Introduction to Computational Physics Lectures, FYS4411/9411

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Aims

- Be able to apply two central many-particle methods, Variational Monte Carlo and Hartree-Fock theory (and density functional theory) theory to properties of many-fermion systems, mainly quantum dots.
- Understand how to simulate quantum mechanical systems with many interacting particles. The methods are relevant for atomic, molecular, solid state, materials science, nanotechnology, quantum chemistry and nuclear physics.

Lectures and ComputerLab

- Lectures: Thursday (2.15pm-4pm), remotely via adobe connect. First time January 26.
- Computerlab: Thursday (4.15pm-7pm), first time January 19, last lab session May 11.
- Weekly plans and all other information are on the webpage
- Intensive week starts March 6 and ends March 10.
- **First project to be handed in March 10**.
- **Second and final project to be handed in May 31.**
- There is no final exam, only project work.

Course Format

- Two compulsory projects. Electronic reports only. You are free to choose your format.
- Evaluation and grading: The two projects count 1/2 each of the final mark. No exam.
- The computer lab (room FV329) consists of 16 Linux PCs, but many prefer own laptops. C/C++ is the default programming language, but Fortran2008 and Python are also used. All source codes discussed during the lectures can be found at the webpage of the course. We recommend either C/C++, Fortran2008 or Python as programming languages.

Topics covered in this course

- Parallelization (MPI and OpenMP), high-performance computing topics. Choose between Fortran2008 and/or C++ as programming languages. Python also possible as programming language.
- Algorithms for Monte Carlo Simulations (multidimensional integrals), Metropolis-Hastings and importance sampling algorithms. Improved Monte Carlo methods.
- Statistical analysis of data from Monte Carlo calculations, blocking method.
- Eigenvalue solvers

Topics covered in this course

- Search for minima in multidimensional spaces (conjugate gradient method, steepest descent method, quasi-Newton-Raphson, Broyden-Jacobian).
- Iterative methods for solutions of non-linear equations.
- Object orientation
- Variational Monte Carlo for 'ab initio' studies of quantum mechanical many-body systems.
- Simulation of two-dimensional systems like quantum dots.
- Hartree-Fock theory to study quantum dots

Quantum Monte Carlo Motivation

Most quantum mechanical problems of interest in for example atomic, molecular, nuclear and solid state physics consist of a large number of interacting electrons and ions or nucleons.
The total number of particles N is usually sufficiently large that an exact solution cannot be found.
Typically, the expectation value for a chosen hamiltonian for a system of N particles is

$$\langle H \rangle = \frac{\int d\boldsymbol{R}_1 d\boldsymbol{R}_2 \dots d\boldsymbol{R}_N \Psi^*(\boldsymbol{R_1}, \boldsymbol{R}_2, \dots, \boldsymbol{R}_N) H(\boldsymbol{R_1}, \boldsymbol{R}_2, \dots, \boldsymbol{R}_N) \Psi(\boldsymbol{R_1}, \boldsymbol{R}_2}{\int d\boldsymbol{R}_1 d\boldsymbol{R}_2 \dots d\boldsymbol{R}_N \Psi^*(\boldsymbol{R_1}, \boldsymbol{R}_2, \dots, \boldsymbol{R}_N) \Psi(\boldsymbol{R_1}, \boldsymbol{R}_2, \dots, \boldsymbol{R}_N)}$$

an in general intractable problem.
This integral is actually the starting point in a Variational Monte Carlo calculation. **Gaussian quadrature: Forget it**! Given 10 particles and 10 mesh points for each degree of freedom and an ideal 1 Tflops machine (all operations take the same time), how long will it take to compute the above integral? The lifetime of the universe is of the order of 10^{17} s.

