Quantum Interference and Out-of-Equilibrium Effects in Nano-interferometers

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The Aharonov-Bohm interferometer provides a probe to study coherent properties of electrons in nano-scale electron devices. Coherent electron transport has been investigated in an Aharonov-Bohm interferometer consisting of two quantum dots. For nonequilibrium situations, three coherent contributions to the current in the interferometer are identified as
(i) a transport current,
(ii) a persistent current by Aharonov-Bohm flux, and
(iii) a magnetic polarization current due to quantum interference effects.

We discuss the characteristics of the currents in the case where one dot is in the Kondo regime and the other dot is in the non-Kondo regime.
How important is the *kink* in the angle resolved photo-emission spectra of high Tc superconductors?

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Recently high resolution angle resolved photo-emission experiments reveal a *kink* in the electron energy dispersion spectrum in a number of hole-doped high Tc materials. This special feature is reproduced now by several groups. In conventional metal physics the *kink* occurs due to renormalisation of energy of the quasi-particles involving the electron-phonon interaction. In this talk we shall analyse and identify carefully the relevant low energy scales concerning the origin of the *kink*. This may help to understand the correct microscopic mechanism in high Tc materials.
Spin-resolved correlation kinetic energy of the spin-polarised electron gas, for applications in spintronics

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Detailed modelling of spintronic devices will require tractable descriptions of spin current response in inhomogenous systems. Spin current density functional theory is a promising approach, but, as expounded by Vignale and coworkers, this theory brings some novel difficulties requiring new inputs from the spin-polarised uniform electron gas. This paper will describe an approximate calculation of the required spin-resolved kinetic correlation energy components.
Compressibility and Mesoscopic Transport: an Odd Couple

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Many phenomena related to mesoscopic transport have been popularly explained, in simple terms, as purely one-electron processes. In reality, transport in a "mesoscopic" electron gas presents all sorts of many-body problems which defy naive single-electron explanations. In a most dramatic way, this is shown by the central role of the compressibility - a collective electronic property - in the excess current noise of a quantum point contact driven at high currents. That the compressibility (a static, equilibrium object) should couple to current correlations (a highly dynamic, nonequilibrium object), so intimately as to dictate their spectral form, seems very odd. Their relationship is, in fact, the consummation of a fundamental conservation law: gauge invariance. We discuss this.
Maximizing the Hilbert space for a finite number of distinguishable quantum states

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We consider a quantum system with a finite number of distinguishable quantum states, which may be partitioned freely by a number of quantum particles, assumed to be maximally entangled. We show that if we partition the system into a number of qudits, then the Hilbert space dimension is maximized when each quantum particle is allowed to represent a qudit of order $e$. We find that the dimensionality of an entangled system, constrained by the total number quantum states, partitioned into qutrits will always exceed the dimensionality when partitioned into qubits or a combination of qubits and qutrits. We then show that if we relax the requirement of partitioning the system into qudits, but instead let the particles exist in any given state, that the Hilbert space dimension is greatly increased.
Bilayer Quantum Hall Systems from spontaneously broken symmetries to superfluidity

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This talk will review the unusual properties of bilayer quantum Hall systems, and discuss recent experimental results on bilayer coherent states in double layer two-dimensional hole systems.

Bilayer quantum Hall systems consist of a pair of two dimensional systems separated by a distance \( d \) that is comparable to the interparticle spacing within each layer. In the presence of a strong magnetic field the interplay of interlayer and intralayer correlations, spin, tunnelling and density imbalance combine to produce a rich variety of physical phenomena that have no counterpart in single layer systems. One of the most striking examples occurs at total filling factor \( \nu = 1 \): At large layer separations there is no quantum Hall effect, as each layer forms a compressible state with filling factor \( \nu = \frac{1}{2} \). However at small layer separations spontaneous phase coherence develops between the two layers, so that the ground state can be regarded as an easy plane pseudospin ferromagnet, as a condensate of electrons in one layer and holes in the Landau level of the other layer, or as a superfluid of Chern-Simons composite bosons. The close similarity between the composite boson theory and that of a Josephson junction has even led to suggestions that these systems should exhibit a dc Josephson effect – i.e. that persistent currents can flow between the layers in the absence of an interlayer bias.

