

FYS3150/4150 Project 5

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Abstract

The aim of this project was to model the behaviour of two electrons in a harmonic oscillator potential using the variational Monte Carlo (VMC) method. We proposed two trial wave functions, Ψ_{T1} and Ψ_{T2} , to use in the VMC approach. The expectation values of the energy, energy variance and mean distance between the electrons were calculated at the ground state for both trial wave functions. The results show that while the unperturbed Ψ_{T1} coincides with the exact wave function, both trial wave functions yield energy expectation values that are too high when the repulsive Coloumb interaction is included. Thus indicating that they are bad approximations for the exact wave function. Additionally, we compared the results obtained with the VMC approach to the results found using the Jacobi method to solve the eigenvalue equation in project 2, and the results from the VMC approach were far superior. The source code and benchmarks of the project can be found on GitHub: <https://github.com/ingridavh/compphys1/tree/master/Project%205/QuantumMC>. Note that this work has been a collaboration between Ingrid A. V. Holm (FYS4150) and Johannes K. Kjernlie (FYS3150). We will deliver separate reports, since we are in different courses.

1 Introduction

One of the few exactly solvable systems with genuine Coulomb interactions is one comprised of two electrons in an external harmonic oscillator potential [5]. These electrons are sometimes referred to as *quantum dots* (QD) – small semiconductor particles with electronic properties different to those of larger particles. QDs can emit light of different colours, depending on the size of the dot. They are of much interest in transistors, solar cells, quantum computing and more.

In this project we wish to model a system of quantum dots with two electrons using variational Monte Carlo (VMC) methods, with emphasis on correlations due to electron-electron repulsion. We will introduce two trial wave functions to use in the VMC method as an attempt to approximate the exact wave function precisely. We will examine the stability of the approximation as a function of the number of Monte Carlo cycles, and find the optimal values of the variational parameters of the trial functions by minimizing the ground state energy. The results are presented in Sec. (4), before we give our conclusions in Sec. (5).

2 Physical background

2.1 Quantum dots

The quantum dots are represented as two electrons, $N = 2$, moving in three dimensions in an isotropic harmonic oscillator potential. The idealized Hamiltonian is 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 we have used natural units $\hbar = c = e = m_e = 1$, and all energies are in atomic units a.u. All distances r_j and r_{ij} are unitless. The first two terms describe the kinetic energy and potential energy from

the harmonic oscillator. The Coulomb force between charged particles is given by

$$F_C = k_e \frac{q_1 q_2}{r_{12}}, \quad (2)$$

and gives rise to a repulsive interaction between the equally charged electrons, as illustrated in Fig. (1). Since $q_1 = q_2 = e = 1$ and we use atomic units ($k_e = 1$), the contribution to the Hamiltonian is

$$\hat{H}_1 = \sum_{i < j} \frac{1}{r_{ij}}, \quad (3)$$

where the distance between electrons is given by $r_{ij} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$. The modulus for the position of a single electron is given as $r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}$.

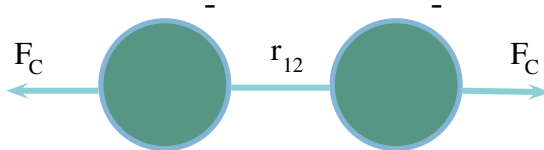


Figure 1: The Coulomb interaction between same-sign charges is repulsive, and inversely proportional to the distance between them.

2.2 The Non-Interacting Case

For the unperturbed system the Hamiltonian is

$$\hat{H}_0 = \sum_{i=1}^N \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right). \quad (4)$$

The *wave function* that satisfies this Hamiltonian is given by

$$\phi_{n_x, n_y, n_z}(x, y, z) = A H_{n_x}(\sqrt{\omega}x) H_{n_y}(\sqrt{\omega}y) H_{n_z}(\sqrt{\omega}z) \exp(-\omega(x^2 + y^2 + z^2)/2), \quad (5)$$

where the functions $H_{n_x}(\sqrt{\omega}x)$ are the Hermite polynomials, and A is a normalization constant. Some additional material on Hermite polynomials is given in App. (A). The wave functions are eigenstates of the Hamiltonian with energy eigenvalues. For a single electron the expression for the energy is $\epsilon_{n_x, n_y, n_z} = \omega(n_x + n_y + n_z + 3/2)$. In the ground state all quantum numbers are zero, $n_i = 0$, and the energy is thus

