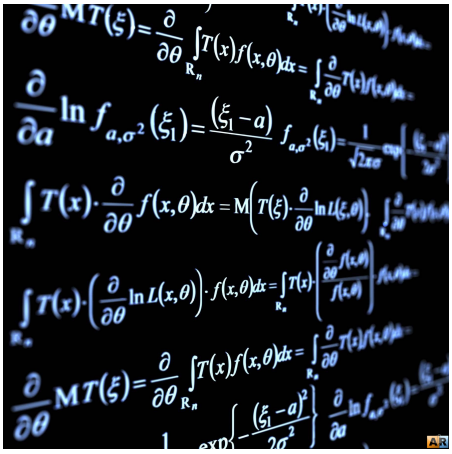

Project 3

FYS3150 - Computational physics

Quantum dots

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November 21, 2014

Abstract

Here is a short summary of the project.

Contents

1 Introduction

Quantum mechanics is an exciting field.

2 Theory

Here is all the theory needed to understand the project.

2.1 The physical system

This is the section explaining the physics of the system. Throughout the project, *natural units* are used ($\hbar = 1$,$c = 1$,$e = 1$,$m_e = 1$) and all energies are in so-called *atomix units* a.u.

2.1.1 The quantum mechanics and the variational principle

2.1.1.1 The quantum mechanics

In this project we will look at a system of N electrons in a so-called *quantum dot*. That is, a two dimensional harmonic oscillator with potential

$$V(\vec{r}) = \frac{1}{2}\omega^2 r^2 \tag{2.1.1}$$

This potential gives rise to a multi-particle Hamiltonian $\hat{H}$ given as the sum of an ordinary Hamiltonian and an electron repulsive part

$$\hat{H} = \sum_{i=1}^{N}\left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{r_{ij}} \tag{2.1.2}$$

Where $r_{ij} = |\vec{r}_i - \vec{r}_j|$ is the distance between the electrons i and j and $r_i = |\vec{r}_i| = \sqrt{x_i^2 + y_i^2}$ when $\vec{r}_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix}$. Our goal in this project is to find the ground eigenstate and energy of this multi-particle Hamiltonian numerically.

2.1.1.2 The variational principle

We will approach this by constructing a real test function $\Psi_T(\vec{r}_0, \vec{r}_1, ..., \vec{r}_{N-1}, \alpha, \beta)$ dependent on two parameters α and β and calculate the expextation value of the hamilton operator $\langle\hat{H}\rangle$. As we know, the orthonormal eigenstates Ψ_i of the Hamiltonian forms a complete basis, so any state, including our test state Ψ_T, can be written as a linear combination of the eigenstates

$$\Psi_T = \sum_i c_i \Psi_i \tag{2.1.3}$$

Inserting this expression into the equation for the expectation value of $\hat{H}$ gives

$$\langle \hat{H} \rangle = \frac{\int \Psi_T \hat{H} \Psi_T d\vec{r}}{\int \Psi_T \Psi_T d\vec{r}} = \frac{\int \left(\sum_i c_i^* \Psi_i^*\right) \hat{H} \left(\sum_i c_i \Psi_i\right) d\vec{r}}{\int \left(\sum_i c_i^* \Psi_i^*\right) \left(\sum_i c_i \Psi_i\right) d\vec{r}} = \frac{\int \left(\sum_i c_i^* \Psi_i^*\right) \left(\sum_i c_i E_i \Psi_i\right) d\vec{r}}{\int \left(\sum_i c_i^* \Psi_i^*\right) \left(\sum_i c_i \Psi_i\right) d\vec{r}}$$
$$= \frac{\sum_i |c_i|^2 E_i}{\sum_i |c_i|} \tag{2.1.4}$$

The energy of the ground state E_0 is smaller than all other E_i's so

$$\frac{\sum_i |c_i|^2 E_i}{\sum_i |c_i|} \geq \frac{\sum_i |c_i|^2 E_0}{\sum_i |c_i|} = E_0 \frac{\sum_i |c_i|^2}{\sum_i |c_i|} = E_0 \tag{2.1.5}$$

$$\langle H \rangle \geq E_0 \tag{2.1.6}$$

This simple observation is called *the variational principle* and is what we will use to narrow our search for the optimal parameters α and β. We will look for the parameters α and β that gives us the smallest value of $\langle \hat{H} \rangle$ and this will be our estimate for the ground state energy.

2.1.1.3 Finding the expectation value of $\hat{H}$

We have

$$\langle \hat{H} \rangle = \frac{\int \Psi_T \hat{H} \Psi_T d\vec{r}}{\int \Psi_T \Psi_T d\vec{r}} = \int \frac{\Psi_T \Psi_T}{\int \Psi_T \Psi_T d\vec{r}} \frac{1}{\Psi_T} \hat{H} \Psi_T d\vec{r} \tag{2.1.7}$$

If we rename probability density function of the particles

$$\frac{\Psi_T \Psi_T}{\int \Psi_T \Psi_T d\vec{r}} = P(\vec{r}) \tag{2.1.8}$$

And introduce the local energy

$$E_L(\vec{r}) = \frac{1}{\Psi_T} \hat{H} \Psi_T \tag{2.1.9}$$

The integral becomes

$$\langle \hat{H} \rangle = \int P(\vec{r}) E_L(\vec{r}) d\vec{r} = \langle E_L \rangle \tag{2.1.10}$$

Thus, to calculate the expectation value of $\hat{H}$ we can just calculate the expectation value of the local energy.

