

## **Coherence and Correlation in Electronic Nanostructures**

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We are studying quantum interference (coherence) and electron-electron interaction (correlations) over a wide range of spatial scales, from nm to  $\mu\text{m}$ . The interplay of correlations and coherence is one of the deepest topics in current chemistry and physics – it plays a critical role, for instance, in the 2D metal-insulator transition, interaction corrections in mesoscopic systems, and efforts towards molecular electronics. Nanostructures provide a novel controlled environment for studying these effects: both interactions and interference can be manipulated by changing the size and shape of the nanostructure, thereby directly gaining information on their interplay.

Results have been obtained in five areas [1] to date:

### **1. Spin and Conductance Peak-Spacing Distributions in Isolated and Realistic Quantum Dots: A Density-Functional Theory Study**

*[with Hong Jiang (student) and Denis Ullmo (visiting professor)]*

A semiconductor quantum dot – a nanodevice in which electron motion is quantized in all three directions – is a particularly simple system in which to study coherence/interaction interplay.[2] In Coulomb blockade experiments in the electron tunneling regime, the conductance through the dot varies strongly as a function of gate voltage, forming a series of sharp peaks. For closed dots at low temperature, both the positions and heights of the peaks encode information about the dot's ground state. In particular, the spacing between adjacent peaks is proportional to the second difference of the ground state energy, which is often called the addition energy. Furthermore, the ground state spin of the quantum dot can be inferred from the shift in position of the conductance peaks upon applying a magnetic field.

We use spin-density-functional theory to study electron-electron interaction effects in quantum dots with up to 200 electrons.[3] We have investigated two types of 2D quantum dots: (1) an isolated quantum dot with classically chaotic external potential, and (2) a more realistic quantum dot with irregular confining gate. The statistical properties of both the ground state spin and the spacing between conductance peaks are calculated at different interaction strengths and electron number. Results for the first model show a large fraction of high-spin ground states and a weak even/odd effect in the conductance peak spacing. This indicates that e-e interaction effects are much stronger than expected from statistical theories. The study of the realistic quantum dot demonstrates the effect of the electrostatic gate, which is an important component in experimental studies of quantum dots.

### **2. Electron Tunneling Into Ferromagnetic Nanoparticles: The Role of Spin-Orbit Coupling**

*[with Gonzalo Usaj (post-doc)]*

We calculate the fluctuation of the anisotropy constant in ferromagnetic nanoparticles and compare with experimental [4] tunneling data. Starting from a microscopic spin-orbit

Hamiltonian and considering it as a perturbation of the much stronger exchange interaction, we derive an explicit expression for the anisotropy tensor. Assuming a simple random matrix model for the spin-orbit coupling allows us to describe the fluctuation of such a tensor. In the case of uniaxial anisotropy, we calculate the probability distribution of the anisotropy constant for a given number of electrons and its variation upon increasing this number by one. The magnitude of the latter is sufficient to account for the experimental data. Finally, we discuss the relevance of our model for the tunneling excitation spectrum, both for the number of resonances and for the change in intensity as a function of the magnetic field.

### **3. Addition Energy of Fullerenes and Carbon Nanotubes as Quantum Dots**

*[with San-Huang Ke (post-doc)]*

Quantum dots have recently been made using finite pieces of carbon nanotubes. In the case of tunneling contacts so that one is in the Coulomb blockade regime, transport spectroscopy probes the ground state properties of these molecules. Using density functional theory calculations, we find a robust even/odd oscillation in the addition energy of carbon nanotube quantum dots, while such oscillation is absent in fullerene balls. For the fullerene balls ( $C_{60}$ ,  $C_{76}$ ,  $C_{240}$ , and  $C_{540}$ ), high symmetry causes a high degeneracy in their energy levels. Thus high-spin configurations are preferred when electrons are added to or removed from the balls (Hund's rule), and as a result, there is no even/odd oscillation in the addition energy. For the carbon nanotubes ( $C_{250}$ ,  $C_{510}$ ,  $C_{640}$ , and  $C_{1010}$ ), the low density of states near the Fermi energy gives an average level spacing, which is much larger than the exchange-induced level shift ( $J/\Delta \ll 1$ ). Consequently, there is a strong even/odd oscillation in the addition energy. We find that this is quite robust against effects from native defects, structure deformation and disturbance by an external electrostatic potential. Far from the Fermi energy (where the density of states increases), this even/odd oscillation tends to vanish.

### **4. Superconductivity With Disorder: A Quantum Monte Carlo Study**

*[with James Osborn (post-doc) and Anand Priyadarshie (student)]*

We use cluster algorithms to study superconductivity with disorder in two-dimensional systems. This problem is a classic example of the competition between coherence (superconductivity) and interference (localization caused by the disorder): as the strength of the disorder increases, one expects a quantum phase transition from the superconducting to the insulating state. We compare the effects of disorder on quantum spin-1/2 models with fermionic models for s-wave superconductivity [5]. The former can be studied efficiently using the directed loop quantum Monte Carlo algorithm [6], while the latter can be studied using the meron cluster algorithm [7]. We use the pairing susceptibility and the superfluid density as observables to identify and characterize the superconducting phase, paying particular attention to how interference causes the coherent order to disappear at the transition.

### **5. Fluctuations of the Kondo Effect in Quantum Dots**

*[with Ribhu Kaul (student) and Denis Ullmo (visiting professor)]*

Correlations between the most energetic electron in a quantum dot and the electrons in the metallic lead connected to the dot have been of great interest since the observation of the Kondo

effect a few years ago.[8] The coupling of a quantum dot to its leads depends sensitively on the realization of the dot; thus, in the Kondo regime, the Kondo temperature itself becomes a mesoscopic quantity. This is in contrast to the conventional Kondo effect where the coupling is a fixed material parameter. Assuming chaotic dynamics for the dot, we use Random Matrix Theory to describe the wavefunctions. We calculate the distributions of the Kondo temperature and of the Kondo enhanced conductance in the Coulomb Blockade valleys, finding that they are very broad because of the exponential sensitivity inherent in the Kondo effect. We also investigate parametric correlations of the conductance.

#### References

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