

# Diffusion Monte Carlo studies of systems of confined fermions

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MSc thesis in Computational Physics

## Aims

The aim of this thesis is to develop a diffusion Monte Carlo (DMC) code that can be used to study properties of confined fermions. The code should be flexible enough to deal with both closed-shell and open-shell systems. The project here is an ambitious one and has enough material for two independent Master of Science thesis projects.

The applications will be directed towards studies of electron-electron correlations in quantum dots as function of the density of the systems. Properties like single-particle and pair densities will be studied as the density is lowered towards the eventual Wigner crystallization. Quantum dot molecules can also be studied and the first step would be to repeat calculations done with large-scale diagonalization techniques for two-electron quantum dot molecules.

## 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.

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  $\Delta_N$  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  $r_s$  (this 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). (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. 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 very 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  $N = 56$  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. Hartree, restricted Hartree-Fock, spin- and/or space-unrestricted Hartree-Fock and local spin-density, and 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

The first task of this thesis is to develop a variational (VMC) and diffusion Monte Carlo (DMC) code that are fully object oriented and parallelized and can tackle both closed-shell systems and open shell systems. This code should be able to use different single-particle basis functions as input for the Slater determinants used in the VMC and DMC calculations. A single-particle basis of interest is the one represented by confining double well potential, see the discussion below. The first step in such a development is to study a system of two electrons in a double oscillator like well. This means that we could study the two-electron 'quantum dot molecule' (QDM) with for example the two-dimensional Hamiltonian

The second part includes applications of the codes and studies of quantum dot systems at different densities, computing both single-electron densities and pairing densities in order to understand better electron-electron correlations towards the Wigner crystallization limit.

The Hamiltonian of the system to study is given by

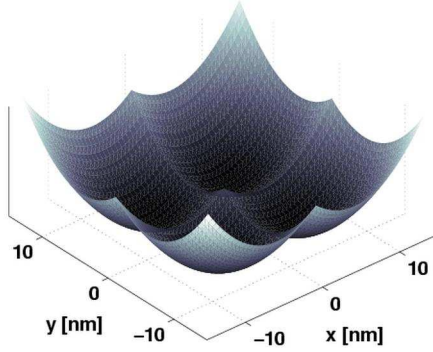
$$H = \sum_{i=1}^2 \left( \frac{(-i\hbar\nabla_i - \frac{e}{c}\mathbf{A})^2}{2m^*} + V_c(\mathbf{r}_i) \right) + \frac{e^2}{\epsilon r_{12}},$$

where  $V_c$  is the external confinement potential taken to be

$$V_c(\mathbf{r}) = \frac{1}{2}m^*\omega_0^2 \min \left[ \sum_j^M (\mathbf{r} - \mathbf{L}_j)^2 \right],$$

where the coordinates are in two dimensions  $\mathbf{r} = (x, y)$  and the  $L_j$ 's ( $L_j = (\pm L_x, \pm L_y)$ ) give the positions of the minima of the QDM potential, and  $M$  is the number of minima. When  $\mathbf{L}_1 = (0, 0)$  (and  $M = 1$ ) we have a single parabolic QD. With  $M = 2$  and  $\mathbf{L}_{1,2} = (\pm L_x, 0)$  we get a double-dot potential.

One can also study four-minima QDM ( $M = 4$ ) with minima at four possibilities of  $(\pm L_x, \pm L_y)$  (see the figure here).



We can study both square-symmetric ( $L_x = L_y$ ) and rectangular-symmetric ( $L_x \neq L_y$ ) four-minima QDMs. The confinement potential can also be written using the absolute values of  $x$  and  $y$  coordinates as

$$V_c(x, y) = \frac{1}{2} m^* \omega_0^2 [r^2 - 2L_x|x| - 2L_y|y| + L_x^2 + L_y^2] .$$

For non-zero  $L_x$  and  $L_y$ , the perturbation to the parabolic potential comes from the linear terms of  $L_x$  or  $L_y$  containing also the absolute value of the associated coordinate.

## Progress plan and milestones

The aims and progress plan of this thesis are as follows

- Fall 2016: Develop a program which diagonalizes the single-electron problem in different potentials, starting with a harmonic oscillator basis.
- Fall 2016: Expand the solutions of a general potential well in terms of harmonic oscillator functions.

- Fall 2016: Develop a Hartree-Fock program which finds a self-consistent basis expressed in terms of Harmonic Oscillator basis functions.
- Fall 2016: Use the optimal self-consistent basis expressed as a linear combination of harmonic oscillator functions as input to the Slater determinant for a variational Monte Carlo (VMC) calculation. Perform studies of several quantum dot systems with and without a Jastrow factor for the VMC trial functions.
- Spring 2017: Develop and finalize a fully object-oriented and parallelized diffusion Monte Carlo (DMC) code that can tackle closed-shell quantum dot systems.
- Spring 2017: Study one and two-body operators like spin-correlation operators and onebody densities for various quantum dot systems.
- Spring 2017: The last part deals with a proper write-up of the thesis.

The thesis is expected to be handed in May/June 2017.