$$E_{0, \text{single particle}} = \frac{3}{2} \omega. \quad (6)$$

In the case of two electrons with no interaction the total energy is just the sum of individual energies $H\Psi = (H_1 + H_2)\Psi_1\Psi_2 = (E_1 + E_2)\Psi$. Hence, the ground state energy is

$$E_{0, 2 \text{ particles}} = \frac{3\omega}{2} + \frac{3\omega}{2} = 3\omega$$

Spin

It follows from the wave function that the total spin in the ground state should be zero. Electrons belong to a group of particles called *fermions*, which are required to have antisymmetric wave functions. That is, no two electrons can be in the *exact* same state. If the quantum numbers are all the same $n_i = 0$, the electron spins must be different, giving $S_{\text{total}} = \frac{1}{2} - \frac{1}{2} = 0$. This is illustrated in Fig. (2).

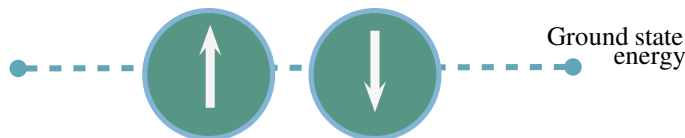


Figure 2: There can only be two electrons in the ground state energy of our system, and they must have different spin. The next level, where one $n_i = 1$, can contain electrons of the same spin configurations since the spatial part of the wave function is antisymmetric.

2.3 Comparison with Eigenvalue Approach

The Schrödinger's equation can be separated into two parts; one for the relative motion \mathbf{r} of the particles of the system, and one for the center-of-mass motion $\mathbf{R}_{COM} = 0.5 \times (\mathbf{r}_1 + \mathbf{r}_2)$. In a previous project the equation for the relative motion was solved, providing $E_{\mathbf{r}}$ for the total energy $E = E_{\mathbf{r}} + E_{\mathbf{R},com}$. To compare these results with those from the VMC approach, we simply add the contribution from the center-of-mass energy. For the ground state in three dimensions the center-of-mass energy is

$$E_{\mathbf{R},com} = \frac{3}{2} \hbar \omega. \quad (7)$$

Thus, for $\omega = 1.0$ we have that $E_{\mathbf{R},com} = 1.5$.

2.4 The Virial Theorem

The *virial theorem* states that for a system in equilibrium the expectation value of the total kinetic energy $\langle T \rangle$ is proportional to the expectation value of the total potential energy $\langle V \rangle$. In quantum mechanics the time derivative of the expectation value of some operator can be written as, using that \hat{H} is hermitian [1],

$$\frac{d}{dt} \langle Q \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{Q}] \rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle. \quad (8)$$

We choose $\hat{Q} = xp$, and remember that the representation of momentum in position space is $-i\hbar \frac{\partial}{\partial x_i}$. The commutator between xp and \hat{H} is

$$\frac{i}{\hbar} [\hat{H}, xp] = -\frac{\hbar^2}{m} \frac{\partial^2}{\partial x^2} - x \frac{\partial V}{\partial x}, \quad (9)$$

where the first term equals two times the kinetic energy. By setting this into Eq. (8) we find

$$\frac{d}{dt} \langle xp \rangle = 2 \langle T \rangle - \left\langle x \frac{dV}{dx} \right\rangle. \quad (10)$$

At a stationary state there will be no change in momentum or position. Using this, and the expression for the potential for a pure harmonic oscillator, we find

$$\langle T \rangle = \langle V \rangle. \quad (11)$$

The ratio between kinetic and potential energy should thus approach 1 in the ground state of a pure harmonic oscillator.

3 Implementation

3.1 Variational Monte Carlo

The ground state energy can be calculated using variational Monte Carlo (VMC). The VMC method uses a trial wave function $\Psi_T(\mathbf{R})$ regulated by a set of variational parameters α, β , with similar behaviour as the exact wave function. \mathbf{R} represents the spatial coordinates of the particles in the system. The amplitude of a particle is given by $\Psi^* \Psi$, and the total amplitude is normalized, i.e. $\int d\mathbf{R} |\Psi(\mathbf{R})|^2 = 1$. We can insert unity in the denominator and write the probability distribution as

$$P(\mathbf{R}; \alpha) = \frac{|\Psi_T(\mathbf{R})|^2}{\int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}}, \quad (12)$$

and the Hamiltonian expectation value as

$$\langle \hat{H} \rangle = \frac{\int d\mathbf{R} \Psi^*(\mathbf{R}) \hat{H}(\mathbf{R}) \Psi(\mathbf{R})}{\int d\mathbf{R} \Psi^*(\mathbf{R}) \Psi(\mathbf{R})}. \quad (13)$$

