Thesis title: Monte-Carlo simulations 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.

In this thesis, the study of such a system of two-dimensional electrons entails more specifically the use of many-body techniques through the development of variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC) programs to solve Schrödinger's equation, in order to obtain various expectation values of interest, such as the energy of the ground state, magnetization etc. The DMC approach allows, in principle, for a numerically exact solution of Schrödinger's equation. However, it needs a reasonable starting point. It is here where a variational Monte Carlo calculation of the same system provides a variationally optimal trial wave function of a many-body system.

In the next section we give a brief description of the physics behind quantum dots and their potential for constructing quantum gates. Thereafter, we sketch the ideas behind both the VMC and DMC approaches to be used.

A progress plan for this thesis project is given at the end.

Introduction to quantum dots

Quantum computing has attracted much interest recently as it opens up the possibility of outperforming classical computation through new and more powerful quantum algorithms such as the ones discovered by Shor and by Grover. There is now a growing list of quantum tasks such as cryptography, error correcting schemes, quantum teleportation, etc. that have indicated even more the desirability of experimental implementations of quantum computing. In a quantum computer each quantum bit (qubit) is allowed to be in any state of a quantum two-level system. All quantum algorithms can be implemented by concatenating one- and two-qubit gates. There is a growing number of proposed physical implementations of qubits and quantum gates. A few examples are: Trapped ions, cavity QED, nuclear spins, superconducting devices, and our qubit proposal based on the spin of the electron in quantum-confined nanostructures.

Coupled quantum dots provide a powerful source of deterministic entanglement between qubits of localized but also of delocalized electrons. E.g., with such quantum gates it is possible to create a singlet state out of two electrons and subsequently separate (by electronic transport) the two electrons spatially with the spins of the two electrons still being entangled–the prototype of an EPR pair. This opens up the possibility to study a new class of quantum phenomena in electronic nanostructures such as the entanglement and non-locality of electronic EPR pairs, tests of Bell inequalities, quantum teleportation, and quantum cryptography which promises secure information transmission.

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 mechanical studies of such many-body systems are also interesting per se. This thesis deals with a numerical *ab initio* solution of Schrödinger's equation for quantum dots, from few electrons to many. A critical understanding of our ability to solve such many-body systems through Monte Carlo methods is one of the aims of this thesis project. Presently, Monte Carlo methods are the only ones which allow us to solve, in principle exactly, systems with many interacting particles. These techniques are briefly sketched in the next two sections.

Variational Monte Carlo

The variational quantum Monte Carlo (VMC) has been widely applied to studies of quantal systems. The recipe consists in choosing a trial wave function $\psi_T(\mathbf{R})$ which we assume to be as realistic as possible. The variable $\mathbf{R}$ stands for the spatial coordinates, in total dN if we have N particles present. The variable d is the dimension of the system. The trial wave function serves then as a mean to define the quantal probability distribution

$$P(\mathbf{R}) = \frac{|\psi_T(\mathbf{R})|^2}{\int |\psi_T(\mathbf{R})|^2 d\mathbf{R}}. \tag{1}$$

This is our new probability distribution function (PDF).

The expectation value of the energy E is given by

$$\langle E \rangle = \frac{\int d\mathbf{R}\Psi^*(\mathbf{R})H(\mathbf{R})\Psi(\mathbf{R})}{\int d\mathbf{R}\Psi^*(\mathbf{R})\Psi(\mathbf{R})}, \tag{2}$$

where Ψ is the exact eigenfunction. Using our trial wave function we define a new operator, the so-called local energy,

$$E_L(\mathbf{R}) = \frac{1}{\psi_T(\mathbf{R})} H\psi_T(\mathbf{R}), \tag{3}$$

which, together with our trial PDF allows us to rewrite the expression for the energy as

$$\langle H \rangle = \int P(\mathbf{R}) E_L(\mathbf{R}) d\mathbf{R}. \tag{4}$$

This equation expresses the variational Monte Carlo approach. For most hamiltonians, H is a sum of kinetic energy, involving a second derivative, and a momentum independent potential. The contribution from the potential term is hence just the numerical value of the potential.

