Format for delivery of report and programs

The format of the project is that of a printed file or hand-written report. The programs should also be included with the report. Write **only your candidate number** on the first page of the report and state clearly that this is your report for the last project of FYS3150/FYS4150, fall 2014. The project counts 50% of the final mark. If you have collaborated with one or more fellow students, please state the respective candidate number(s). There will be a box marked 'FYS3150/FYS4150' at the reception of the Department of Physics (room FV128).

We encourage you to work two and two together. Optimal working groups consist of 2-3 students. You can then hand in a common report.

Project 3 - Variational Monte Carlo project (version 1), deadline December 1 at noon

The aim of this project is to use the Variational Monte Carlo (VMC) method to evaluate the ground state energy, onebody densities, expectation values of the kinetic and potential energies and single-particle energies of quantum dots with $N = 2$ and $N = 6$ electrons, so-called closed shell systems. The project requires some reading background. The essential background is given in chapters 11, 12, 14 and 16 of the lecture notes, with the latter being the most important one, containing code examples as well. The project contains also optional paths where programming of the Monte Carlo solver on GPUs can be done.

The systems we will focus on are two-dimensional ones, with electrons confined to move in harmonic oscillator like traps. As such, this project can be seen as a continuation of project 2, except that we now focus on two dimensions only. We have again some analytical results for the interacting two-electron case thans to M. Taut, see the reference list below.

These systems are called quantum dots and constitute a lively research area in condensed matter physics and materials science, with applications spanning from the contruction of quantum circuits to applications to solar cells and nano-medicine, see `http://en.wikipedia.org/wiki/Quantum_dot` for a general overview.

Our aim here is to use the variational Monte Carlo method to study such systems, with an emphasis on understanding correlations due to the repulsive interaction between electrons.

Theoretical background and description of the physical system

We consider a system of electrons confined in a pure two-dimensional isotropic harmonic oscillator potential, with an idealized total Hamiltonian given by

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 \right) + \sum_{i<j} \frac{1}{r_{ij}}, \tag{1}$$

where natural units ($\hbar = c = e = m_e = 1$) are used and all energies are in so-called atomic units a.u. We will study systems of many electrons N as functions of the oscillator frequency ω using the above Hamiltonian. The Hamiltonian includes a standard harmonic oscillator part

$$\hat{H}_0 = \sum_{i=1}^{N} \left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 \right),$$

and the repulsive interaction between two electrons given by

$$\hat{H}_1 = \sum_{i<j} \frac{1}{r_{ij}},$$

with the distance between electrons given by $r_{ij} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$. We define the modulus of the positions of the electrons (for a given electron i) as $r_i = \sqrt{r_{i_x}^2 + r_{i_y}^2}$.

1a) In exercises 1a-1d we will deal only with a system of two electrons in a quantum dot with a frequency of $\hbar\omega = 1$. The reason for this is that we have exact closed form expressions for the ground state energy from Taut's work for selected values of ω, see M. Taut, J. Phys. A **27**, 1045 (1994). The energy is given by 3 a.u. (atomic units) when the interaction between the electrons is included. If we only include the harmonic oscillator part of the Hamiltonian, the so-called unperturbed part,

$$\hat{H}_0 = \sum_{i=1}^{N} \left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 \right),$$

the energy is 2 a.u. This serves as an excellent benchmark when we develop our code. The wave function for one electron in an oscillator potential in two dimensions is

$$\phi_{n_x,n_y}(x,y) = A H_{n_x}(\sqrt{\omega}x) H_{n_y}(\sqrt{\omega}y) \exp\left(-\omega(x^2+y^2)/2\right).$$

The functions $H_{n_x}(\sqrt{\omega}x)$ are so-called Hermite polynomials, discussed in the appendix here while A is a normalization constant. For the lowest-lying state we have $n_x = n_y = 0$ and an energy $\epsilon_{n_x,n_y} = \omega(n_x + n_y + 1) = \omega$. Convince yourself that the lowest-lying energy for the two-electron system is simply 2ω.