To find the energy of the trial function we introduce the local energy operator

$$\hat{E}_L(\mathbf{R}; \alpha) = \frac{1}{\Psi_T(\mathbf{R}; \alpha)} \hat{H} \Psi_T(\mathbf{R}; \alpha). \quad (14)$$

The expectation value can now be found using the probability distribution and local energy

$$\langle E_L(\alpha) \rangle = \int P(\mathbf{R}) \hat{E}_L(\mathbf{R}) d\mathbf{R}. \quad (15)$$

The integral in Eq. (15) is computed for different trial functions, using various α in order to minimize the energy expectation value $\langle E_L(\alpha) \rangle$. $\langle E_L \rangle$ should approach $\langle \hat{H} \rangle$ [3]. The trial wave functions and corresponding local energies used in this project are given in Sec. (3.2). We will use the Monte Carlo method (MC) with the Metropolis algorithm for the calculation of Eq. (15). The algorithm for calculating the ground state is outlined in the text box below.

Variational Monte Carlo Algorithm

- Set the number the number of Monte Carlo cycles, and initial values for the variational parameters and the step length, δ . Initialize a random set of initial spatial coordinates, \mathbf{R} .
- Set energy and variance to zero.
- Start Monte Carlo simulation
 1. Calculate the new trial positions

$$\mathbf{R}_p = \mathbf{R} + r \times \delta,$$

where r is a random variable $r \in [-0.5, 0.5]$.

2. Find $|\Psi(\mathbf{R}_p; \alpha)|$ and $|\Psi(\mathbf{R}; \alpha)|$, and use the Metropolis algorithm to accept or reject the proposed move by calculating the ratio

$$w = P(\mathbf{R}_p)/P(\mathbf{R}).$$

If $w \geq s$, where s is a random number $s \in [0, 1]$, the new state is accepted and we set $\mathbf{R} = \mathbf{R}_p$. Otherwise the new configuration is rejected and we continue using \mathbf{R} .

3. Update the local energy and variance.
- Average energy and variance.

3.2 Trial Wave Functions

We will call the exact wave function Ψ_0 . Two trial wave functions, i.e. approximations to Ψ_0 , are used in the simulations

$$\Psi_{T1}(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2), \quad (16)$$

$$\Psi_{T2}(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \exp\left(\frac{r_{12}}{2(1 + \beta r_{12})}\right), \quad (17)$$

where α, β are variational parameters. Notice that Ψ_{T2} is just Ψ_{T1} with an added Jastrow factor to account for the distance between the electrons r_{12} . To find the energy of the first trial state, we use the hamiltonian operator on the state

$$\begin{aligned} \hat{H}_0 \Psi_{T1} &= \frac{1}{2} \left(-(\nabla_1^2 + \nabla_2^2) + \omega^2 r_1^2 + \omega r_2^2 \right) C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \\ &= \frac{1}{2} (\alpha\omega(\nabla_1 + \nabla_2)(x_1 + y_1 + z_1 + x_2 + y_2 + z_2) + \omega^2(r_1^2 + r_2^2)) C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \\ &= \frac{1}{2} (6\alpha\omega - \alpha^2\omega^2(r_1^2 + r_2^2) + \omega^2(r_1^2 + r_2^2)) C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \\ &= 3\alpha\omega - \frac{\omega^2}{2} (1 - \alpha^2) C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \\ &= E_{T1} \Psi_{T1}, \end{aligned}$$

where we have used that $\nabla x_1 e^{-\alpha\omega(r_1^2 + r_2^2)/2} = (1 - \alpha\omega x_1^2) e^{-\alpha\omega(r_1^2 + r_2^2)/2}$. The local energy of the first test function is thus

$$E_{L1} = 3\alpha\omega + \frac{\omega^2}{2} (1 - \alpha^2) (r_1^2 + r_2^2). \quad (18)$$

Notice that for $\alpha = 1$ this equals the exact energy, so $\Psi_{T1}(\alpha = 1)$ equals the exact wavefunction for the unperturbed case. Adding the repulsive Coloumb interaction gives

$$E_{L1} = 3\alpha\omega + \frac{\omega^2}{2} (1 - \alpha^2) (r_1^2 + r_2^2) + \frac{1}{r_{12}}. \quad (19)$$