2.1.1.4 Verifying that we have found an eigenstate

We could very well find a minimum of $\langle \hat{H} \rangle$ that is not an eigen energy of the system, i.e. still larger than E_0. To address this problem, let's look at the variance V_{E_L} of $\langle E_L \rangle$.

$$V_{E_L} = \langle E_L^2 \rangle - \langle E_L \rangle^2 = \int P(\vec{r}) \left(\frac{1}{\Psi_T} \hat{H} \Psi_T \right)^2 d\vec{r} - \left(\int P(\vec{r}) \frac{1}{\Psi_T} \hat{H} \Psi_T d\vec{r} \right)^2 \tag{2.1.11}$$

Since

$$\begin{aligned}\langle (E_L - \langle E_L \rangle)^2 \rangle &= \langle E_L^2 - 2E_L\langle E_L\rangle + \langle E_L\rangle^2 \rangle = \langle E_L^2\rangle - 2\langle E_L\rangle\langle E_L\rangle + \langle E_L\rangle^2 \\ &= \langle E_L^2\rangle - \langle E_L\rangle^2 = V_{E_L}\end{aligned} \tag{2.1.12}$$

We have that if $V_{E_L} = 0$, then

$$\langle (E_L - \langle E_L \rangle)^2 \rangle = 0 \tag{2.1.13}$$

$$0 = \int \left(P(\vec{r}) E_L(\vec{r}) - \int P(\vec{r}) E_L(\vec{r}) d\vec{r} \right)^2 d\vec{r} = \int \left(\frac{1}{\Psi_T} \hat{H}\Psi_T - \int \Psi_T \hat{H} \Psi_T d\vec{r} \right)^2 d\vec{r} \tag{2.1.14}$$

When the Hamiltonian acts on a real function, it gives a real function. And since Ψ_T is real $\frac{1}{\Psi_T}\hat{H}\Psi_T - \int \Psi_T \hat{H}\Psi_T d\vec{r}$ is real. By consequence

$$\left(\frac{1}{\Psi_T} \hat{H}\Psi_T - \int \Psi_T \hat{H} \Psi_T d\vec{r} \right)^2 > 0 \tag{2.1.15}$$

Which means that for the integral in equation 2.1.14 to be zero, the following must be true for all $\vec{r}$

$$\frac{1}{\Psi_T} \hat{H}\Psi_T - \int \Psi_T \hat{H} \Psi_T d\vec{r} = 0 \tag{2.1.16}$$

$$\Psi_T \hat{H}\Psi_T = \int \Psi_T \hat{H} \Psi_T d\vec{r} \tag{2.1.17}$$

The right hand side of this equation is just a real number. Naming this number E gives

$$\frac{1}{\Psi_T} \hat{H}\Psi_T = E \tag{2.1.18}$$

$$\hat{H}\Psi_T = E\Psi_T \tag{2.1.19}$$

Which is nothing but the eigenvalue equation stating that Ψ_T is an eigenstate of $\hat{H}$. This will serve as a test to see if the state we have found when minimizing the expectation value of E_L is an eigenstate of the Hamilton operator. It is just as easily (perhaps easier) shown that if Ψ_T *is* and eigenstate of $\hat{H}$, then the variance of the local energy is 0. This means that if the variance of our test function is *not* 0, then it is *not* an eigenfunction of $\hat{H}$. We can summarize this discussion as follows

$$\boxed{V_{E_L} = 0 \quad \text{if and only if} \quad \Psi_T \text{ is an eigenstate of } \hat{H}} \tag{2.1.20}$$

2.1.2 The test function Ψ_T

We will in this project use the trial wavefunctions of $\vec{r}_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix}$ given by

$$\Psi_T(\vec{r}_0, ..., \vec{r}_{N-1}) = \mathrm{Det}_M(\phi_0, ..., \phi_{N-1}) \cdot \mathrm{J}(\vec{r}_0, ..., \vec{r}_{N-1}) \tag{2.1.21}$$

2.1.2.1 The modified Slater determinant $\mathbf{Det}_M(\phi_0, ..., \phi_{N-1})$

$\mathrm{Det}_M(\phi_0, ..., \phi_{N-1})$ is a modified *Slater determinant* defined as

$$\mathrm{Det}_M(\phi_0, ..., \phi_{N-1}) = |U| \cdot |D|$$
$$\begin{vmatrix} \phi_0(\vec{r}_0) & \phi_2(\vec{r}_0) & ... & \phi_{N-2}(\vec{r}_0) \\ \phi_0(\vec{r}_2) & \phi_2(\vec{r}_2) & ... & \phi_{N-2}(\vec{r}_2) \\ ... & ... & ... & ... \\ \phi_0(\vec{r}_{N-2}) & \phi_2(\vec{r}_{N-2}) & ... & \phi_{N-2}(\vec{r}_{N-2}) \end{vmatrix} \cdot \begin{vmatrix} \phi_1(\vec{r}_1) & \phi_3(\vec{r}_1) & ... & \phi_{N-1}(\vec{r}_1) \\ \phi_1(\vec{r}_3) & \phi_3(\vec{r}_3) & ... & \phi_{N-1}(\vec{r}_3) \\ ... & ... & ... & ... \\ \phi_1(\vec{r}_{N-1}) & \phi_3(\vec{r}_{N-1}) & ... & \phi_{N-1}(\vec{r}_{N-1}) \end{vmatrix} \tag{2.1.22}$$

Where $\phi_i(\vec{r}_i)$ is a wavefunction resembling one of the eigenfunctions of the Hamilton operator for *one* particle in a two dimensional harmonic oscillator, but parameterized by α in the following way:

$$\phi_i(\vec{r}_j) = H_{n_x}(\sqrt{\alpha\omega}x_j)H_{n_y}(\sqrt{\alpha\omega}y_j)\exp(-\alpha\omega(x^2+y^2)/2) \tag{2.1.23}$$

The reason for this modified version of the Slater determinant (whose real form can be explored elsewhere[1]) is that the spin parts of the wavefunctions are not incorporated in the expressions of $\phi_i(\vec{r}_j)$. The result is that if we were to insert these into a regular Slater determinant we would get 0, everytime. The modified Slater determinant Det_M avoids this issue while still conserving some of the most important properties of the Slater determinant.

$n_x(i)$ and $n_y(i)$ corresponds to the quantum numbers needed to "fill up" the system from the lowest energy levels twice (one for each spin configuration). For $i < 12$, the explicit depence of n_x, n_y on i is given in table 2.1.1.

$i =$	0	1	2	3	4	5	6	7	8	9	10	11
$n_x =$	0	0	1	1	0	0	2	2	1	1	0	0
$n_y =$	0	0	0	0	1	1	0	0	1	1	2	2

Table 2.1.1: The explicit dependence of n_x and n_y on i in the construction of the trial wavefunctions.