The unperturbed wave function for the ground state of the two-electron system is given by

$$\Phi(\mathbf{r_1}, \mathbf{r_2}) = C \exp\left(-\omega(r_1^2 + r_2^2)/2\right),$$

with C being a normalization constant and $r_i = \sqrt{r_{i_x}^2 + r_{i_y}^2}$. Note that the vector $\mathbf{r_i}$ refers to the x and y position for a given particle. What is the total spin of this wave function? Find arguments for why the ground state should have this specific total spin.

1b) We want to perform a Variational Monte Carlo calculation of the ground state of two electrons in a quantum dot well with different oscillator energies, assuming total spin $S = 0$ using the Hamiltonian of Eq. (1). In our first attempt we will use a brute force Metropolis sampling with a trial wave function which has the following form

$$\psi_T(\mathbf{r_1}, \mathbf{r_2}) = C \exp\left(-\alpha\omega(r_1^2 + r_2^2)/2\right) \exp\left(\frac{ar_{12}}{(1 + \beta r_{12})}\right), \qquad (2)$$

where a is equal to one when the two electrons have anti-parallel spins and $1/3$ when the spins are parallel. Finally, α and β are our variational parameters.

Your task is to perform a Variational Monte Carlo calculation using the Metropolis algorithm to compute the integral

$$\langle E \rangle = \frac{\int d\mathbf{r_1} d\mathbf{r_2} \psi_T^*(\mathbf{r_1}, \mathbf{r_2}) \hat{H}(\mathbf{r_1}, \mathbf{r_2}) \psi_T(\mathbf{r_1}, \mathbf{r_2})}{\int d\mathbf{r_1} d\mathbf{r_2} \psi_T^*(\mathbf{r_1}, \mathbf{r_2}) \psi_T(\mathbf{r_1}, \mathbf{r_2})}. \qquad (3)$$

You should parallelize your program. As an optional possibility, to program GPUs can be used instead of standard parallelization with MPI throughout the project. The GPU part is optional, see below. Chapter 14 of the lecture notes contain all relevant material.

Find the energy minimum and compute also the mean distance $r_{12} = \sqrt{\mathbf{r_1} - \mathbf{r_2}}$ (with $r_i = \sqrt{r_{i_x}^2 + r_{i_y}^2}$) between the two electrons for the optimal set of the variational parameters. A code for doing a VMC calculation for a two-electron system (the three-dimensional helium atom) can be found on the webpage of the course, see under programs for chapter 14. To find the energy you can use numerical derivation. To perform the calculations with an analytical expression for the local energy is an optional exercise, see below.

It is convenient to make modules or classes of trial wave functions, both many-body wave functions and single-particle wave functions and the quantum numbers involved, such as spin, value of n_x and n_y quantum numbers.

1c) Introduce now importance sampling and study the dependence of the results as a function of the time step δt. Compare the results with those obtained in the previous exercise and comment eventual differences. The code has to run in parallel.

1d) With the optimal parameters for the ground state wave function, and compute the expectation value of the kinetic energy and potential energy using $\omega = 0.01$, $\omega = 0.28$ and $\omega = 1.0$. How important are the correlations introduced by the Jastrow factor? Comment your results.

The previous exercises have prepared you for extending your calculational machinery to other systems. Here we will focus on quantum dots with $N = 6$ electrons.

The new item you need to pay attention to is the calculation of the Slater Determinant. This is an additional complication to your VMC calculations. If we stick to harmonic oscillator like wave functions, the trial wave function for say an $N = 6$ electron quantum dot can be written as

$$\psi_T(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_6}) = Det\,(\phi_1(\mathbf{r_1}), \phi_2(\mathbf{r_2}), \ldots, \phi_6(\mathbf{r_6})) \prod_{i<j}^{6} \exp\left(\frac{ar_{ij}}{(1 + \beta r_{ij})}\right), \qquad (4)$$

where Det is a Slater determinant and the single-particle wave functions are the harmonic oscillator wave functions for the $n_x = 0, 1$ and $n_y = 0, 1$ orbitals. Observe that $r_i = \sqrt{r_{i_x}^2 + r_{i_y}^2}$. Use the Hermite polynomials defined in the appendix.

