List of Computational Physics Projects for Senior Sophister Theoretical Physics Students
Michaelmas Term 2012

1 Transport properties of Magnetic Nanowire Networks

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Thin films composed of nanowire networks have their transport properties regulated by the junctions formed between neighbouring wires. Experimental measurements show very intriguing behaviour in the way these materials conduct electricity and there is now a growing interest in understanding how these materials behave when the nanowires are modified, in particular, when the wires become magnetic. The goal of the present project is to develop simple theoretical models capable of describing the transport properties of such networks. The project is divided in two separate yet complementary parts: one involving the development of a macroscopic model and another which consists of the microscopic details of the charge transport in magnetic disordered media.

2 The dynamics of the dipping bird

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The dipping bird is a toy which, based on thermodynamic and mechanic principles, displays cyclic motion which may last for days. This project concerns the development of the simplest form of equations which qualitatively describe the key aspects of the bird's motion. Furthermore it will be investigated how this motion could be rendered chaotic.

Guemez et al., *Experiments with the drinking bird,*
Am. J. Phys. 71, 1257-1263 (2003)
Lorentz R, *Finite-time thermodynamics of an instrumented drinking bird toy,*
Am. J. Phys. 74, 677-682 (2006)

3 Static and time-dependent theory for electron-spin correlated systems

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One of the possible models for describing magnetism is the so-called s-d model [1], where conducting electrons, s, couples to localized spins, d, by means of a local Heisenberg-type interaction. If the local spins are treated at the quantum level the problem becomes many-body in nature. In this case the Hilbert space of the problem grows exponentially with the number of electrons and only small systems are tractable. In this project we will first construct an exact solution for such a many-body problem and then we will look at two particular aspects:
1. Time-dependent simulations: one student will extend the method to the time domain by essentially solving the Liouville equation for the density matrix in real time [2]. Results will be then compared with approximated solutions taking into account a single particle expansion for the electronic degrees of freedom.
2. Construction of a density functional theory: the second student will construct, by reverse potential engineering, a lattice density functional theory [3] for the s-d model. This will allow us calculations of ground-state properties of the same system at a much smaller computational cost, but at an equal high level of accuracy.

[1] A. Hurley, N. Baadji and S. Sanvito, Phys. Rev. B 84, 035427 (2011).
[2] A. Pertsova, M. Stamenova and S. Sanvito, Phys. Rev. B 84, 155436 (2011).
[3] K. Schönhammer, O. Gunnarsson and R.M. Noack, Phys. Rev. B 52, 2504 (1995).

4 Controlling quantum-dot excitons with light pulses

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Quantum dots are discrete quantum systems - "artificial atoms" - formed from islands of reduced bandgap in a semiconductor. They allow us to study the dynamics of a simple quantum-mechanical system inside a solid, and are leading candidates for implementing quantum devices such as single-photon sources. A key requirement is the ability to precisely prepare a quantum dot in a particular quantum state, which can in principle be done by exciting them with specially shaped laser pulses. In this project you will use Matlab and the Chebfun package (http://www2.maths.ox.ac.uk/chebfun/) to develop a simulation of a quantum dot excited with a laser pulse, and use this to try to identify the most accurate and reliable control schemes.

5 Electron scattering by surfaces and interfaces

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Electrons are inelastically scattered by elementary excitations in matter such as phonons. Vibrations at semiconductor surfaces are observed using electron energy loss spectroscopy (EELS) [1]. In this technique, a monoenergetic beam of electrons is scattered from a surface and phonon quanta are found by measuring energies of inelastically scattered electrons. The theory of EELS was originally developed for scattering by a vacuum-surface interface by Evans and Mills [2]. This project will be to extend the theory of Evans and Mills to include scattering at the interface between an oxide insulator and a semiconductor. It will require derivation of the equations by Evans and Mills and extension to a metal/oxide/semiconductor system. Applications of the project include electron scattering in the channels of transistors which have high-k oxide gates.

[1] *Validity of the HREELS surface dipole selection rule at semiconductor surfaces*, C. H. Patterson EPL **98**, 66001 (2012).
[2] E. Evans and D. L. Mills, Phys. Rev. B **5**, 4126 (1972) 4126.

6 Simulation of nanoscale mechanics

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In this project, we will solve nonlinear mechanics problems related to the fabrication of nanostructures used for semiconductor, storage and nanomedicine applications. Finite element analysis (FEA) is a numerical technique to solve partial differential equations including time-dependent solutions to continuum mechanics problems. FE models of nanoscale deformation processes in polymer glasses will be built and tested and compared to experimental results.

7 Contact number distribution of jammed packings

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Disordered packings of spheres have been used as model systems of amorphous matter such as glasses, granular media and foams. These systems can be characterized by their contact number distribution which depends on the polydispersity of the spheres. While the average contact number of the spheres in the packing is known from mechanical constraints, their distribution is not. Recently, a granocentric model has been proposed to explain the shape of the contact number distribution of polydisperse packings at the random close packing (RCP) density. In this project you will investigate whether this model can be extended and suitably modified to packings above the RCP density. In this project you will create simulated packings at different densities and study their contact number distribution. The results are compared with a suitably modified granocentric model.