2.1.2.2 The Jastrow factor $\mathbf{J}(\vec{r}_0, ..., \vec{r}_{N-1})$

$\mathrm{J}(\vec{r}_0, ..., \vec{r}_{N-1})$ is a so-called *Jastrow factor*, which represents the electron repulsion part of the wavefunction, defined as

$$\mathrm{J}(\vec{r}_0, ...\vec{r}_{N-1}) = \prod_{i<j}^{N} \exp\left(\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}\right)$$
$$\text{where} \quad r_{ij} = |\vec{r}_i - \vec{r}_j| \quad \text{and} \quad a_{ij} = \begin{cases} 1/3 & \text{if spin(i) and spin(j) are parallell} \\ 1 & \text{if spin(i) and spin(j) are anti-parallell} \end{cases} \tag{2.1.24}$$

[1] http://en.wikipedia.org/wiki/Slater_determinant

From the expression of the Jastrow factor, we see that it is zero whenever $r_{ij} = 0$ for any pair $i \neq j$. This is what we want from such a factor, namely that the wavefunction is zero whenever there is no distance between two particles (i.e. $r_{ij} = 0$).

2.1.2.3 Motivation

The motivation of such a trial wavefunction is that it is partly made of the unperturbed harmonic oscillator ground states. See figure 2.1.1.

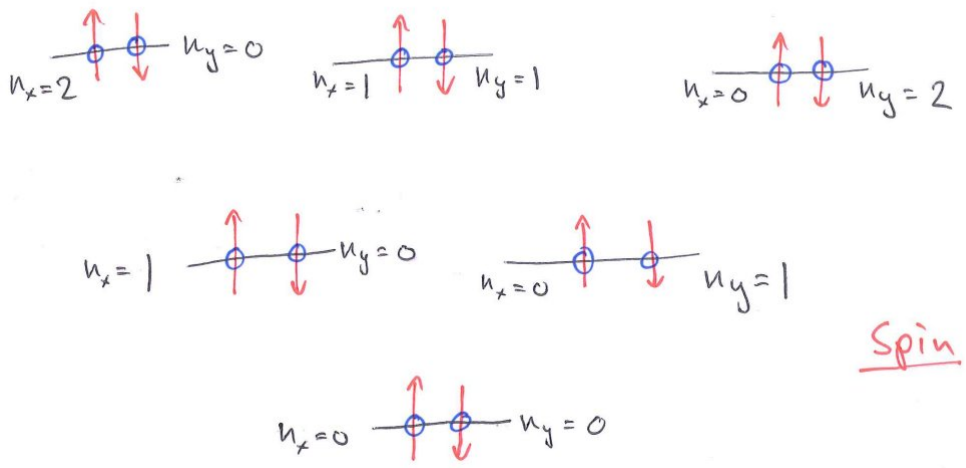

Figure 2.1.1: The wave function levels. The blue dots represent electrons filling up the states from $n_x = n_y = 0$ to the third lowest states. 2 electrons fill up the lowest level, 6 electrons the two lowest levels and 12 electrons all three first energy levels. The net spin of each level must be 0 due to the Pauli Exclusion principle.

The energies of these levels are given by the well known 2D-harmonic oscillator energy formula

$$E_{n_x,n_y} = \hbar\omega(1 + n_x + n_y) \tag{2.1.25}$$

So if we have two electrons in the lowest state ($n_x = n_y = 0$), we would expect the energy of this state to be

$$2 \cdot \hbar\omega(1 + 0 + 0) = 2\hbar\omega = 2\omega \tag{2.1.26}$$

When using natural units.

To have two electrons in the same state, their spin must be opposite due to the Pauli exclusion principle. This means that the total spin of the $n_x = n_y = 0$ state is 0. It can be shown that the wavefunction given by equation 2.1.21 when $N = 2$ (i.e. two electrons) is given by the following equation

$$\Psi_T(\vec{r}_0, \vec{r}_1) = \exp(-\alpha\omega(r_0^2 + r_1^2)/2) \cdot \mathrm{J} \tag{2.1.27}$$

If we do not include the repulsion part of the system, there is no need to include the Jastrow Factor (for details, see section 2.1.2.2). It can be shown that this state is an eigenstate of the unperturbed harmonic oscillator with energy 2ω when $\alpha = 1$. This analogy can be extended to the $N = 6$ and $N = 12$ electron case as well. When $N = 6$ the unperturbed energy should be the sum of the energies in the first level (i.e. 2ω) and the collective energies of the electrons in the second level states ($n_x = 1,\ n_y = 0 \vee n_x = 0,\ n_y = 1$) which is $4 \cdot 2\omega = 8\omega$, resulting in a total energy of 10ω. Equivalently, the energy for the $N = 12$ electron case should be 28ω. These energies will all serve as benchmarks and we should get the exact results when there is no repulsion, $\alpha = 1$ and the jastrow factor is omitted.

2.1.2.4 Closed form expression of the local energy

To evaluate the local energy

$$E_L(\vec{r}) = \frac{1}{\Psi_T}\hat{H}\Psi_T = \frac{1}{\Psi_T}\left(\sum_i -\frac{1}{2}\nabla_i^2 + \sum_i V(\vec{r}_i)\right)\Psi_T = \sum_i V(\vec{r}_i) - \frac{1}{2}\sum_i \frac{1}{\Psi_T}\nabla_i^2\Psi_T \quad (2.1.28)$$

We need a lot of computational power. This is mainly due to the fact that we need to compute the sum of the laplacian operators on each particle. This is an easy task to do "brute force", but if we were able to find an analytical expression for the local energy, it would possibly simplify calculations by alot. Let's look at one of the terms in the laplacian sum, naming it LSP (Laplacian sum part)

$$LSP = \frac{1}{\Psi_T}\nabla_i^2\Psi_T \quad (2.1.29)$$

Inserting the trial wavefunction expression (equation 2.1.21) into the latter gives

$$\frac{1}{\Psi_T}\nabla_i^2\Psi_T = \frac{1}{\mathrm{Det}_M\mathrm{J}}\nabla_i^2(\mathrm{Det}_M\mathrm{J}) \quad (2.1.30)$$