(1e) Write a function which sets up the Slater determinant in order to be able to handle larger systems as well. Find the Hermite polynomials which are needed for $n_x = 0, 1, 2$ and obviously n_y as well. Compute the ground state energies of quantum dots for $N = 6$ electrons for $\omega = 0.01$, $\omega = 0.28$ and $\omega = 1.0$. The calculations should include parallelization and importance sampling. To test your Slater determinant code, you should reproduce the unperturbed single-particle energies when the electron-electron repulsion is switched off. Convince yourself that the unperturbed ground state energy for $N = 6$ is 10ω. What is the expected total spin of the ground states?

The Slater determinant for six electrons is given by a 6×6 matrix which can rewritten as the product of two 3×3 Slater determinants, one for electrons with spin up and one for electrons with spin down, as described in chapter 16 of the lecture notes. The simplest way to calculate these Slater determinants is to set up a function which calculates a 3×3 determinant using Cramer's rule. You can then place the first three electrons to have spin up and electrons four to six to have spin up down. If you get time, you can also implement the optimal algorithm for setting up the update of the Slater determinant as discussed in chapter 16 of the lecture notes. The latter is optional.

1f) Finally, we want to test the virial theorem for a range of frequencies. The virial theorem states that the expectation value of the total kinetic energy $\langle T \rangle$ is proportional to the expectation value of the total potential energy $\langle V \rangle$. For a pure harmonic oscillator this proportionality is given by

$$\langle T \rangle = \langle V \rangle.$$

Use your optimal results for $\omega = 0.01$, $\omega = 0.28$ and $\omega = 1.0$ and add to these other values in the range $\omega \in [0.01, 1]$ and compute the expectation value of the kinetic energy and potential energy with and without the repulsive interaction between electrons for $N = 2$ and $N = 6$. Plot the ratio $\langle T \rangle / \langle V \rangle$ as function of ω and comment your results.

1g) This exercise is optional and gives an additional 30%. You can choose between two options here: 1) Find closed-form expressions for the local energy and the quantum force used in importance sampling and compare the results of these calculations (in terms of CPU time) with the calculations that perform a brute force numerical derivation for both $N = 2$ and $N = 6$. Discuss the results for the total energy only. The second alternative 2) is to implement exercises 1a-1f) using GPUs without setting up the closed form expressions for the local energy and the quantum force.

Additional material on Hermite polynomials

The Hermite polynomials are the solutions of the following differential equation

$$\frac{d^2 H(x)}{dx^2} - 2x\frac{dH(x)}{dx} + (\lambda - 1)H(x) = 0. \tag{5}$$

The first few polynomials are

$$H_0(x) = 1,$$
$$H_1(x) = 2x,$$
$$H_2(x) = 4x^2 - 2,$$
$$H_3(x) = 8x^3 - 12x,$$

and

$$H_4(x) = 16x^4 - 48x^2 + 12.$$

They fulfil the orthogonality relation

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x)^2 dx = 2^n n! \sqrt{\pi},$$

and the recursion relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

Literature

1. M. Taut, J. Phys. A **27**, 1045 (1994).

2. B. L. Hammond, W. A. Lester and P. J. Reynolds, *Monte Carlo methods in Ab Initio Quantum Chemistry*, World Scientific, Singapore, 1994, chapters 2-5 and appendix B.

3. B.H. Bransden and C.J. Joachain, Physics of Atoms and molecules, Longman, 1986. Chapters 6, 7 and 9.

4. A. K. Rajagopal and J. C. Kimball, see Phys. Rev. B **15**, 2819 (1977).

5. M. Pedersen Lohne, G. Hagen, M. Hjorth-Jensen, S. Kvaal, and F. Pederiva, Phys. Rev. B **84**, 115302 (2011).