Similarly, the energy of the second wave function is

$$E_{L2} = E_{L1} + \frac{1}{2(1 + \beta r_{12})^2} (\alpha\omega r_{12} - \frac{1}{2(1 + \beta r_{12})} - \frac{2}{r_{12}} + \frac{2\beta}{1 + \beta r_{12}}) \quad (20)$$

The exact value of the ground state energy is 3.558 for $\omega = 1$ [2]. The addition of the perturbation can for some wave functions give rise to divergence for small r_{12} , see Sec. (3.3) about cusp conditions.

3.3 Cusp Conditions

The trial wave functions should satisfy the cusp condition when $r_{12} \rightarrow 0$. Cusp conditions are to ensure that the test functions behave like the actual wave functions in various limits, and are related to the derivatives of the wave function [3]. When the two electrons approach eachother, the hamiltonian and thus the energy has a singularity at $\frac{1}{r_{12}} \rightarrow \infty$. We can write the local energy as

$$E_L(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} H \Psi_T(\mathbf{R}) = \frac{1}{\Psi_T(\mathbf{R})} \frac{1}{2} \left(-\nabla_1^2 + \nabla_2^2 + \omega^2(r_1^2 + r_2^2) + \frac{2}{r_{12}} \right) \Psi_T(\mathbf{R}) + \text{finite terms},$$

which we can rewrite in spherical coordinates and use the radial part of the wave function. We consider the terms in the wave function that depend on the relative distance

$$\lim_{r_{12} \rightarrow 0} E_L(R) = \frac{1}{R_T(r_{12})} \left(2 \frac{d^2}{dr_{ij}^2} + \frac{4}{r_{ij}} \frac{d}{dr_{ij}} + \frac{2}{r_{ij}} - \frac{l(l+1)}{r_{ij}^2} + 2E \right) R_T(r_{12}) = 0,$$

where l is the orbital momentum. As r_{12} becomes very small, the terms that will dominate are

$$\lim_{r_{12} \rightarrow 0} E_L(R) = \frac{1}{R_T(r_{12})} \left(\frac{4}{r_{ij}} \frac{d}{dr_{ij}} + \frac{2}{r_{ij}} - \frac{l(l+1)}{r_{ij}^2} \right) R_T(r_{12}) = 0,$$

which implies that

$$\begin{aligned} \frac{1}{R_T(r_{12})} 4 \frac{dR_T(r_{12})}{dr_{ij}} &= -2 + \frac{l(l+1)}{r_{ij}} \\ \frac{dR_T(r_{12})}{dr_{12}} &= -\frac{1}{2(l+1)} R_T(r_{12}). \end{aligned}$$

This results in

$$R_T \propto \begin{cases} \exp(r_{12}/2) & \text{for antiparallel spins, } l = 0, \\ \exp(r_{12}/4) & \text{for parallel spins, } l = 1. \end{cases}$$

Like we mentioned in Sec. (3.2), the first test function ignores the cusp condition, and the second test function reflects the condition for antiparallel spins.

4 Results

4.1 Trial Wave Function T1

Fig. (3) shows the expectation value of the unperturbed energy as a function of α for $\omega = 1.0$. The simulations using VMC yield the exact result for $\omega = 1.0$ and $\alpha = 1.0$, namely $\langle E_L \rangle = \langle \hat{\mathbf{H}} \rangle = 3.0$. For the unperturbed ground state the trial function with $\alpha = 1.0$ simulations give the exact result for the energy, even for a low number of MC cycles.

