Thesis title: Thesis title: Time-evolution of systems of quantum dots

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Aims

The aim of this thesis is to study the time evolution of a system of quantum dots (electrons confined in two dimensional traps) using the multi-configuration time-dependent Hartree-Fock method, as discussed in Ref. [1]. The first step, based on a code developed by a fellow Master of Science student (Frank Olsen) is to study the structure of quantum dots using large-scale diagonalization techniques. Thereafter, time-dependence via an external time-dependent field will be included. The large-scale diagonalization results for various quantum dots will also be benchmarked against virtually exact variational and diffusion Monte Carlo results.

General introduction to possible physical systems

What follows here is a general introduction to systems of confined electrons in two or three dimensions. However, although the thesis will focus on such systems, the codes will be written so that other systems of trapped fermions or eventually bosons can be handled. Examples could be neutrons in a harmonic oscillator trap, see for example Ref. [2], or ions in various traps [3].

Strongly confined electrons offer a wide variety of complex and subtle phenomena which pose severe challenges to existing many-body methods. Quantum dots in particular, that is, electrons confined in semiconducting heterostructures, exhibit, due to their small size, discrete quantum levels. The ground states of, for example, circular dots show similar shell structures and magic numbers as seen for atoms and nuclei. These structures are particularly evident in measurements of the change in electrochemical potential due to the addition of one extra electron, $\Delta_N = \mu(N+1) - \mu(N)$. Here N is the number of electrons in the quantum dot, and $\mu(N) = E(N) - E(N-1)$ is the electrochemical potential of the system. Theoretical predictions of Δ_N and the excitation energy spectrum require accurate calculations of ground-state and of excited-state energies. Small confined systems, such as quantum dots (QD), have become very popular for experimental study. Beyond their possible relevance for nanotechnology, they are highly tunable in experiments and introduce level quantization and quantum interference in a controlled way. In a finite system, there cannot, of course, be a true phase transition, but a cross-over between weakly and strongly correlated regimes is still expected. There are several other fundamental differences between quantum dots and bulk systems: (a) Broken translational symmetry in a QD reduces the ability of the electrons to delocalize. As a result, a Wigner-type cross-over is expected for a smaller value of r_s[37]. (b) Mesoscopic fluctuations, inherent in any confined system, lead to a rich interplay with the correlation effects. These two added features make strong correlation physics particularly interesting in a QD. As clean 2D bulk samples with large r_s are regularly fabricated these days in semiconductor heterostructures, it seems to be just a matter of time before these systems are patterned into a QD, thus providing an excellent probe of correlation effects.

The above-mentioned quantum mechanical levels can, in turn, be tuned by means of, for example, the application of various external fields. The spins of the electrons in quantum dots provide a natural basis for representing so-called qubits [4]. The capability to manipulate and study such states is evidenced by several recent experiments [5, 6]. Coupled quantum dots are particularly interesting since so-called two-qubit quantum gates can be realized by manipulating the exchange coupling which originates from the repulsive Coulomb interaction and the underlying Pauli principle. For such states, the exchange coupling splits singlet and triplet states, and depending on the shape of the confining potential and the applied magnetic field, one can allow for electrical or magnetic control of the exchange coupling. In particular, several recent experiments and theoretical investigations have analyzed the role of effective spin-orbit interactions in quantum dots [7–10] and their influence on the exchange coupling.