The function Det_M is a product of two matrice-determinants $|U|$ and $|D|$ where $|U|$ handles all the particles assigned spin up and $|D|$ the ones assigned spin down. Particle i has either spin up or down, so let $|S_i|$ denote the matrix determinant which handles particle i and $|S_{j\neq i}|$ denote the one that doesn't, then

$$\frac{1}{\Psi_T}\nabla_i^2\Psi_T = \frac{1}{|S_i||S_{j\neq i}|\mathrm{J}}\nabla_i^2(|S_i||S_{j\neq i}|\mathrm{J}) = \frac{1}{|S_i||S_{j\neq i}|\mathrm{J}}|S_{j\neq i}|\nabla_i^2(|S_i|\mathrm{J}) = \frac{1}{|S_i|\mathrm{J}}\nabla_i^2(|S_i|\mathrm{J}) \quad (2.1.31)$$

Using the product rule of the laplacian operator gives

$$\boxed{\frac{1}{\Psi_T}\nabla_i^2\Psi_T = \frac{\nabla_i^2|S_i|}{|S_i|} + \frac{\nabla_i^2\mathrm{J}}{\mathrm{J}} + 2\frac{\nabla_i\mathrm{J}}{\mathrm{J}}\cdot\frac{\nabla_i|S_i|}{|S_i|}} \quad (2.1.32)$$

It is possible to find analytical expression for all these terms, and that has been already been done in a master thesis written by Jørgen Høgberget [3]. The arguments will not be repeated

but the results are as follows (with names added for code reference)

$$NSS = \frac{\nabla_i |S_i|}{|S_i|} = \sum_{k=0}^{N/2} \left[(S^{-1})_{ki} \cdot \nabla_i \phi_{2k}(\vec{r}_i) \right] \tag{2.1.33a}$$

$$N2SS = \frac{\nabla_i^2 |S_i|}{|S_i|} = \sum_{k=0}^{N/2} \left[(S^{-1})_{ki} \cdot \nabla_i^2 \phi_{2k}(\vec{r}_i) \right] \tag{2.1.33b}$$

$$NJJ = \frac{\nabla_i \mathrm{J}}{\mathrm{J}} = \sum_{k \neq i} \frac{a_{ik}}{r_{ik}} \frac{\vec{r}_i - \vec{r}_k}{(1 + \beta r_{ik})^2} \tag{2.1.33c}$$

$$N2JJ = \frac{\nabla_i^2 \mathrm{J}}{\mathrm{J}} = \left| \frac{\nabla_i J}{J} \right|^2 + \sum_{k \neq i} \frac{a_{ik}}{r_{ik}} \frac{1 - \beta r_{ik}}{(1 + \beta r_{ik})^3} \tag{2.1.33d}$$

$\nabla_i \phi_k(\vec{r}_i)$ and $\nabla_i^2 \phi_k(\vec{r}_i)$ scan be found simply by inserting and taking the derivative of the Hermite polynomials. The explicit formulas for ϕ_k for k in the range 0 to 11 is given in table 2.1.2 and are also taken from the master thesis by Jørgen Høgberget.

k	(n_x, n_y)	$\phi_k(\vec{r})$	$\nabla_i \phi_k(\vec{r}_i) = [\nabla_x, \nabla_y]$	$\nabla_i^2 \phi_k(\vec{r}_i)$
0	(0,0)	1	$-\left[l^2 x, l^2 y\right]$	$l^2(l^2 r^2 - 2)$
2	(1,0)	$2lx$	$-2l\left[(lx-1)(lx+1), l^2 xy\right]$	$2l^3 x(l^2 r^2 - 4)$
4	(0,1)	$2ly$	$-2l\left[l^2 xy, (ly-1)(ly+1)\right]$	$2l^3 y(l^2 r^2 - 4)$
6	(2,0)	$4l^2 x^2 - 2$	$-2\left[l^2 x(2l^2 x^2 - 5), l^2 y(2l^2 x^2 - 1)\right]$	$2l^2(l^2 r^2 - 6)(2l^2 x^2 - 1)$
8	(1,1)	$4l^2 xy$	$-4l^2\left[y(lx-1)(lx+1), x(ly-1)(ly+1)\right]$	$4l^4 xy(l^2 r^2 - 6)$
10	(0,2)	$4l^2 y^2 - 1$	$-2\left[l^2 x(2l^2 y^2 - 1), l^2 y(2l^2 y^2 - 5)\right]$	$2l^2(l^2 r^2 - 6)(2l^2 y^2 - 1)$

Table 2.1.2: Table of derivatives of $\phi_k(\vec{r}_i)$ where $l = \sqrt{\alpha\omega}$. The factor $e^{-\frac{1}{2}l^2 r^2}$ is ommitted from all expressions. The formula for $k+1$ is the same as for k if k is even (e.g. $\phi_0 = \phi_1$).

2.1.3 The virial theorem

2.2 The numerical foundation

This is the section explaining the numerical theory upon which the project is built.

2.2.1 Monte Carlo simulations

A Monte Carlo simulation is a way of solving a mathematical or physical problem by generating a random (or pseudorandom [2]) sequence of numbers and evaluating some quantity on the assumption that our the random sequence of numbers is representative of the domain from which the

[2] No electronic random number generator of today is truly random. The sequence of numbers generated will repeat itself after a long period. These periods however, are increadibly long and we will for this report consider the random number generators to be truly random.

quantity is evaluated. An example is evaluating the area of the unit circle by randomly placing points in a $[-1, 1] \times [-1, 1]$ grid and find the fraction points whose distance to the origin is ≤ 1 and multiply this fraction by the area of the grid (i.e. 4). Such a simple Monte Carlo simulation can give the result as shown in figure 2.2.1.

