, and, just as our correction to the coarse structure only hints at an understanding which does not make artificial use of reciprocal sums of squares, this, our final correction to the fine structure only hints at a comprehension of ordinary angles in Euclidean space which does not confound the two interpretations.

Electron spin and Pauli exclusion

In the case of both ‘spin’ and ‘exclusion,’ the intuition which the familiar names sometimes connote is that an electron is a ball, such as a ball in a sports game, and it might be spinning; and that somehow these balls cannot occupy the same space when you put them away on the shelf.

There is nothing wrong with thinking like this, except it is dangerous if it gives a person confidence that they can understand the way ideas change or generalize in a similar manner.

I like the way that the formulism works nowadays, that people write down a potential function, say ‘this is the Hamiltonian,’ and then there is a sort of dogma that where the Hamiltonian has p_x you write $\partial/\partial x$, and transport yourself into a different world by a sort of analogy.

And to have analogies for understanding ‘spin’ and ‘exclusion’ etc. And it is maybe appealling to have discussions like a footnote in Atkins chemistry book, speaking of the relativistic correction, as if one is standing upon the nucleus and watching the electron orbiting, and applying a relativistic correction.

The notion of a relativistic ‘correction’ is an interesting notion too. The notion that relativity means everything is sort of right in a classical limit, but not quite right, and we have to correct things to explain why propogatin of electromagnetic radiation is ‘always at a constant speed.’

But, one has to understand that all this type of thinking is dangerous too. It is saying, as long as you follow the dogma, you can be *completely sure* that your conclusions will be right.

And, here is where I should mention Becky Sloan and Joseph Pelling’s video ‘Don’t hug me I’m scared.’ The notepad character says “Come one! Take another look!” and leads the other characters to think creatively in one way, “I can see a cat, I can see a hat,...”

The notion of standing on the nucleus of an atom and imagining what you might see is creative, and it is along the lines of admired creative thinking of earlier physicists, or earlier explorers, adventurers, exploring the sea for new continents, or fictional heroes exploring space as in Star Trek for ‘new life, new civilizations.’

The notion is as if to say, ‘this is where we will be, right there on the nucleus, standing there.’ It is like the film ‘Honey, I shrunk the kids,’ or countless fictions, Gulliver’s travels, for example.

And that it is admirable to say ‘If we can’t physically do it, we can imagine it, there are no limits to where our imagination takes us.’

But one has to understand that one is following one's own wish to combine ideas, in a way that yes has worked for humans throughout our existence.

I have written before about how an animal rights scholar, some time ago, had written about the experiences of a sow in captivity, that when it is about to give birth, it uses its snout to push along the concrete, as if it were building a nest. That, if the natural plants that had been there during the significant part of the creature's evolution had gone extinct, we could see what they should have been, by the animal's behaviour. That it is unintentionally drawing for us a painting of nature which no longer exists.

When human thought is disconnected from nature as it now is, then in looking at how people interpret chemical spectra and chemical reactions, at the things which they write on their blackboards, one sees not anything related to the phenomena they see in front of them, but things with more depth, more detail.

Yet, this depth is clearly connected to things that no longer exist in the abstract context in which the person is thinking. The confidence that our imagination will take us to a new and wonderful place when we think creatively, has become a dogmatic concept, not because anyone has been evil, but because of false hope.

It was not the right conclusion

Now having thought about this for a few hours, the conclusion seems very naive.

Having explained the spectrum of Hydrogen by the notion of energy levels – that the frequencies in the spectrum are differences of frequencies corresponding to fixed energy levels – there was maybe some elation, some wish to generalize the success further. Some infectious enthusiasm, perhaps.

I had forgotten some of my own papers, where I'd realized that this type of thing does happen, for polynomial vector fields in the plane, as Poincare had asked. But the reason why it did happen was essentially a grungy reason. And not what will happen in general.

The whole point of Chaos theory had been to show that general dynamical systems can never in any way fall into energy levels like that. And, the hope for a Hamiltonian, of course, was two-pronged. On the one hand was the notion that a single closed one-form, when it is locally a differential of a function H, then however one may write a particular associated one form as $\sum p_i d' q_i$ the ordinary, as it were Euclidean, partial derivatives of H with respect to the q_i determine everything that happens. And so one form and function do also. But a second aspect of it, which I'd not been paying attention to, is that the orbits locally preserve level sets of H.

But, really, very honestly, one has to ask whether any enthusiasm for such a phenomenon was a disguised reflection of a residue of hope for the notion that there is such a phenomenon in nature as 'conservation of energy,' or a consistent notion of 'energy.'