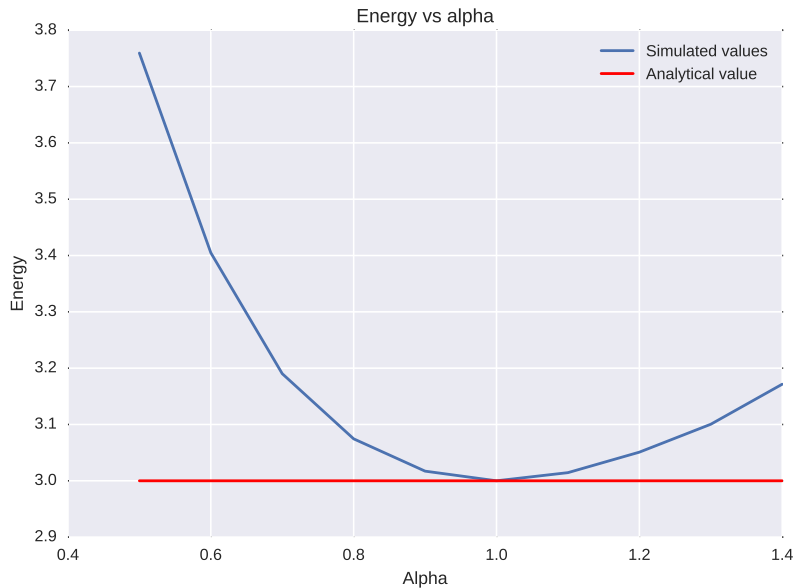


Figure 3: Unperturbed energy expectation value as a function of α for $\omega = 1.0$ and step length 1.0. $N = 1 \cdot 10^6$ MC cycles was used with a step length of $h = 0.00001$ for the numerical differentiation.

The repulsive Coulomb interaction was added to the local energy E_{L1} , as in Eq. (19). We proceeded to investigate the stability of the calculations as a function of MC cycles. The resulting energies are presented in Fig. (4), where a total of $N = 4 \cdot 10^6$ MC cycles is used for $\omega = 1.0$. The optimal value for $\omega = 1$, $\alpha = 0.9$ was used. The energy expectation value seems to stabilize at around $2.5 \cdot 10^6$ MC cycles.

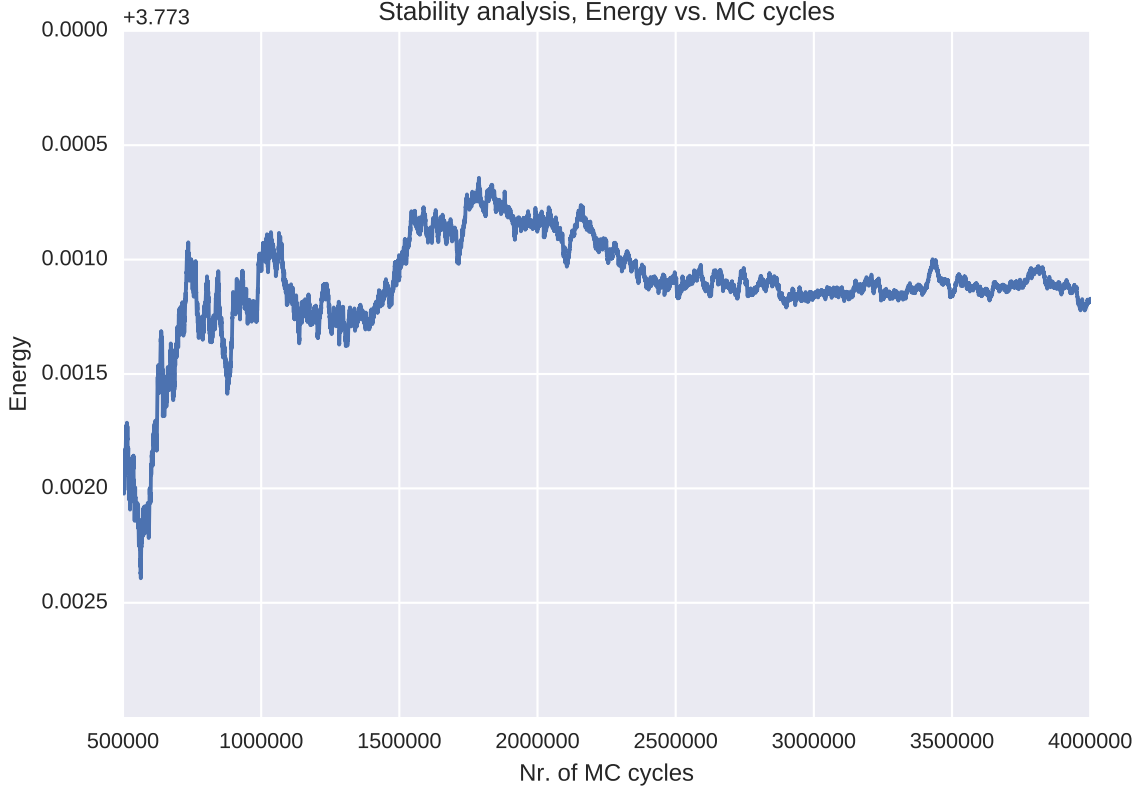


Figure 4: Stability analysis. The expectation value for the perturbed energy as a function of the number of MC cycles, for $\omega = 1.0$ and $\alpha_{opt.} = 0.9$. Here, the number of MC cycles used was $N = 4 \cdot 10^6$ and the step length used for the numerical differentiation was $h = 0.00001$.