Using the Metropolis algorithm and the Monte Carlo evaluation of Eq. (4), a detailed algorithm is as follows

- Initialisation: Fix the number of Monte Carlo steps and thermalization steps. Choose an initial $\mathbf{R}$ and variational parameters α and calculate $|\psi_T^{\alpha}(\mathbf{R})|^2$. Define also the value of the stepsize to be used when moving from one value of $\mathbf{R}$ to a new one.
- Initialise the energy and the variance.
- Start the Monte Carlo calculation
  1. Thermalise first.
  2. Thereafter start your Monte carlo sampling.
  3. Calculate a trial position $\mathbf{R}_p = \mathbf{R} + r * step$ where r is a random variable $r \in [0,1]$.
  4. Use then the Metropolis algorithm to accept or reject this move by calculating the ratio

     $$w = P(\mathbf{R}_p)/P(\mathbf{R}).$$

     If $w \geq s$, where s is a random number $s \in [0,1]$, the new position is accepted, else we stay at the same place.
  5. If the step is accepted, then we set $\mathbf{R} = \mathbf{R}_p$.
  6. Update the local energy and the variance.
- When the Monte Carlo sampling is finished, we calculate the mean energy and the standard deviation.

Diffusion Monte Carlo

The DMC method is based on rewriting the Schrödinger equation in imaginary time, by defining $\tau = it$. The imaginary time Schrödinger equation is then

$$\frac{\partial \psi}{\partial \tau} = -\widehat{\mathbf{H}}\psi, \tag{5}$$

where we have omitted the dependence on τ and the spatial variables in ψ. The wave function ψ is again expanded in eigenstates of the Hamiltonian

$$\psi = \sum_i^{\infty} c_i \phi_i, \tag{6}$$

where

$$\widehat{\mathbf{H}}\phi_i = \epsilon_i \phi_i, \tag{7}$$

ϵ_i being an eigenstate of $\widehat{\mathbf{H}}$. A formal solution of the imaginary time Schrödinger equation is

$$\psi(\tau_1 + \delta\tau) = e^{-\widehat{\mathbf{H}}\delta\tau}\psi(\tau_1) \tag{8}$$

where the state $\psi(\tau_1)$ evolves from an imaginary time τ_1 to a later time $\tau_1 + \delta$. If the initial state $\psi(\tau_1)$ is expanded in energy ordered eigenstates, following Eq. (6), then we obtain

$$\psi(\delta\tau) = \sum_i^{\infty} c_i e^{-\epsilon_i \delta\tau}\phi_i. \tag{9}$$

Hence any initial state, ψ, that is not orthogonal to the ground state ϕ_0 will evolve to the ground state in the long time limit, that is

$$\lim_{\tau\to\infty} \psi(\delta\tau) = c_0 e^{-\epsilon_0\tau}\phi_0. \tag{10}$$

This derivation shares many formal similarities with that given for the variational principle discussed in the previous section. However in the DMC method the imaginary time evolution results in excited states decaying exponentially fast, whereas in the VMC method any excited state contributions remain and contribute to the VMC energy.

The DMC method is a realisation of the above derivation in position space. Including the spatial variables as well, the above equation reads

$$\lim_{\tau\to\infty} \psi(\mathbf{R}, \delta\tau) = c_0 e^{-\epsilon_0\tau}\phi_0(\mathbf{R}). \tag{11}$$

By introducing a constant offset to the energy, $E_T = \epsilon_0$, the long-time limit of Eq. (11) can be kept finite. If the Hamiltonian is separated into the kinetic energy and potential terms, the imaginary time Schrödinger equation, takes on a form similar to a diffusion equation, namely

$$-\frac{\partial\psi(\mathbf{R},\tau)}{\partial\tau} = \left[\sum_i^N -\frac{1}{2}\nabla_i^2\psi(\mathbf{R},\tau)\right] + (V(\mathbf{R}) - E_T)\psi(\mathbf{R},\tau). \tag{12}$$

