

Introduction to numerical projects

Here follows a brief recipe and recommendation on how to write a report for each project.

- Give a short description of the nature of the problem and the eventual numerical methods you have used.
- Describe the algorithm you have used and/or developed. Here you may find it convenient to use pseudocoding. In many cases you can describe the algorithm in the program itself.
- Include the source code of your program. Comment your program properly.
- If possible, try to find analytic solutions, or known limits in order to test your program when developing the code.
- Include your results either in figure form or in a table. Remember to label your results. All tables and figures should have relevant captions and labels on the axes.
- Try to evaluate the reliability and numerical stability/precision of your results. If possible, include a qualitative and/or quantitative discussion of the numerical stability, eventual loss of precision etc.
- Try to give an interpretation of your results in your answers to the problems.
- Critique: if possible include your comments and reflections about the exercise, whether you felt you learnt something, ideas for improvements and other thoughts you've made when solving the exercise. We wish to keep this course at the interactive level and your comments can help us improve it.
- Try to establish a practice where you log your work at the computerlab. You may find such a logbook very handy at later stages in your work, especially when you don't properly remember what a previous test version of your program did. Here you could also record the time spent on solving the exercise, various algorithms you may have tested or other topics which you feel worthy of mentioning.

Format for electronic delivery of report and programs

The preferred format for the report is a PDF file. You can also use DOC or postscript formats or an ipython notebook file ipynb. As programming language we prefer that you choose between C/C++, Fortran2008 or Python. The following prescription should be followed when preparing the report:

- Use Devilry to hand in your projects, log in at <http://devilry.ifi.uio.no> with your normal UiO username and password and choose either 'fys3150' or 'fys4150'. There you can load up the files within the deadline.

- Upload **only** the report file! For the source code file(s) you have developed please provide us with your link to your github domain.
- Comments from us on your projects, approval or not, corrections to be made etc can be found under your Devilry domain and are only visible to you and the teachers of the course.

Finally, 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 $N = 2$, $N = 6$ and $N = 12$ electrons, so-called closed shell systems. The project requires some reading background. The essential background is given in chapters 11, 12 and 14 of the lecture notes, with the latter being the most important one, containing code examples as well. Additional teaching sessions will be held during week 41. 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 thanks 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 construction 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

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

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 $r_{ij} = \sqrt{\mathbf{r}_i - \mathbf{r}_j}$. We define the modulus of the positions of the electrons (for a given electron i) as $r_i = \sqrt{r_{ix}^2 + r_{iy}^2}$.

- 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, Phys. Rev. A **48**, 3561 (1993). 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

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

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

$$\Phi(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\omega(r_1^2 + r_2^2)/2),$$

with C being a normalization constant and $r_i = \sqrt{r_{ix}^2 + r_{iy}^2}$. 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

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \exp\left(\frac{ar_{12}}{(1 + \beta r_{12})}\right), \quad (2)$$

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

$$\langle E \rangle = \frac{\int d\mathbf{r}_1 d\mathbf{r}_2 \psi_T^*(\mathbf{r}_1, \mathbf{r}_2) \hat{H}(\mathbf{r}_1, \mathbf{r}_2) \psi_T(\mathbf{r}_1, \mathbf{r}_2)}{\int d\mathbf{r}_1 d\mathbf{r}_2 \psi_T^*(\mathbf{r}_1, \mathbf{r}_2) \psi_T(\mathbf{r}_1, \mathbf{r}_2)}. \quad (3)$$

You should parallelize your program. As an optional possibility, to program GPUs can be used instead of standard parallelization with MPI throughout the project. 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 $r_i = \sqrt{r_{ix}^2 + r_{iy}^2}$) 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.

You should also find a closed-form expression for the local energy. Compare the results of this calculation (in terms of CPU time) compared with a calculation which performs a brute force numerical derivation.

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, compute the one-body density. Discuss your results and compare the results with those obtained with a pure harmonic oscillator wave functions. Run a Monte Carlo calculations without the Jastrow factor as well and compute the same quantities. How important are the correlations induced by the Jastrow factor? Compute also the expectation value of the kinetic energy and potential energy using $\omega = 0.01$, $\omega = 0.28$ and $\omega = 1.0$. 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 $N = 6$ and $N = 12$ 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

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_6) = \text{Det}(\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \dots, \phi_6(\mathbf{r}_6)) \prod_{i < j}^6 \exp\left(\frac{ar_{ij}}{(1 + \beta r_{ij})}\right), \quad (4)$$

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. For the $N = 12$ quantum dot, the trial wave function can take the form

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_{12}) = \text{Det}(\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \dots, \phi_{12}(\mathbf{r}_{12})) \prod_{i < j}^{12} \exp\left(\frac{ar_{ij}}{2(1 + \beta r_{ij})}\right), \quad (5)$$

In this case you need to include the $n_x = 2$ and $n_y = 2$ wave functions as well. Observe that $r_i = \sqrt{r_{ix}^2 + r_{iy}^2}$. 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 $N = 6$ and $N = 12$ 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 energies for $N = 6$ is 10ω and for $N = 12$ we obtain 28ω . What is the expected total spin of the ground states?
- 1f) With the optimal parameters for the ground state wave function, compute again the onebody density. Discuss your results and compare the results with those obtained with a pure harmonic oscillator wave functions. Run a Monte Carlo calculations without the Jastrow factor as well and compute the same quantities. How important are the correlations induced by the Jastrow factor?
- 1g) 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 $N = 2$, $N = 6$ and $N = 12$. Plot the ratio $\langle T \rangle / \langle V \rangle$ as function of ω and comment your results.

Additional material on Hermite polynomials

The Hermite polynomials are the solutions of the following differential equation

$$\frac{d^2 H(x)}{dx^2} - 2x \frac{dH(x)}{dx} + (\lambda - 1)H(x) = 0. \quad (6)$$

The first few polynomials are

$$\begin{aligned} H_0(x) &= 1, \\ H_1(x) &= 2x, \\ H_2(x) &= 4x^2 - 2, \\ H_3(x) &= 8x^3 - 12x, \end{aligned}$$

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, Phys. Rev. A **48**, 3561 - 3566 (1993).
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).