I will summarise the experimental evidence which strongly points towards the existence of such a bilayer coherent state, and discuss recent results which examine the evolution of this state as the densities in the two layers are unbalanced.
The role of inhomogeneity in the exact diagonalization solution of the single band Hubbard Model has recently been investigated for finite linear cluster systems consisting of non-magnetic (N) and magnetic (M) atoms [1]. The inhomogeneity leads to magnetic induction (i.e., spin-polarization) of the N-type sites. Separation of the ground state spin-correlation profiles occur due to variations in the local chemical potential, finite size effects and the linear geometry of the system. The induction mechanism is an energy minimization process, which is used to tune the local magnetic properties. Comparison with homogeneous and inhomogeneous magnetic and non-magnetic structures gives additional understanding to the role of inhomogeneity in the mixed Hubbard system. The potential application of this model in finite system device design will also be explored. In particular, a progressive spin-switching device, of type NNMMMN, will be introduced. This device is an extension to the previous proposal of the NMMMMM spin-switching system [2].

A theory for a site-disordered system of spins is constructed as a means of determining the low-dimensional behaviour of glassy structures. The goal of this work is to develop a theory capable of describing competing interactions in dipolar coupled spin systems and clustered metal alloys. In this theory, a wide range of functional forms may be used to model interactions between the spins. This allows for analysis of long range interactions, which introduce a simple means of examining dimensionality effects. Preliminary results showing spin glass transitions will be discussed using model interactions in two and three dimensions.
The decay of a metastable state is quite often initiated by formation of a `bubble' or 'droplet' of the more stable state. An example being a super-cooled vapour, where a droplet of critical size must form before condensation proceeds. The 'bubble' is generally an intermediate state providing the lowest energy barrier a system must pass over to access an energetically more favourable state. This concept is widely known as nucleation, and is used in a range of fields from condensed matter to cosmology. The present discussion will focus on recent theoretical models used to describe the reversal of magnetic dipole moments in ferromagnetic wires with diameters in the nanometer range. Magnetic nanowires are currently of intense interest due to advancements in fabrication, their possible use as sensors and for magnetic data storage, as well as providing a low dimensional system in which to study magnetization dynamics and reversal. In both experimental observations, and the proposed theory, nucleation of reversed regions or domains is shown to provide the key for reversal to take place. In particular domain wall configurations are used in a statistical theory to calculate the rate at which a magnetic nanowire reverses due to thermal activation. Research done at The University of Western Australia in this area is centered on describing nucleation at defect sites such as interfaces and point defects.
Temperature dependence of polaronic transport through single molecules and quantum dots

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Motivated by recent experiments on electric transport through single molecules and quantum dots, we investigate a model for transport that allows for significant coupling between the electrons and a boson mode isolated on the molecule or dot. We focus our attention on the temperature dependent properties of the transport. In the Holstein picture for polaronic transport in molecular crystals the temperature dependence of the conductivity exhibits a crossover from coherent (band) to incoherent (hopping) transport. Here, the temperature dependence of the differential conductance on resonance does not show such a crossover, but is mostly determined by the lifetime of the resonant level on the molecule or dot.
We investigate phase coherent weak localisation effects in high quality two dimensional (2D) hole systems, and show how the values of phase coherence time extracted from the raw data depends critically on the method used to fit the weak localisation correction to the magneto-conductivity. We compare four different methods commonly used in the literature and discuss the differences and relative merits of each of them.

All four methods are then used to fit magneto-conductivity data from high quality 2D GaAs hole systems over a range of carrier densities and temperatures. We compare the extracted phase coherence time, $\tau_\phi$, to the phase breaking rate expected from Fermi liquid theory and show that the method of Dmitriev et al.\(^1\) (the most sophisticated method, used for the first time here) is in good quantitative agreement with Fermi liquid theory despite the presence of strong hole-hole interactions, $r_s$~20.

Enhancement of the electron electric dipole moment in Gadolinium garnets

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Effects caused by the electron electric dipole moment (EDM) in Gadolinium garnets are considered. Experimental studies of these effects could improve current upper limit on the electron EDM by several orders of magnitude.
We suggest a consistent theoretical model and perform calculation of the voltage across a garnet sample induced due to the electron EDM as a response to applied magnetic field.
Two-Parameter Scaling near the Metal-Insulator Bifurcation in Two-Dimensions

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We consider a two-parameter scaling picture for the resistivity of two-dimensional weakly disordered interacting electron systems at low temperature with the aim of describing both the vicinity of the bifurcation and the low resistance metallic regime in the same framework. We contrast the essential features of one-component and two-component scaling theories. We discuss why the conventional lowest order renormalization group equations do not show a bifurcation in two dimensions, and a semi-empirical extension is proposed which does lead to bifurcation. A fit to published experimental data for the resistance of silicon near the bifurcation yields estimates of parameters, including the critical exponent $z_u$. Implications of the proposed scaling for a possible quantum critical point in the ground state limit are considered.
Structural Properties of Transition-Metal@Si\(_n\) (n=14-16) Atomic Clusters