In order to fit the trial function with the optimal variational parameters the ground state energy should be minimized. We are therefore interested in how the energy and variance develop as functions of α . In Fig. (5) expectation values of the energy and variance are plotted as functions of α for $\omega = 0.01, 0.5$ and 1.0 . The results provide a rough estimate of what the optimal α should be. We see that although α varies with the given ω , it approaches 1 for increasing ω . The optimal values of α for $\omega = 0.01, 0.5$ and 1.0 are listed in Tab. (1), and were found by minimizing the local energy for a set of α .

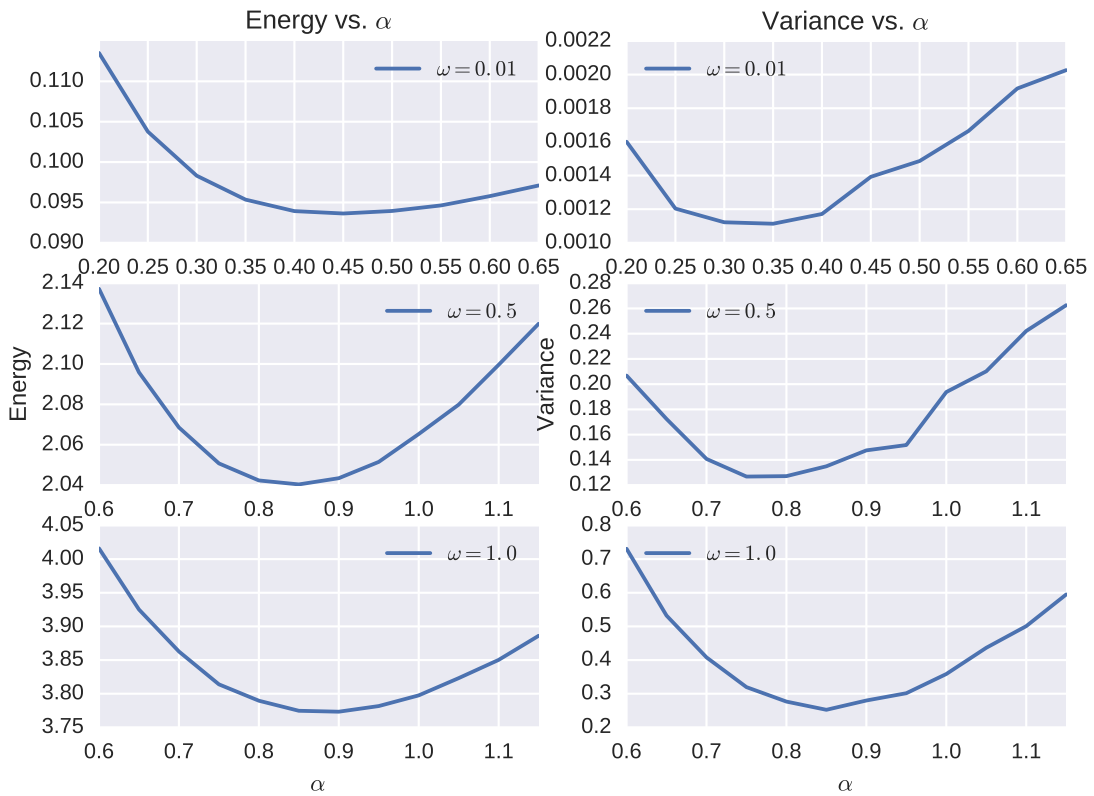


Figure 5: Expectation value for the perturbed energy and variance as a function of α for $\omega = 0.01, 0.5, 1.0$. $N = 2 \cdot 10^6$ Monte Carlo cycles and differentiation step length $h = 0.00001$ were used.

