Thesis project for Espen Flage-Larsen: 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 large scale shell-model diagonalization techniques. These results will be compared with those from diffusion Monte Carlo (DMC) and variational Monte Carlo (VMC) 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 shell-model and VMC/DMC approaches allow, in principle, for a numerically exact solution of Schrödinger's equation.

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, large scale shell-model diagonalization and Monte Carlo methods are the only ones which allow us to solve, in principle exactly, systems with many interacting particles. The main focus is on large scale shell-model techniques. If possible these results will be compared with existing Variational Monte Carlo results. A diffusion Monte Carlo program is under development and can also be used to compare the results from shell-model diagonalizations.

The ability to study different methods is crucial to the reliability of each method. This thesis project will thus be able to shed light on differences between VMC and DMC calculations using the shell-model calculations as the exact frame. Presently, see Ref. [1] below, discrepancies exist between DMC and VMC calculations regarding the spin of the ground and excited states.

The shell-model program is briefly sketched in the next section.

Shell-model studies

Here we describe the philosophy behind the shell-model code developed here in Oslo by Torgeir Engeland. This code will be used in order to deal with the diagonalization of the hamiltonian for several electrons confined in a quantum dot.

The shell model problem requires the solution of a real symmetric $n \times n$ matrix eigenvalue equation

$$H \left| vec_k \right\rangle = E_k \left| vec_k \right\rangle , \tag{1}$$

with $k = 1, \ldots, K$. The eigenvalues E_k are understood to be numbered in increasing order. In a typical shell model problem we are interested in only the lowest eigenstates of Eq. (1), so K may be of the order of 10 to 50. The total dimension n of the eigenvalue matrix H can be large, up to $n \approx 2 \times 10^8$ or more. Different computational approaches to solve Eq.(1) can be distinguished based on the size of n. For n small, i.e. $10^2 < n < 10^3$ and with the number of matrix elements of H less than 10^6 such problems can be accomodated within the direct access memory of a modern work station and can be diagonalized by standard matrix routines. In a second domain with $n > 10^3$ but small enough that H has no more than 10^8 elements. This will require ≈ 1.5 Gbyte of storage.Then all matrix elements may be stored in memory or alternatively on a standard disk. In these cases the complete diagonalization of H will not be of physical interest and efficient iteration procedures have been developed to find the lowest energy eigenvalues and eigenvectors.

Based on the present computer methods we have developed a code which is under continuous improvement to solve the eigenvalue problem given in Eq. (1). The basic requirement is to be able to handle problems with $n > 10^6$. In the following we discuss some of the important elements which enter the algorithm.

We separate the discussion into two parts:

- The m–scheme representation of the basic states.
- The Lanczos iteration algorithm.

The m–scheme representation.

We write the eigenstates in Eq. (1) as linear combinations of Slater determinants. In a second quantization representation a Slater determinant (SD) is given by

$$\left| SD_\nu(N) \right\rangle = \prod_{(jm)\in\nu} a^\dagger_{jm} \left| 0 \right\rangle , \tag{2}$$

and the complete set is generated by distributing the N particles in all possible ways throughout the basic one–particle states constituting the P–space. This is a very efficient representation. A single $|SD\rangle$ requires only one computer word (32 or 64 bits) and in memory a $|SD\rangle$ with N particles is given by

$$\left| SD \right\rangle \longrightarrow (\underbrace{00111101010\cdots}_{N 1's}), \tag{3}$$

where each 0 and 1 corresponds to an m–orbit in the valence P–space. Occupied orbits have a 1 and empty orbits a 0. Furthermore, all important calculations can be handled in Boolean algebra which is very efficient on modern computers. The action of operators of the form $a^\dagger_\alpha a_\beta$ or $a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta$ acting on an $|SD\rangle$ is easy to perform.

The m-scheme allows also for a straightforward definition of many-body operators such as one–, two– and three–particle operators

$$a^\dagger_\alpha a_\beta, \tag{4}$$

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a_{\beta_1} a_{\beta_2}, \tag{5}$$

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a^\dagger_{\alpha_3} a_{\beta_1} a_{\beta_2} a_{\beta_3}, \tag{6}$$

respectively.

The Lanczos iteration process.

At present our basic approach to finding solutions to Eq. (1) is the Lanczos algorithm. For the present discussion we outline the basic elements of the method.

1. We choose an initial Lanczos vector $|lanc_0\rangle$ as the zeroth order approximation to the lowest eigenvector in Eq. (1). Our experience is that any reasonable choice is acceptable as long as the vector does not have special properties such as good angular momentum. That would usually terminate the iteration process at too early a stage.