A proper theoretical understanding of the exchange coupling, correlation energies, ground state energies of quantum dots, the role of spin-orbit interactions and other properties of quantum dots as well, requires the development of appropriate and reliable theoretical few- and many-body methods. Furthermore, for quantum dots with more than two electrons and/or specific values of the external fields, this implies the development of few- and many-body methods where uncertainty quantifications are provided. For most methods, this means providing an estimate of the error due to the truncation made in the single-particle basis and the truncation made in limiting the number of possible excitations. For systems with more than three or four electrons, *ab initio* methods that have been employed in studies of quantum dots are variational and diffusion Monte Carlo [11, 13, 14], path integral approaches [15], large-scale diagonalization (full configuration interaction) [16–18, 20], and to a very limited extent coupled-cluster theory [21–25]. Exact diagonalization studies are accurate for a very small number of electrons, but the number of basis functions needed to obtain a given accuracy and the computational cost grow very rapidly with electron number. In practice they have been used for up to eight electrons[16, 17, 20],

but the accuracy is very limited for all except $N \leq 3$. Monte Carlo methods have been applied up to $N = 24$ electrons [13, 14]. Diffusion Monte Carlo, with statistical and systematic errors, provide, in principle, exact benchmark solutions to various properties of quantum dots. However, the computations start becoming rather time-consuming for larger systems. Hartree[29], restricted Hartree-Fock, spin- and/or space-unrestricted Hartree-Fock[30–32] and local spin-density, and current density functional methods[33–36] give results that are satisfactory for a qualitative understanding of some systematic properties. However, comparisons with exact results show discrepancies in the energies that are substantial on the scale of energy differences.

Specific tasks

The specific task here is to develop a multi-configuration time-dependent Hartree-Fock (MCTHF) code, in order to be able to study the time evolution of an interacting quantum mechanical system. In this case, the system we will start with is that of electrons confined in two-dimensional regions, so-called quantum dots. If properly object-oriented, the codes could also be used to study atoms or electrons confined to three dimensions. The algorithmic details behind the MCTHF method are exposed in Ref. [1].

Progress plan and milestones

The aims and progress plan of this thesis are as follows

- Fall 2012: In order to become familiar with the large-scale diagonalization method, the first step is to solve the two-electron problem in an oscillator basis. A fellow Master of Science student (Frank Olsen) has already developed a large-scale diagonalization code. To build upon this code is the starting point for this thesis. These results will be compared with the exact ones from either the diffusion Monte Carlo code, or existing exact results from Coupled-cluster theory or exact diagonalization[25]. To achieve this, the first step is to set up the Coulomb interaction in an oscillator basis. This has been done in for example Ref. [25]. The code and its details can be looked up from the slides for FYS4411 from 2011.

- Fall 2012: In order to perform the large-scale diagonalization part, one will need first to set up a Hartree-Fock basis. Such codes are also available from previous Master of Science theses, see for example Christoffer Hirth's thesis. This part will also be included in Sarah Reimann's Master of Science thesis.

- Fall 2012 and begin Spring 2013: The Hartree-Fock interaction (and possibly effective interactions as well, see Ref. [25]), is then used as input to the large-scale diagonalization code, a code which is part of Frank Olsen's Master thesis. It is expected that Sigve will be able to build his MCTHF code based on these earlier developments. The results will be compared with available results from variational and diffusion Monte Carlo and coupled-cluster techniques for closed-shell systems.

- Fall 2012 and Spring 2013: The last step is to implement the MCTHF method, as exposed in Ref. [1]. The first step is to test the code for a system of two electrons in two dimensions using a time-independent Hamiltonian. For this case, closed-form expressions are well-known for the time-evolution of the wave function. Thereafter a simple time-dependent electromagnetic field will be included and tested against existing results for two electrons. The final stage is to explore the stability of limits of this method for systems with more than two electrons.

This method has never before been applied to systems of strongly confined electrons. This method can also be benchmarked against the popular time-dependent density functional approach to be developed by a fellow Master of Science student, Jørgen Høgberget. This can bode for fruitful collaborations. The Hartree-Fock part for two electrons only and the diagonalization procedure can be benchmarked against the the similarity renormalization group approach to be implemented by another fellow Master of Science student, Sarah Reimann. Similarly, the diffusion Monte Carlo results can be benchmarked against the thesis work of Karl Leikanger.

The thesis is expected to be handed in June 1 2013.

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