# Quantum Monte Carlo Studies of Quantum Dots

In my research for Prof. Morten Hjorth-Jensen, I will be using Variational Monte Carlo techniques to simulate systems of quantum dots. Semiconductor quantum dots are structures where charge carriers are confined in all three spatial dimensions. The sizes of these dots range from 10 nm and 1$\mu$m, the size of the Fermi Wavelength for the host material. The dots are confined by electrical gating of a two-dimensional electron gas (2DEG) and etching techniques. Quantum dots have numerous intriguing potential applications in solid-state physics, such as improving the efficiency of energy production from solar cells. Thus, modeling systems of quantum dots can yield insights on their interactions and the effects that have been observed.

Variational Monte Carlo (VMC) is widely used in the studies of many-body quantal systems in order to numerically evaluate multi-dimensional integrals. My project involves writing a VMC program to calculate spherical quantum dots as functions of an applied magnetic field. Different types of quantum dot confinements will be tested in this project, from harmonic oscillator traps to square well traps, which can be compared to quantum dot experiments. A properly written VMC program can be further extended to study three-dimensional electronic systems as well other interacting fermionic or bosonic systems.

Numerous benchmarks have to be met throughout the building of this program. The first step of building this program is to accurately simulate a system of two electrons in a quantum dot. This result can then be compared to the closed form solutions formulated by Taut. I must then perform a VMC calculation of the ground state of two electrons in a quantum dot well with different oscillator energies. Using VMC and the Metropolis algorithm, I will compute the expectation value of the energy using both the analytical expression for the local energy and numerical derivation of the kinetic energy and compare their computational times, with and without important sampling. This program must then be parallelized to make more efficient after I find the most optimal variational parameters. These calculations will be repeated for different oscillator frequencies and the results will be analyzed and compared to Taut's work.

After I create this simple model for just two electrons, I can later extend this program to bigger systems of N = 6 and N = 12 electrons. I will repeat the calculations as stated before for these systems. The performance of this program will be analyzed for at least $10^6$ cycles. I expect the parallelized program to be sped up by about 100%. Done correctly, this program should provide the basis for making comparisons with experiment and other theories, thus opening up many possibilities for simulating other quantum systems.