2. The next step involves generating a new vector through the process $|new_{p+1} >= H|lanc_p >$. Throughout this process we construct the energy matrix elements of H in this Lanczos basis. First, the diagonal matrix elements of H are then obtained by

$$\langle lanc_p| \, H \, |lanc_p\rangle = \langle lanc_p| \; new_{p+1}\rangle \, , \tag{7}$$

3. The new vector $|new_{p+1}\rangle$ is then orthogonalized to all previously calculated Lanczos vectors

$$\left|new^{'}_{p+1}\right\rangle = |new_{p+1}\rangle - |lanc_p\rangle \cdot \langle lanc_p| \; new_{p+1}\rangle - \sum_{q=0}^{p-1} |lanc_q\rangle \cdot \langle lanc_q| \; new_{p+1}\rangle \, , \tag{8}$$

   and finally normalized

$$|lanc_{p+1}\rangle = \frac{1}{\sqrt{\langle new^{'}_{p+1}| \; new^{'}_{p+1}\rangle}} \left|new^{'}_{p+1}\right\rangle , \tag{9}$$

   to produce a new Lanczos vector.

4. The off–diagonal matrix elements of H are calculated by

$$\langle lanc_{p+1}| \, H \, |lanc_p\rangle = \left\langle new^{'}_{p+1}\right| \; new^{'}_{p+1}\right\rangle , \tag{10}$$

   and all others are zero.

5. After n iterations we have an energy matrix of the form

$$\left\{ \begin{array}{ccccc} H_{0,0} & H_{0,1} & 0 & \cdots & 0 \\ H_{0,1} & H_{1,1} & H_{1,2} & \cdots & 0 \\ 0 & H_{2,1} & H_{2,2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & H_{p-1,p} \\ 0 & 0 & 0 & H_{p,p-1} & H_{p,p} \end{array} \right\} \tag{11}$$

   as the p'th approximation to the eigenvalue problem in Eq. (1). The number p is a reasonably small number and we can diagonalize the matrix by standard methods to obtain eigenvalues and eigenvectors which are linear combinations of the Lanczos vectors.

6. This process is repeated until a suitable convergence criterium has been reached.

In this method each Lanczos vector is a linear combination of the basic $|SD\rangle$ with dimension n.

Progress plan

A program for solving the diffusion Monte Carlo problem for fermions is under development as part of two other Master of Science thesis projects and will be used in this thesis in order to compare with the shell-model results. The task here is to use two-body effective interactions for a given set of single-particle orbits and perform a shell-model diagonalization. The effective interaction will be provided by Morten Hjorth-Jensen but will also be developed by Espen. A variational Monte Carlo program has already been developed and is documented in Victoria Popsueva's thesis. She will also work closely with Espen. She is presently a PhD student at UiB working on quantum dot related problems.

The thesis is expected to be finished towards the end of the spring semester of 2006.

- Fall 2004: Exams in FYS4520 (Subatomic Many-Body Physics I), FYS4170 (Relativistic Quantum Field Theory) and INF-MAT4350 Numerical Linear Algebra. Thesis work: Set up a given model space using harmonic oscillator energies with and without a finite B-field and obtain the energies for the ground state and excited states with no interaction. Use also the shell-model code to chech that the results are the same. Develop a numerical code which computes the two-body interaction matrix elements using a two-dimensional harmonic oscillator basis.

- Spring 2005: Exams in FYS4530 Subatomic Many-Body Physics II, FYS5120 Advanced Quantum Field theory and INF5620 Numerical methods for partial differential equations.

  Thesis work: Read in the two-body interaction and study the spectra of two electrons confined in a quantum dot. Compare the results with the analytic ones of Ref. [2].

- Fall 2005: Thesis work: extensive shell-model calculations for systems with many electrons in several shells. Compare the results with the Variational Monte Carlo code.

- Spring 2006: Finalize thesis and final exam. Eventually also compare the results with the diffusion Monte Carlo code.

Literature

1. S.M. Reimann and M. Manninen, Reviews of Modern Physics **74**, 1283 (2002).

2. M. Dyneykhan and R.G. Naszmitdinov, Physical Review **B 55**, 13707 (1997). Exact solution for two electrons.

3. A. Harju, V.A. Sverdlov, R.M. Nieminen and V. Halonen, Physical Review **B 59**, 5622 (1999). Variational Monte Carlo paper

4. F. Bolton, Physical Review **B 54**, 4780 (1996). Diffusion Monte Carlo paper.

5. W. D. Heiss and R. G. Nazmitdinov, Physical Review **B 55**, 16310 (1997). Shell-model paper.

6. A useful text on Matrix computations is Golub and Van Loan.