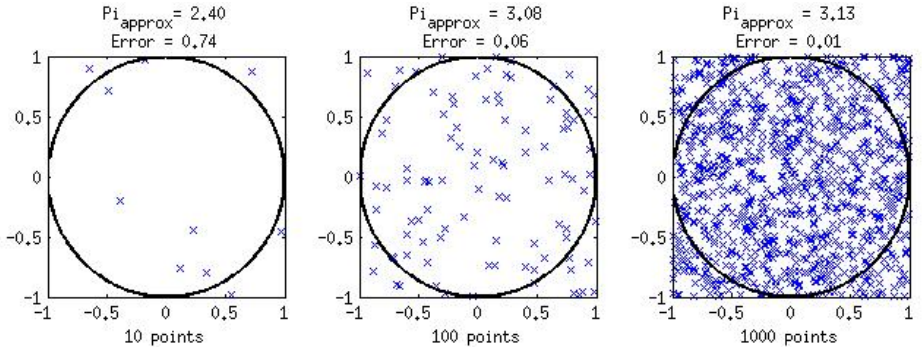

Figure 2.2.1: The results from a very simple Monte Carlo simulation of estimating the circle constant π. The precision increases with the number of points.

However, the method is not confined to this sort of problem, but can be applied to a variety of mathematical and physical problems. In this report, the method, through the Metropolis algorithm (see section 2.2.2) has been applied to a quantum mechanical system.

2.2.2 The Metropolis algorithm

The Metropolis algorithm is a method which cleverly employs a stoichastic approach in order to quickly estimate certain mathematical objects. The method is explained at lengths elsewhere[2], but in this section we will look at an example which captures the main idea of the method.

Suppose we have a PDF[3] $P(x)$ in a domain $[a, b]$ for which we want to calculate the expectation value $\langle g \rangle$ of some function $g(x)$. The integral we need to solve is then

$$\langle g \rangle = \int_a^b P(x)g(x)dx \tag{2.2.1}$$

This integral can be approximated as follows

$$\int_a^b P(x)g(x)dx \approx \frac{b-a}{N} \sum_i P(x_i)g(x_i) \equiv I \tag{2.2.2}$$

Where x_i are some uniformly chosen values in the interval $[a, b]$. Now, imagine instead of picking values x_i uniformly and weighing them by multiplying $g(x)$ with $P(x)$ instead chose the values of $\tilde{x_i}$ from the PDF $P(x)$ and calculated the quantity $\tilde{I}$ given by

$$\tilde{I} = \frac{1}{N} \sum_i g(\tilde{x_i}) \tag{2.2.3}$$

[3]Probability Distribution Function

It can be shown mathematically that for large enough N, these two quantities I and $\tilde{I}$ approach the same value. The problem with such an approach is that we need the precise expression for the PDF $P(x)$ and a robust algorithm for choosing random values from it. With the Metropolis algorithm however, we can use this approach *without* knowing the precise expression of the PDF and the relevant values from the domain come naturally.

The algorithm requires that we are able to calculate $\tilde{P}(x)$, an unnormalized version of $P(x)$ (i.e. some function $aP(x)$ proportional to $P(x)$). This may seem like a very strong requirement, but in many applications, as in this project, this is a much easier task than to calculate the precise PDF. The algorithm goes as follows. Starting with a position x choose a new trial position x_p by

$$x_p = x + \Delta x \tag{2.2.4}$$

Where Δx is a random step according to some rule (see subsections). Then generate a probability criteria s, a random number between zero and one. If

$$\frac{P(x_p)}{P(x)} = \frac{aP(x_p)}{aP(x)} = \frac{\tilde{P}(x_p)}{\tilde{P}(x)} \equiv w \geq s \tag{2.2.5}$$

We accept the trial position as our new x and if not we reject it. If we choose new values of x_i in this manner, the collection of x_i's will in fact reflect the PDF $P(x)$, which was what we needed in order to use equation 2.2.3. Note how equation 2.2.5 doesn't require us to have the exact form of the probability distribution function, only a function $\tilde{P}(x)$ proportional to it.

The intuition behind the algorithm is that for each new position x_i we generate is drawn towards the part of the domain where $P(x)$ is bigger. To see this, we note that if $P(x_p) > P(x)$ then $\frac{P(x_p)}{P(x)} > 1$ which is always bigger than $s \in [0, 1]$ and the new move is always accepted. Whereas if $P(x_p) < P(x)$, the move might be rejected. This allows new values of x_i to be chosen from where $P(x)$ is big, but at the same time allows values with lower values of $P(x)$ to be chosen. Which is what we expect from a PDF. The fact that for a large number M of such steps, the values x_i picked actually reflects the PDF requires some more mathematics, and once again we refer to the lecture notes of the course [2].

2.2.2.1 Brute force Metropolis

If we have no information about the physical nature of the system a reasonable way to model Δx is the following

$$\Delta x = r\Delta x_0 \tag{2.2.6}$$

Where r is a random number between 0 and 1 and Δx_0 is a predefined step length. The step length Δx_0 is affecting the effectiveness of the algorithm in two contradicting ways. A small step length increases the probability of each suggested move x_p being accepted, but weakens the ergodicity[4] of the method. Increasing the acceptance probability reduces the amount of times we need to evaluate the probability ratio w, but also increses the amount of Monte Carlo simulations needed in order to get a representative collection of x_i's. It can be argued that a good balance

[4]The way in which the walker is able to reach all positions within a finite number of steps.

between these two aspects is to achieve an acceptance ratio (i.e. the ratio between accepted and rejected moves) of around 0.5.

This is called the "Brute Force Metropolis algorithm".

2.2.2.2 Importance sampling

If our current position x is in a region where the probability distribution is important, i.e. has a large value, a small step Δx would be favorable. This is because we want to sample many points in this region, which is what a small step allows. In contrast, if the current position x is in an unimportant region, we want a large step Δx since we don't mind moving a bit farther from the region we're in. The brute force approach produced a step independent of the PDF value in each point, which resulted in an optimal acceptance ratio of around 0.5. If we could introduce some sort of rule which adjusts the step Δx according to the value of the PDF in the point we currently are, this could allow us to achieve an acceptance rate of around 0.9 with the same ergodicity.