If one thinks about it, such a notion would be an attempt to continue to capitalize on the success of finding that the spectrum of Hydrogen had been explained by 'energy levels.' The source of these comes down to two things, that we are describing things by polynomials, and polynomials have degrees l, and secondly that the ordinary differential equation $xy'' + (2+2l)y' - Ayx - By = 0$ for y as a function of x has particular entire solutions. But, for example, the notion that we describe things by polynomials and polynomials have degrees, comes down to multilinear algebra, and this to a belief in a Euclidean structure. Perhaps if we anyway have accepted manifolds, we should accept a local Euclidean structure in this precise sense.

The fact that different atoms of Hydrogen have the same energy levels would be because we'd assumed the same constants (which played the role of the mass, charge of the electron, etc), and the three-dimensional differential equation from which this ordinary differential equation arises is applied as though space has Euclidean translations, etc.

Then the hope for a local Hamiltonian would be a hope that energy levels make sense locally without any contradiction.

One of the things which I didn't mention is another hope which people have, that the form $\eta\omega$ would be the 'canonical' form on a cotangent bundle, somehow, by some transformation of thought. That is, that there is some notion of relativity that gives rise to a canonical local consistency of energy levels.

But if one really is honest about the source for such a hope, it is a hope to continue the success of finding that the spectrum of hydrogen had been explained as differences of a quantity that takes fewer, simpler values and in that sense can be seen as more intrinsic, and which agrees with conservation of energy in Newtonian physics.

By the way, regarding the closed form ω, we know it cannot be in general an exact form. Results of chaos theory prove that it is impossible, and of course this is just the same old notion that classical integrals do not in general exist at all.

It may easily be possible to prove using methods like Sard's theorem that there is always a locally consistent definition of energy. But that is different from saying that there is a canonical locally consistent definition of energy.

What I really have to question is why I was said I 'hope' for such a thing.

One reason is that I had thought of the local Hamiltonian as like a nice new computer, something that will do work for me, or maybe for people in the future, in helping me understand the action of nature, and to calculate what will happen in any situation. Surely, like the magic bag of Felix the Cat cartoons, this would be a nice thing.

Yet, at the time radiation was being discovered, people loved the idea so much that they put radioactive materials into their food, into their cosmetics, into their toys. They believed that since electromagnetic radiation is a generalization of sunlight, it may have all the health giving properties of sunlight.

Even after Madame Curie had ruined her health, and generations of scientists had died terrible deaths from cancer, there was a notion that there is a consistent physics that will explain the future to us, that there is something called electromagnetic radiation.

In the popular mind there is a mistaken connection between the work of physicists like Schroedinger, and of those like Madame Curie; she discovered by trial and error what was interpreted as lots of energy stored in atoms, and the concept does make sense certainly, locally. Perhaps the vast range of orders of magnitude, from such tiny differences of energy as changes in the values of l create, to the vast differences that Curie's work and others brought about on a larger scale, made it convincing that there should be a Euclidean scale of values from the very large to the very small, a consistent ruler or thermometer, against which all things can be measured.

For me to have concluded that such a scale, even locally, depends on relativistic notions, really is also, though unintentionally, a political statement. Because, relativistic notions, when they are analyzed, become notions of agreement. This is not agreement in the sense of diplomacy, only, but agreement of ideas, when considered from different perspectives, and by different conscious entities.

Links:

Northern Lights http://spectrograph.uk/index.html?pmult=1.5&allowForbidden=true&panLeft=160&scal
They represent transitions between even functions,

The green Magnesium star triplet. Press ‘next config’ a few times after the calculation is definitely done, waiting each time, to see the yellow one. http://spectrograph.uk/index.html?panLeft=160&scaleWidth=4&p
Both are reversed because the p orbital is more than half full.

The familiar bright yellow Sodium Doublethttp://spectrograph.uk/index.html?autocorrect.

the Carbon spectrum, perhaps reminiscent of fire, http://spectrograph.uk/index.html?pan

The variables in the url such as panLeftSpeed or scaleWidth refer to the spectrograph display, and can be changed with the arrow keys.

And the unadorned explorer http://spectrograph.uk.

The arrow keys are for looking closer, and ‘compare external’ compares with what is actually found in nature.

References.

1. Alex Freire, Spherical harmonics and homogeneous harmonic polynomials (8 pages)

2. E. Schroedinger, An undulatory theory of the mechanics of atoms and molecules, the Physical Review 28, 1049-1070

3. Helene Esnault and Eckard Viehweg, Notes on vanishing theorems, Birkhauser-Verlag (with permission to be shown on the web).

4. E. U. Condon, G. H. Shortley, The theory of Atomic Spectra, 1935 - 1959

5. M. Geller, E. W. Ng, A table of integrals of the exponential integral, Journal of research of the National Bureau of Standards B, vol 73 B (1969)