Thesis title: Coupled-cluster and density functional theory studies of quantum dots

The aim of this thesis is to study numerically systems consisting of several interacting electrons in two dimensions, confined to small regions between layers of semiconductors. These electron systems are dubbed quantum dots in the literature. Semiconductor quantum dots are structures where charge carriers are confined in all three spatial dimensions, the dot size being of the order of the Fermi wavelength in the host material, typically between 10 nm and 1 μm. The confinement is usually achieved by electrical gating of a two-dimensional electron gas (2DEG), possibly combined with etching techniques. Precise control of the number of electrons in the conduction band of a quantum dot (starting from zero) has been achieved in GaAs heterostructures. The electronic spectrum of typical quantum dots can vary strongly when an external magnetic field is applied, since the magnetic length corresponding to typical laboratory fields is comparable to typical dot sizes. In coupled quantum dots Coulomb blockade effects, tunneling between neighboring dots, and magnetization have been observed as well as the formation of a delocalized single-particle state.

Quantum dots have been used to fabricate quantum gates and are also used in the emerging field of quantum nano medicine.

More specifically, this thesis aims at studying the reliability of the coupled-cluster method for studies of quantum dots in two dimensions. The coupled-cluster method has been extremely succesful in providing almost exact ab initio results in quantum chemistry, atomic physics, molecular physics and nuclear physics. These calculations will in turn provide the basis for determining a as good as possible ground state wave function. This wave function will in turn be used to define the quantum mechanical density. The density will be used to construct a density functional for quantum dots using the adiabatic-connection method as described by Teale *et al* in J. Chem. Phys. **130**, 104111 (2009). The results will be compared with existing density functional for quantum dots.

The reliability of the coupled-cluster method as function of the externally applied magnetic field will be compared with ab initio Monte Carlo and large-scale diagonalization techniques. The latter two calculations will be performed by other Master of science students.

The results are expected to be published in leading journals.

The aims of this thesis are as follows

- Develop first a Hartree-Fock code for electrons trapped in a single harmonic oscillator in two dimensions. This part entails developing a code for computing the Coulomb interaction in two dimensions in the laboratory system.
- Compare the Hartree-Fock results with available large scale diagonalization techniques.
- The Hartree-Fock interaction is then used as input to our exsisting coupled-cluster codes. The results will be compared with large scale diagonalization and Monte Carlo techniques for 2, 6, 12 and 20 electrons in a single harmonic oscillator well.
- The obtained ground states will in turn be used to define a as exact as possible density functional for quantum dots using the adiabatic-connection method. The density functional can in turn be used to model systems with a large number of quantum dots. Possible applications of these quantum dots functionals are studies of applications to solar cells.

Progress plan and milestones

The thesis is expected to be handed in June 1 2010.

- Fall 2009: Develop a Hartree-Fock code for quantum dots and derive a self-consistent interaction to be used in the coupled cluster codes. Make comparisons with large-scale diagonalization and Monte Carlo techniques.

- Spring 2010: Derive a density functional for quantum dots and compare with existing parameterizations. Writeup of thesis and final thesis exam.

References

[1] A. M. Teale, S. Coriani, and T. Helgaker, J. Chem. Phys. **130**, 104111 (2009).