ω	$\alpha_{opt.}$	Accept. ratio	Energy	Variance	r_{12}
0.01	0.44	0.600723	0.0935443	0.00129839	24.0666
0.5	0.84	0.452264	2.04121	0.423179	2.46084
1.0	0.9	0.432763	3.77279	0.272852	1.68181

Table 1: Expectation values of the mean distance $r_{12} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$ between the two electrons for the optimal set of variational parameters, α , for $\omega = 1, 0.5, 1.0$. $N = 2 \cdot 10^6$ MC cycles, step length $h = 0.00001$, for the numerical differentiation and the first trial wave function, Ψ_{T1} .

Also listed in Tab. (1) are acceptance ratios and energy-, variance-, and mean distance r_{12} expectation values for the optimal value of α for $\omega = 0.01, 0.5$ and 1.0 . By decreasing the harmonic oscillator frequency ω , we notice an increase in r_{12} . This coincides with the prediction made in the article by M. Taut [5] that turning down the oscillator frequency will make the wave function spread out more and more.

Furthermore, the acceptance ratio is defined as the ratio between accepted and proposed states, as determined by the Metropolis algorithm. Ideally, the acceptance ratio should lay close to 0.5, so as to pick states that are well inside the probability distribution. In order to ensure an acceptance ratio in the interval $[0.40, 0.60]$ the step size was adjusted accordingly. Finally, we want to compare the expectation value of the energy to the exact value. From the assignment text we have that the exact ground state energy for $\omega = 1.0$ is 3.558. The computed value for $\omega = 1.0$ found in Tab. (1), namely 3.773, is thus too high compared to the exact value. This indicates that the trial function T1 is not an optimal fit to the exact wave function when the Hamiltonian includes the Coulomb perturbation.

4.2 Trial Wave Function T2

To account for the change in the exact wave function when the energy includes a perturbation, we examine the trial wave function $\Psi_{T2}(\mathbf{R})$ with the added Jastrow factor introduced in Sec. (3.2). Note that we now have two variational parameters which we need to optimize to find the minima of the local energy. The optimized α , β , energies and corresponding variances for $\omega = 0.01, 0.5$ and 1.0 are listed in Tab. (2). The energy expectation value for $\omega = 1.0$ is 3.730. Despite being lower than the value found using $\Psi_{T1}(\mathbf{R})$, it is still too high compared to the exact value of 3.55, which suggests that $\Psi_{T2}(\mathbf{R})$ is not an ideal fit to the wave function. The mean r_{12} values in Tab. (2) indicate the same trend as for Ψ_{T1} , that is, decreasing ω gives an increase in r_{12} . r_{12} -values are slightly higher for $\Psi_{T2}(\mathbf{R})$. Further, the expectation values of the energy and variance are both generally lower than for $\Psi_{T1}(\mathbf{R})$.

ω	$\alpha_{opt.}$	$\beta_{opt.}$	Accept. ratio	Energy	Variance	r_{12}
0.01	0.9	0.05	0.472582	0.0793664	$4.00715e - 06$	28.5248
0.5	1.0	0.2	0.443651	2.00009	0.0001725	2.69138
1.0	1.0	0.25	0.434202	3.73028	0.000618212	1.81957

Table 2: Expectation values of the mean distance $r_{12} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$ using Ψ_{T2} with optimal α for $\omega = 1, 0.5, 1.0$. $N = 2.5 \cdot 10^6$ Monte Carlo cycles and differentiation step length $h = 0.00001$ were used.

4.3 Comparison with Eigenvalue Approach

In Tab. (3) the energy expectation values from the eigenvalue approach and the VMC approach are listed together with the exact value for $\omega = 1.0$. Neither the Jacobi approach for the eigenvalue problem [4] nor the VMC approach correctly estimates the energy. In fact, the result from project 2 deteriorates with the addition of the center-of-mass energy.

Analytical	$E_{Project\ 2}$	$E_{Project\ 2} + E_{R,com}$	$E_{Project\ 5,T1}$	$E_{Project\ 5,T2}$
3.588	4.05466	5.55466	3.77279	3.73028

Table 3: Energy expectation values calculated using Jacobi approach for the eigenvalue system in project 2, and VMC approach with $\Psi_{T1}(\mathbf{R})$ and $\Psi_{T2}(\mathbf{R})$ listed with the analytical value.