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Structure has a central role in cluster science and is a prerequisite for elucidating many of the properties of clusters. As a consequence, much experimental and theoretical effort has been expended in order to characterize cluster structures. The properties of fullerens can be rationalised by the topological properties of buckyball-cages and chemical properties of C. Attempts to explain the stability of the newly discovered endohedral Si clusters have led to the formulation of the "octet rule" and the "effective atomic number" principle. While both explain the stability of the Group VI metals encapsulated in a Si\(_{12}\) cage, they fail to explain the stability of the tetrahedral Ti@Si\(_{16}\) cluster and, possibly, other endohedral Si clusters. In this talk we will demonstrate that the most energetically stable M@Si\(_n\) clusters (n = 12, 14, 15, and 16) for Group IV elements are conformally limited to the so-called Frank-Kasper (FK) 14, 15 and 16 structures. By exploring the FK configuration space we have also found that the rearrangement of a M@Si FK-type cluster – by attachment of additional Si atoms - transforms the cluster to another FK-type cluster. The latter shows the preferential growth mode for the M@Si\(_n\) clusters and indicates on the strong magic behaviour of the FK cluster topologies.
Calculation of the electronic band structure, electronic density and total density of state of paraelectric and ferroelectric BaTiO$_3$

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The electronic structure, total density of states (DOS) and electronic density in paraelectric cubic crystal and ferroelectric tetragonal crystal of BaTiO$_3$ are studied using full potential–linearized augmented plane wave (FP-LAPW) method in the framework of the density functional theory (DFT) with the generalized gradient approximation (GGA) by WIEN2k package. The results show a direct band gap of 1.8eV at the Γ point in the Brillouin zone and indirect gap of 2.3eV for the tetragonal phase. The calculated band structure and density of state of BaTiO$_3$ in both phases are in good agreement with previous theoretical and experimental results. The nature of the chemical bonds and the measure of the hybridization is also discussed through the calculations of the electron density distribution which indicates the ionic nature of the bond between Ba and TiO$_3$ and the covalent nature of the bond between Ti and O. The calculation of the optical properties are in progress.

4. P Blaha, K Schwarz, WIEN2k, Vienna University of Technology, Austria(2002).
Hartree-Fock simulations of 2D quantum dots

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We perform unrestricted Hartree-Fock simulations of 2D quantum dots of various shapes, with up to 80 electrons and with 0.8<r_s<1.3. The spins of the electrons are fully accounted for. We obtain the statistics of the conductance peak spacings and the ground state spins. A good agreement with experimental data is observed.
Precipitation hardening of alloys is carried out by the addition of small amounts of solute element to the pure metal. With increasing computational power, atomic scale effects can now be better simulated to determine the nature of the hardening mechanism. Density functional theory computations have been used to study the optimal geometry of very small size clusters in aluminium with initial convergence conditions tested by determination of binding energies for a variety of super cell sizes of the aluminium host crystal. These are compared with total energy calculations for small size precipitates of noble metals with fixed geometry. Comparisons are also reported between Kohn-Sham eigenvalues interpreted as excitation energies in density-functional theory and previous empirical pseudopotential work. Extensions using the GW approximation for the electronic self-energy are indicated which help improve the accuracy of quantitative band-structure calculations.
Detection of qubit states by a non-ideal quantum point contact

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Most proposals for quantum measurements of states of quantum systems using various devices are idealised. That is, the uncertainty in the conditioned state of the quantum system is due purely to the stochastic nature of the quantum processes. However in a real laboratory the measurements cannot be perfect due to practical devices and circuits. The models using ideal devices are not necessarily sufficient for describing the detection information of the states of the quantum systems. We present a model for detection of the states of a coupled quantum dots by a quantum point contact that includes the extension to a non-ideal measurement device case using an equivalent circuit.

We derive a realistic quantum trajectory that describes the stochastic evolution of the state of the system of the qubit and the measuring device. We calculate the noise power spectrum of tunnelling events in an ideal and a non-ideal quantum point contact measurement respectively. The influence of the non-ideal components on the noise spectrum is analysed by comparing the spectra of two cases. We found that, for the strong inter-dot coupling case it is difficult to obtain information of the quantum processes in the qubit by measurements using a non-ideal quantum point contact. The noise spectra can also be used to estimate the limits of applicability of the ideal model.
Coupled Plasmon-Phonon Modes in a Two-Dimensional Electron Gas in Presence of Spin Orbit Interaction

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A theoretical study of the collective excitation is presented for a two-dimensional electron gas in the presence of spin orbit (SO) interaction induced by Rashba effect. It is found that in such a system, coupled plasmon-phonon excitation can be achieved via intra- and inter-SO electronic transitions. As a result, six branches of the coupled plasmon-phonon oscillations can be observed. The interesting features of these coupled plasmon-phonon modes are examined.