This equation is a diffusion equation where the wave function ψ may be interpreted as the density of diffusing particles (or "walkers"), and the term $V(\mathbf{R}) - E_T$ is a rate term describing a potential-dependent increase or decrease in the particle density. The above equation may be transformed into a form suitable for Monte Carlo methods, but this leads to a very inefficient algorithm. The potential $V(\mathbf{R})$ is unbounded in coulombic systems and hence the rate term $V(\mathbf{R}) - E_T$ can diverge. Large fluctuations in the particle density then result and give impractically large statistical errors.

These fluctuations may be substantially reduced by the incorporation of importance sampling in the algorithm. Importance sampling is essential for DMC methods, if the simulation is to be

efficient. A trial or guiding wave function $\psi_T(\mathbf{R})$, which closely approximates the ground state wave function is introduced. This is where typically the VMC result enters. A new distribution is defined as

$$f(\mathbf{R},\tau) = \psi_T(\mathbf{R})\psi(\mathbf{R},\tau), \tag{13}$$

which is also a solution of the Schrödinger equation when $\psi(\mathbf{R},\tau)$ is a solution. Eq. (12) consequently modified to

$$\frac{\partial f(\mathbf{R},\tau)}{\partial \tau} = \frac{1}{2}\nabla\left[\nabla - F(\mathbf{R})\right] f(\mathbf{R},\tau) + (E_L(\mathbf{R}) - E_T) f(\mathbf{R},\tau). \tag{14}$$

In this equation we have introduced the so-called force-term F, given by

$$F(\mathbf{R}) = \frac{2\nabla\psi_T(\mathbf{R})}{\psi_T(\mathbf{R})}, \tag{15}$$

and is commonly referred to as the "quantum force". The local energy E_L is defined as previously

$$E_L\mathbf{R}) = -\frac{1}{\psi_T(\mathbf{R})}\frac{\nabla^2\psi_T(\mathbf{R})}{2} + V(\mathbf{R})\psi_T(\mathbf{R}), \tag{16}$$

and is computed, as in the VMC method, with respect to the trial wave function.

We can give the following interpretation to Eq. (14). The right hand side of the importance sampled DMC equation consists, from left to right, of diffusion, drift and rate terms. The problematic potential dependent rate term of the non-importance sampled method is replaced by a term dependent on the difference between the local energy of the guiding wave function and the trial energy. The trial energy is initially chosen to be the VMC energy of the trial wave function, and is updated as the simulation progresses. Use of an optimised trial function minimises the difference between the local and trial energies, and hence minimises fluctuations in the distribution f . A wave function optimised using VMC is ideal for this purpose, and in practice VMC provides the best method for obtaining wave functions that accurately approximate ground state wave functions locally.

Progress plan

The thesis is expected to be finished towards the end of the spring semester of 2003.

- Spring 2002: Exam in Fys 372 (Nuclear structure, 3vt). Write a code which solves the variational Monte-Carlo (VMC) problem for two interacting electrons in a harmonic oscillator potential in two dimensions. The role of an external magnetic field is also to be studied. Possible connections to the quantum Hall effect. This code is then expanded in order to account for more electrons (tipycally 10-20 or more) which are localized in the quantum dot.

- Fall 2002: Exam in Fys 303 (Relativistic quantum physics, 4vt). Follow lectures in Fys 305 (many-body physics, 3vt). The next step is to write a Diffusion Monte Carlo (DMC) programme for the same system. The DMC code receives as input the optimal variational energy and wave function from the VMC calculation and solves in principle the Schrödinger equation exactly.

- Spring 2003: Writeup of thesis, thesis exam and exam in Fys 305.