Quantum Monte Carlo Motivation

As an example from the nuclear many-body problem, we have Schroedinger's equation as a differential equation

$$\hat{H}\Psi(\boldsymbol{r}_1,..,\boldsymbol{r}_A,\alpha_1,..,\alpha_A) = E\Psi(\boldsymbol{r}_1,..,\boldsymbol{r}_A,\alpha_1,..,\alpha_A)$$

where

$$\boldsymbol{r}_1,..,\boldsymbol{r}_A,$$

are the coordinates and

$$\alpha_1,..,\alpha_A,$$

are sets of relevant quantum numbers such as spin and isospin for a system of A nucleons ($A = N + Z$, N being the number of neutrons and Z the number of protons).

Quantum Monte Carlo Motivation

There are

$$2^A \times \begin{pmatrix} A \\ Z \end{pmatrix}$$

coupled second-order differential equations in $3A$ dimensions.
For a nucleus like beryllium-10 this number is **215040**. This is a truely challenging many-body problem.
Methods like partial differential equations can at most be used for 2-3 particles.

Quantum Monte Carlo Motivation

- Monte-Carlo methods
- Renormalization group (RG) methods, in particular density matrix RG
- Large-scale diagonalization (Iterative methods, Lanczo's method, dimensionalities 10^{10} states)
- Coupled cluster theory, favoured method in quantum chemistry, molecular and atomic physics. Applications to ab initio calculations in nuclear physics as well for large nuclei.
- Perturbative many-body methods
- Green's function methods
- Density functional theory/Mean-field theory and Hartree-Fock theory

The physics of the system hints at which many-body methods to use.

Quantum Monte Carlo Motivation

Pros and Cons of Monte Carlo

- Is physically intuitive.
- Allows one to study systems with many degrees of freedom. Diffusion Monte Carlo (DMC) and Green's function Monte Carlo (GFMC) yield in principle the exact solution to Schroedinger's equation.
- Variational Monte Carlo (VMC) is easy to implement but needs a reliable trial wave function, can be difficult to obtain. This is where we will use Hartree-Fock theory to construct an optimal basis.
- DMC/GFMC for fermions (spin with half-integer values, electrons, baryons, neutrinos, quarks) has a sign problem. Nature prefers an anti-symmetric wave function. PDF in this case given distribution of random walkers ($p \geq 0$).
- The solution has a statistical error, which can be large.
- There is a limit for how large systems one can study, DMC needs a huge number of random walkers in order to achieve

Quantum Monte Carlo Motivation

Where and why do we use Monte Carlo Methods in Quantum Physics

- Quantum systems with many particles at finite temperature: Path Integral Monte Carlo with applications to dense matter and quantum liquids (phase transitions from normal fluid to superfluid). Strong correlations.
- Bose-Einstein condensation of dilute gases, method transition from non-linear PDE to Diffusion Monte Carlo as density increases.
- Light atoms, molecules, solids and nuclei.
- Lattice Quantum-Chromo Dynamics. Impossible to solve without MC calculations.
- Simulations of systems in solid state physics, from semiconductors to spin systems. Many electrons active and possibly strong correlations.

Quantum Monte Carlo Motivation

Given a hamiltonian H and a trial wave function Ψ_T, the variational principle states that the expectation value of $\langle H \rangle$, defined through

$$E[H] = \langle H \rangle = \frac{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) H(\boldsymbol{R}) \Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) \Psi_T(\boldsymbol{R})},$$

is an upper bound to the ground state energy E_0 of the hamiltonian H, that is

$$E_0 \leq \langle H \rangle.$$

In general, the integrals involved in the calculation of various expectation values are multi-dimensional ones. Traditional integration methods such as the Gauss-Legendre will not be adequate for say the computation of the energy of a many-body system.