To make such a rule, we need to use our physical understanding of the system. One way of doing so is to consider the points to move as a random walker would where the resulting probability is equal to the PDF we're treating. Doing this, and invoking the Fokker-Planck and Langevin equations [5] , it can be shown that the choice of Δx is as follows

$$\Delta x = DF(x)\delta t + \eta \tag{2.2.7}$$

Where D is the diffusion term, $F(x)$ is a drift term which is responsible for pulling the particle towards regions where the PDF is important and η is a gaussian random number.

Using this approach is what we will call the "Metropolis algorithm with importance sampling".

2.2.2.3 The metropolis algorithm for our wavefunction

As discussed in section 2.1.1 we need to solve the integral

$$\langle E_L \rangle = \int P(\vec{r}) E_L(\vec{r}) d\vec{r} \tag{2.2.8}$$

Where we have a trial function

$$\Psi_T(\vec{r}_0, ..., \vec{r}_{N-1}, \alpha, \beta) \tag{2.2.9}$$

dependent on 2 trial parameters α and β where $\vec{r}_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix}$. This is exactly the kind of problem the Metropolis algorithm can solve and the explicit algorithm for calculating $\langle E_L \rangle$ and $\langle E_L^2 \rangle$ is given in algorithm 2.1.

If we move only one particle at a time, each new trial position will be given by

$$\boxed{\mathbf{r_p} = \begin{pmatrix} x_0 & x_1 & ... & x_i & ... & x_{N-1} \\ y_0 & y_1 & ... & y_i + \Delta\vec{r} & ... & y_{N-1} \end{pmatrix}} \tag{2.2.10}$$

[5] Once again we refer to the lecture notes [2] for a more detailed explanation.

Data:
An initial position matrix $\mathbf{r} = (\vec{r}_0, \vec{r}_1 ... \vec{r}_{N-1}) = \begin{pmatrix} x_0 & x_1 & ... & x_{N-1} \\ y_0 & y_1 & ... & y_{N-1} \end{pmatrix}$
A method of chosing the step Method($\mathbf{r}$) $= \Delta\vec{r} = \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix}$
Result:
The expectation value of the local energy: $\langle E_L \rangle$
The expectation value of the local energy squared: $\langle E_L^2 \rangle$

begin
  $cumulative\_local\_energy = E_L(\mathbf{r}, \alpha, \beta)$ // Initialization
  $cumulative\_local\_energy\_squared = 0$
  $counter = 0$
  while $counter < M$ **do**
    $i = \text{randint}(0, 1, ..., N-1)$ // Choose random element index
    $\Delta\vec{r} = \text{Method}(\mathbf{r})$ // Create a random two-dimensional step
    $\mathbf{r_p} = \begin{pmatrix} x_0 & x_1 & ... & x_i & ... & x_{N-1} \\ y_0 & y_1 & ... & y_i & ... & y_{N-1} \end{pmatrix} + \Delta\vec{r}$ // Create a trial position matrix
    $s = \text{randint}(0,1)$ // Generate a probability criteria
    $w = |\psi(\alpha, \beta, \mathbf{r_p})|^2 / |\psi(\alpha, \beta, \mathbf{r})|^2$ // Calulate the probability ratio
    if $w \geq s$ **then**
      $\vec{r} = \vec{r}_p$
      $E_L(\mathbf{r}, \alpha, \beta) = \frac{1}{\Psi_T(\mathbf{r}, \alpha, \beta)} \hat{H} \psi_T(\mathbf{r}, \alpha, \beta)$ // Calculate the local energy
    end
    $cumulative\_local\_energy \stackrel{+}{=} E_L(\mathbf{r}, \alpha, \beta)$ // Update *cumulative_local_energy*
    $cumulative\_local\_energy\_squared \stackrel{+}{=} E_L(\mathbf{r}, \alpha, \beta)^2$ // Update *cumulative_local_energy_squared*
    $counter \stackrel{+}{=} 1$ // Update *counter*
  end
  Calculate $\langle E_L \rangle = \frac{cumulative\_local\_energy}{M}$
  Calculate $\langle E_L^2 \rangle = \frac{cumulative\_local\_energy\_squared}{M}$
end

Algorithm 2.1: The metropolis algorithm used for finding the expecation value of the local energy and the expecation value of the local energy squared. "Method" refers to either the brute force approach or importance sampling.

Where $\mathbf{r} = \begin{pmatrix} x_0 & x_1 & ... & x_{N-1} \\ y_0 & y_1 & ... & y_{N-1} \end{pmatrix}$. If we are using the brute force approach, then $\Delta\vec{r}$ is simply given by

$$\boxed{\Delta\vec{r} = \Delta r \cdot \vec{\text{rand}}} \tag{2.2.11}$$

Where Δr is a predefined step length and $\vec{\text{rand}}$ is a random 2-vector with elements between -1 and 1.

If we want to implement importance sampling however, we need expressions for the terms in equation 2.2.7. These terms can be shown [1] to be

$$D = \frac{1}{2} \tag{2.2.12}$$

Which stems from the fact that the drift is caused by kinetic energy in front of which is a factor $\frac{1}{2}$ and

$$F = 2\frac{1}{\Psi_T}\nabla_i \Psi_T \tag{2.2.13}$$

The formula for using importance sampling when choosing the trial position $\mathbf{r_p}$ for our wavefunction is thus

$$\boxed{\Delta\vec{r} = \left(\frac{1}{\Psi_T}\nabla_i \Psi_T\right)\delta t + \eta} \tag{2.2.14}$$

We can rewrite this, as in section 2.1.2.4

$$\frac{1}{\Psi_T}\nabla_i \Psi_T = \frac{1}{|S_i|\mathrm{J}}\nabla_i(|S_i|\mathrm{J}) = \frac{1}{|S_i|\mathrm{J}}\left(|S_i|\nabla_i \mathrm{J} + \mathrm{J}\nabla_i|S_i|\right) \tag{2.2.15}$$

$$\boxed{\frac{1}{\Psi_T}\nabla_i \Psi_T = \frac{\nabla_i|S_i|}{|S_i|} + \frac{\nabla_i \mathrm{J}}{\mathrm{J}}} \tag{2.2.16}$$

Expressions we can find both from numerical differenciation and the close form expressions in equations 2.1.33. In this report, we will use both these approaches and compare the CPU time needed.

