Thesis title: Effective parallelization of monte Carlo codes for quantum dots

Aim: ?????????????????????? To

The use of compiled low level languages such as fortran and C is a deeply-rooted tradition among computational scientifics and physicians for doing numerical simulations. The extensive use of them is due, mainly, to their high performance. However, the increased demand for more flexibility has motived the deveploment of object oriented languages such as C++ and Fortran 95. Even thought they keep some characteristics of their ancestors, are hard to master.

In recent years, many scientifics and engineers have migrated to slower interpreted high level languages like matlab. The abundant disponibility of documentation, clear and compact sintaxis, interactive execution of commands and the integration of simulation and visualizations make interpreted languages highly attractive. Python is an interpreted object-oriented language that shares with matlab many of its characteristics, but which is much more powerfull and flexible when equipped with tools for numerical simulations and visualization. Because python was designed to be extended with legacy code for efficiency, it is easier to interface it with software written in C++, C and fortran than in other environments.

The numerical solution of quantum mechanical problems containing a large number of degrees of freedom requires the use of parallelization. A balance between computational efficienty, to get fast codes, and programming efficiency, to concentrate more in doing physics, is preferred. The Python package Pypar provides wrapper to the message passing library MPI throught a simple sintax and it has shown to give sufficiently good performance in other applications.

In this thesis we attempt to parallelize quantum mechanical codes using pypar. Concrete applications are the parallelization of variational monte Carlo sequential codes for quantum dots and the extension to diffusion monte Carlo for fermions. 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 the VMC approach to be used.

Introduction to quantum dots

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 the parallelization of serial variational and diffusion monte Carlo code for quantum dots, from few electrons to many. 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 section.

The aims of this thesis are as follows

- Implement the parallelization of VMC codes in plain python and plain C++. (the VMC calculations are done by another Master of Science student, Rune Albrigtsen).
- Provide benchmarks of the parallelization above.
- Move the slow part in python to C++.
- Extend the implementation of VMC to diffusion monte Carlo DMC for quantum dots.

- Provide benchmarks of the DMC codes.

The thesis is expected to be finished towards the end of september 2009.