Quantum Monte Carlo Motivation

The trial wave function can be expanded in the eigenstates of the hamiltonian since they form a complete set, viz.,

$$\Psi_T(\boldsymbol{R}) = \sum_i a_i \Psi_i(\boldsymbol{R}),$$

and assuming the set of eigenfunctions to be normalized one obtains

$$\frac{\sum_{nm} a_m^* a_n \int d\boldsymbol{R} \Psi_m^*(\boldsymbol{R}) H(\boldsymbol{R}) \Psi_n(\boldsymbol{R})}{\sum_{nm} a_m^* a_n \int d\boldsymbol{R} \Psi_m^*(\boldsymbol{R}) \Psi_n(\boldsymbol{R})} = \frac{\sum_n a_n^2 E_n}{\sum_n a_n^2} \geq E_0,$$

where we used that $H(\boldsymbol{R})\Psi_n(\boldsymbol{R}) = E_n \Psi_n(\boldsymbol{R})$. In general, the integrals involved in the calculation of various expectation values are multi-dimensional ones. The variational principle yields the lowest state of a given symmetry.

Quantum Monte Carlo Motivation

In most cases, a wave function has only small values in large parts of configuration space, and a straightforward procedure which uses homogenously distributed random points in configuration space will most likely lead to poor results. This may suggest that some kind of importance sampling combined with e.g., the Metropolis algorithm may be a more efficient way of obtaining the ground state energy. The hope is then that those regions of configurations space where the wave function assumes appreciable values are sampled more efficiently.

Quantum Monte Carlo Motivation

The tedious part in a VMC calculation is the search for the variational minimum. A good knowledge of the system is required in order to carry out reasonable VMC calculations. This is not always the case, and often VMC calculations serve rather as the starting point for so-called diffusion Monte Carlo calculations (DMC). DMC is a way of solving exactly the many-body Schroedinger equation by means of a stochastic procedure. A good guess on the binding energy and its wave function is however necessary. A carefully performed VMC calculation can aid in this context.

Quantum Monte Carlo Motivation

- Construct first a trial wave function $\psi_T(\boldsymbol{R}, \boldsymbol{\alpha})$, for a many-body system consisting of N particles located at positions

$\boldsymbol{R} = (\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N)$. The trial wave function depends on α variational parameters $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_M)$.

- Then we evaluate the expectation value of the hamiltonian H

$$E[H] = \langle H \rangle = \frac{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha}) H(\boldsymbol{R}) \Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha}) \Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}.$$

- Thereafter we vary α according to some minimization algorithm and return to the first step.

Quantum Monte Carlo Motivation

Basic steps

Choose a trial wave function $\psi_T(\boldsymbol{R})$.

$$P(\boldsymbol{R}) = \frac{|\psi_T(\boldsymbol{R})|^2}{\int |\psi_T(\boldsymbol{R})|^2 \, d\boldsymbol{R}}.$$

This is our new probability distribution function (PDF). The approximation to the expectation value of the Hamiltonian is now

$$E[H(\boldsymbol{\alpha})] = \frac{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha}) H(\boldsymbol{R}) \Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha}) \Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}.$$

Quantum Monte Carlo Motivation

Define a new quantity

$$E_L(\boldsymbol{R},\boldsymbol{\alpha}) = \frac{1}{\psi_T(\boldsymbol{R},\boldsymbol{\alpha})} H\psi_T(\boldsymbol{R},\boldsymbol{\alpha}),$$

called the local energy, which, together with our trial PDF yields

$$E[H(\boldsymbol{\alpha})] == \int P(\boldsymbol{R}) E_L(\boldsymbol{R}) d\boldsymbol{R} \approx \frac{1}{N}\sum_{i=1}^{N} P(\boldsymbol{R_i},\boldsymbol{\alpha}) E_L(\boldsymbol{R_i},\boldsymbol{\alpha})$$

with N being the number of Monte Carlo samples.
In this course, the second project deals with a variational Monte Carlo calculation of quantum dots. We need however a good input for the trial wave function. Hartree-Fock theory will provide us with an optimized single-particle basis. Our first project deals thus with the computation of an optimized Hartree-Fock basis for quantum dot calculations.