3 Experimental

3.1 Benchmarks and verification

3.1.1 Benchmarks for the brute force approach, no repulsion or jastrow factor

As discussed in section 2.1.2.3, when $\omega = 1$, the trial wavefunction should be able to reproduce the exact solution $E = 2$ (in atomic units) when we disregard the electron repulsion part of the Hamiltonian and don't include the Jastrow factor. This benchmark was tested [6] with the brute force metropolis method by varying α from 0 to 1.5 with steps of 0.05 using numerical diffrentiation of the wavefunction in the expression of the local energy. 10^7 Monte Carlo simulations were performed for each α with a step length Δr suited to each case to get an acceptance rate of around 0.5 (which is implemented in the code before any monte carlo simulation is begun).

Then then the benchmarks for the $N = 6$ and $N = 12$ electron case was tested[7] , still with the brute force approach and 10^7 monte carlo simulations for the $N = 6$ case and 10^6 for the $N = 12$ case, but this time with a smaller interval around $\alpha = 1$, ranging from 0.9 to 1.1 with steps of 0.05. In order to also verify the correct implementation of the oscillator frequency ω, this was set to 1.5, so the energies to reproduce are $10\omega = 15$ a.u. and $28\omega = 42$ a.u.

[6] /Logs/N2_norep_bruteforce_num/test_investigate.cpp, 21.11.14. See appendix, section B.

[7] /Logs/N12_norep_bruteforce_num/test_investigate.cpp and /Logs/N6_norep_bruteforce_num/test_investigate.cpp, 21.11.14.

3.1.2 Benchmark for the brute force approach, with repulsion and jastrow factor

The exact energy of the two electron state *with* repulsion has been shown [4] to be 3ω. To test this result, first a fast investigation of $\langle E_L \rangle$ was performed as function of α and β to find the region in which the lowest energy is. Then, a more detailed search was made with $\alpha \in [0.9, 1.1]$ and $\beta \in [0.35, 0.45]$, both in steps of 0.01. The brute force approach with numerical evaluation of the local energy was used and ω was set to 0.5. If the exact wavefunction were within our trial parameters, then we would thus expect to get the exact answer $3 \cdot 0.5 = 1.5$ a.u., but since this may not be the case we expect the lowest energy to be larger than this, according to section 2.1.1.2.

3.1.3 Comparation of different methods

As described in the theory section, a variety of different methods for solving the VMC problem has been explained. Firstly, there is a choice whether to use brute force (BF) or importance sampling (IS) when picking new trial positions in the metropolis algorithm. Secondly there is the the possibility of using numerical methods (NLE) or the analytical expressions (ALE) when evaluating the local energy. In addition, if we're using importance sampling in the metropolis algorithm, there is a choice to whether or not we should use numerical (NQF) or analytical (AQF) expressions for the quantum force. All these methods should output the same result for the expectation value of the local energy, and to verify this an investigation[8] of $\langle E_L \rangle$ with the different methods were performed for three different, semi-random[9] , combination of problem and trial function parameters; (Number of electrons N, α, Jastrow Factor on (Jn) or off (Jf), β, ω, Electron repulsion on (En) or off (Ef)) with 10^6 monte carlo simulations.

[8] /Logs/compare_methods/first_example.cpp, second_example.cpp, third_example.cpp, 21.11.14.
[9] Chosen randomly by me, that is.

3.2 Optimizations and differences

3.2.1 Jastrow factor

3.2.2 Importance sampling

3.2.3 Results from the different methods

3.2.4 Timely differences between methods

3.3 Applications

3.3.1 Energies and variances

3.3.2 The virial theorem

4 Results and discussion

4.1 Benchmarks and verification

4.1.1 Benchmarks for the brute force approach, no repulsion or jastrow factor

Table 4.1.1 shows the results from the brute force simulation of the two electron - no repulsion case. A plot of the results is shown in figure 4.1.1.

α	0.0	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.40	0.45
E(a.u)	1.1e5	19.96	10.03	6.77	5.17	4.23	3.61	3.19	2.89	2.66
Variance	7.4e9	2.0e2	4.8e1	2.0e1	1.1e1	7.0e0	4.5e0	3.1e0	2.2e0	1.5e0
α	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95
E(a.u.)	2.49	2.36	2.26	2.18	2.12	2.08	2.047	2.024	2.0096	2.002
Variance	1.1e0	7.9e-1	5.6e-1	3.9e-1	2.6e-1	1.7e-1	1.0e-1	5.3e-2	2.6e-2	5.2e-3
α	1.0	1.05	1.1	1.15	1.2	1.25	1.3	1.35	1.4	1.45
E(a.u)	2	2.0029	2.010	2.021	2.035	2.05	2.07	2.09	2.12	2.14
Variance	3.3e-13	4.7e-3	1.8e-2	3.9e-2	6.7e-2	1.0e-1	1.4e-1	1.8e-1	2.3e-1	2.9e-1

Table 4.1.1: Table showing the results from the brute force VMC simulation of the expectation value of the local energy $\langle E_L \rangle$ for α between 0 and 1.45 in the 2-electron case with no repulsion or Jastrow factor. The results show a minimum for the energy at $\alpha = 1$, as expected, and the variance at this point is so small that we expect it to be an eigenstate of the system.

The figure shows exactly what we would expect from the discussion of section 2.1.2.3. The energy is always larger than 2 a.u. and takes this value only when $\alpha = 1$. We also see a huge drop in the variance just as we reach $\alpha = 1$ which indicates that this is indeed an eigenstate of the system. What little is rest of the variance at $\alpha = 1$ can be due to numerical errors in the calculation of the laplacians. This has in retropspect been verified to be true by using the analytical expression for the local energy.

