Introduction to Computational Physics Lectures, FYS4411/9411

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Aims

- Be able to apply two central many-particle methods like the Variational Monte Carlo method to properties of many-fermion systems and many-boson systems.
- 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. First time January 18.
- Computerlab: Thursday (4.15pm-7pm), first time January 18, last lab session May 10.
- Weekly plans and all other information are on the webpage
- Intensive week starts March 5 and ends March 8, week 10.
- **First project to be handed in March 16**.
- **Second and final project to be handed in June 1.**
- 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
- For project 2 there will be three variants:
  1. Variational Monte Carlo for fermions
  2. Coupled cluster theory for fermions (iterative methods)
  3. Neural networks and Machine Learning to solve the same problems as in project 1

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
- Data analysis and resampling techniques
- Variational Monte Carlo (VMC) for 'ab initio' studies of quantum mechanical many-body systems.
- Simulation of two-dimensional systems like quantum dots (project 2).
- Simulation of trapped bosons using VMC (project 1)
- Machine learning and neural networks (project 2)
- Coupled cluster theory (project 2)

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.

Various many-body methods

- 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.