Time Evolution of Quantum Mechanical systems

Master of Science thesis project

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Aim

The aim of this thesis is to study the time evolution of a system of quantum dots (electrons confined in two- or three-dimensional traps) using the time-dependent Coupled Cluster method method. The first step is to study a system of two electrons in two or three dimensions whose motion is confined to an oscillator potential. This system has, for two electrons only in two or three dimensions, analytical solutions for the energy and the state functions. Similarly, the matrix elements of the Coulomb interaction have analytical expressions when one employs a harmonic oscillator basis in two or three dimensions. The time-evolution of such a system can thus be given in terms of analytical expressions. The first step consists in studying numerically such systems using the coupled cluster method with singles and double excitations.

For two electrons only the singles and doubles excitations provide an exact answer to the quantum mechanical The numerical results will be compared with analytical expressions. The next step is to add time-dependent external potentials and study how the system evolves with time under the influence of externally applied time-dependent fields and more confined electrons. The final steps consists of extending the system to a so-called double potential well and study the time evolution of this system using the time-dependent Coupled Cluster method.

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 or ions in various traps.

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:

1. 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, that is the so-called gas parameter $r_s = (c_d/a_B)(1/n)^d$, where n is the electron density, d is the spatial dimension, a_B the effective Bohr radius and c_d a dimension dependent constant.

2. 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. The capability to manipulate and study such states is evidenced by several recent experiments. 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 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, path integral approaches, large-scale diagonalization (full configuration interaction and to a more limited extent coupled-cluster theory. 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, but the accuracy is very limited for all except $N \leq 3$. Monte Carlo methods have been applied up to $N \sim 100$ electrons. 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. Mean field methods like various Hartree-Fock approaches and/or current density functional methods 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 and milestones. The specific task here is to study the time evolution of quantum mechanical systems using the Coupled Cluster (CC) method, in order to be able to study the time evolution of an interacting quantum mechanical system, in particular for electrons confined to move in two or three dimensions. In this case, the system we will start with is that of electrons confined in two- and three-dimensional regions, so-called quantum dots. If properly object-oriented, the codes could also be used to study atoms or molecules confined to three dimensions. The algorithmic details behind the time-dependent coupled. The final aim is to extend the formalism and algorithms developed in the thesis of Haakon Emil Kristiansen to systems with two or more electrons trapped in more than one oscillator well. Such systems have been used as prototype systems for testing quantum algorithms and building quantum circuits. This method has never before been applied to systems of strongly confined electrons and opens up several interesting avenues for further research programs as well as eventual publications.

The thesis project can easily be split into several parts and form the basis for the collaborations among several students. The milestones are as follows

1. Spring 2020: Start writing a Coupled Cluster code with doubles excitations only that solves a system of two electrons in two or three dimensions in a single Harmonic oscillator well. Finalize eventual remaining courses.

2. Fall 2020: Extend the project to include singles excitations, time evolution and a double potential well as discussed by Nielsen et al.

3. Spring 2021: Include orbital dependencies as discussed in the article by Kvaal. Finalize thesis.

The thesis is expected to be handed in May/June 2021.

References. Highly relevant articles for possible thesis projects are:

1. http://aip.scitation.org/doi/abs/10.1063/1.4718427

2. https://journals.aps.org/prb/abstract/10.1103/PhysRevB.85.035319

3. https://journals.aps.org/prb/abstract/10.1103/PhysRevB.82.075319

4. https://arxiv.org/pdf/1006.2735.pdf

5. https://juser.fz-juelich.de/record/187784/files/PhysRevB.91.075301.pdf