Table 4.1.2 shows the result from the $N = 6$ and $N = 12$ electrons case with no repulsion using

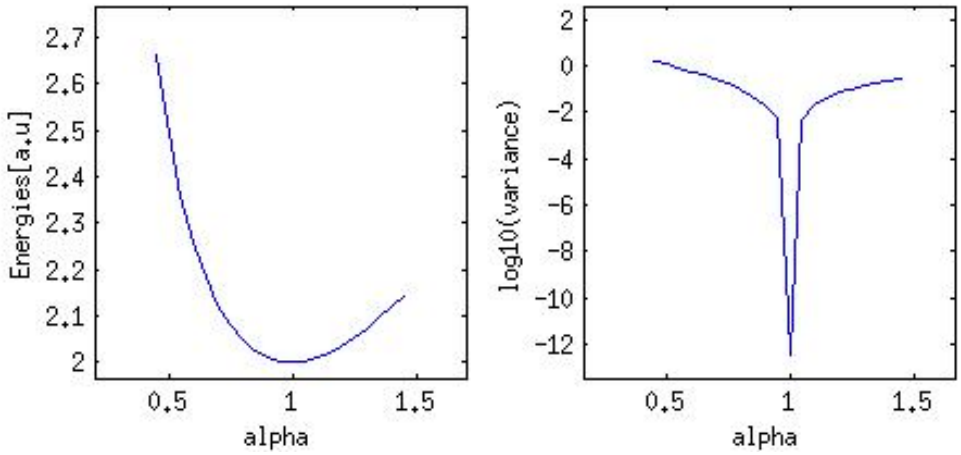

Figure 4.1.1: Plot of the values given in table 4.1.1, the brute force VMC simulation of the two-electron no repulsion or Jastrow factor case. Some of the first values of α has been omitted to make the graph more informative.

the brute force approach with numerical evaluation of the local energy.

	α	0.9	0.95	1	0.105	0.11
N=6	E(a.u)	15.0803	15.0850	15	15.0184	15.0708
	Variance	2.49e-1	5.89e-2	2.56e-13	2.36e-2	2.05e-1
	α	0.9	0.95	1	0.105	0.11
N=12	E(a.u)	42.2114	42.0497	42	42.0563	42.1937
	Variance	6.92e-1	1.66e-1	1.72e-10	1.48e-1	5.69e-1

Table 4.1.2: The results from calculating the expectation value of the local energy and its variance. We see that the code works for the $N = 6$ and $N = 12$ case because we are producing the expected results, $E_6 = 15$ and $E_{12} = 42$ ($\omega = 1.5$). The variance at $\alpha = 1$ is so small that we have probably the exact wavefunction.

The table shows that we are able to produce the results we anticipated. What little there is of variance at $\alpha = 1$ is probably due the numerical evaluation of the local energy, which has been confirmed in retrospect by using the analytical expression for the local energy. It also shows that the code has implemented the oscillator frequency ω correctly.

4.1.2 Benchmark for the brute force approach, with repulsion and jastrow factor

4.1.3 Comparation of different methods

The results from calculation $\langle E \rangle$ for the different method combinations and problem/wave function parameters are shown in table 4.1.3.

	Problem/Wavefunction parameters		
Method parameters	(2, 1, Jf, 0, 1, Ef)	(12, 0.5, Jf, 0, 1.5, En)	(6, 0.82, Jo, 0.22, 3, En)
(BF, NLE)	(2.000, 6e-13)	(92.10, 67.54)	(54.74, 28.11)
(BF, ALE)	(2.000, 0)	(92.18, 161.4)	(54.72, 28.19)
(IS, NLE,NQF)	(2.000, 6e-14)	(92.15, 66.43)	(54.72, 27.33)
(IS, NLE, AQF)	(2.000, 1e-13)	(92.06, 54.49)	(54.72, 27.32)
(IS, ALE, NQF)	(2.000, 0)	()	(54.76, 27.35)
(IS, ALE, AQF)	(2.000, 0)	()	(54.74, 27.44)

Table 4.1.3: A table of the expectation value and variance (Energy,Variance) of the local energy obatined with different Problem/Wavefunction parameters (N,α, Jn/Jf, β, ω, En/Ef). For explanation of abbreviations, see section 3.1.3. For all trials, 10^6 VMC calculations were performed and for the importance sampling methods, a timestep of $\delta t = 0.1$ was used.

4.2 Optimizations and differences

4.2.1 Jastrow factor

4.2.2 Importance sampling

4.2.3 Results from the different methods

4.2.4 Timely differences between methods

4.3 Applications

4.3.1 Energies and variances

4.3.2 The virial theorem

5 Conclusion

References

[1] Morten Hjorth-Jensen. Additional slides for monte carlo project. http://www.uio.no/.../montecarloaddition.pdf, 2014.

[2] Morten Hjorth-Jensen. *Computational Physics - Lecture Notes Fall 2014*. August 2014.

[3] Jørgen Høgberget. Quantum monte-carlo studies of generalized many-body systems, June 2013.

[4] M. Taut. Two electrons in an external oscillator potential: Particular analytic solutions of a coulomb correlation problem. *Phys. Rev. A*, 48:3561–3566, Nov 1993.

A Reference to the questions posed in the project instructions

Since the format of this report does not correspond to the structure of the project instructions, a reference list over the posed questions and where to find the answer is given below.

Section	Instruction	Reference
a)	Convince yourself that ... is simply 2ω. What is the total spin ...? Find arguments for why...	Section 2.1.2.3 Section 2.1.2.3
b)	Perform a Variational Monte Carlo calculation...	Sections 3.1 and 4.1
c)		
d)		
e)	Reproduce the unperturbed ... is switched off. Convince yourself ... for N = 6 is 10ω	Sections 3.1 and 4.1 Section 2.1.2.3
f)		
g)		

Table A.0.1: Reference list over the posed questions and where to find the answer.

B Codes

All codes used in this exercise can be found at GitHub:
https://github.com/vidarsko/Project3.

The class structure of the code is given in the bullet points below

- TrialWavefunction
- QuantumDots
- Investigate

Througout this report, reference to different codes are made as footnotes together with the date at which they were run.