4.4 Virial Theorem

As discussed in Sec. (2.4), the ratio between potential and kinetic energy should be close to 1 in a pure harmonic oscillator for a good approximation. Fig. (6) shows the ratio as a function of ω , where we have calculated the perturbed energy expectation value using $\Psi_{T2}(\mathbf{R})$ and the unperturbed expectation value using $\Psi_{T1}(\mathbf{R})$. For the unperturbed case we see that the ratio is close to 1 for the whole range of ω 's, while for the perturbed case the ratio starts at almost 6 and converges to around 1.7 for $\omega = 1.0$. The perturbed energy ratio behaves in an inversely proportional way as a function of ω .

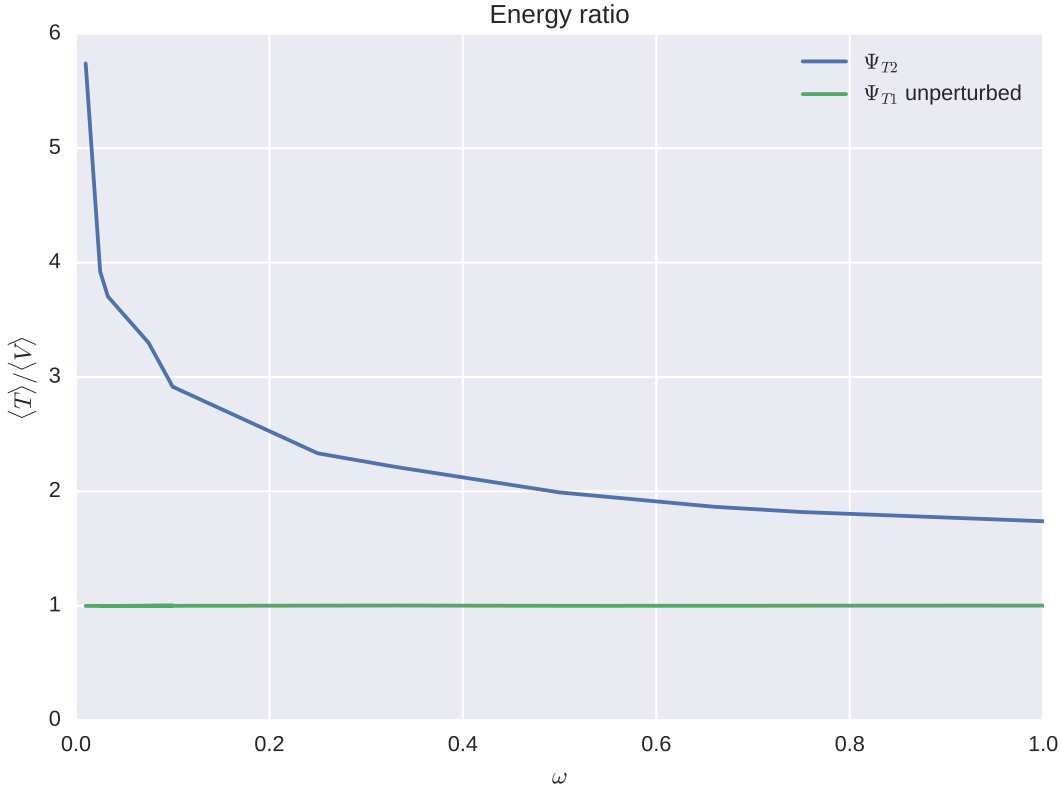


Figure 6: The ratio of the expectation values for the total kinetic energy $\langle T \rangle$ and the total potential energy $\langle V \rangle$ as a function of ω . The second trial wave function $\Psi_{T2}(\mathbf{R})$ with $N = 2.5 \cdot 10^6$ MC cycles and step length $h = 0.00001$ is used.

5 Conclusions

$\Psi_{T1}(\mathbf{R})$ without the Coloumb interaction yields the exact result for $\omega = 1.0$, indicating $\Psi_{T1} = \Psi_0$ for the unperturbed energy. With the Coloumb interaction included, however, the expectation values differ from E_{exact} , indicating that Ψ_{T1} is no longer a good approximation. Ψ_{T2} yields values closer to E_{exact} , but we still have a significant error. $\Psi_{T1}(\mathbf{R})$ and $\Psi_{T2}(\mathbf{R})$ are therefore not optimal approximations for the exact wave function for the perturbed case. The behaviour of the mean distance r_{12} as a function of ω , however, coincides with our expectation that decreasing the oscillator frequency will make the wave function spread out more and more.

The comparison between the analytical, the Jacobi and the VMC value for the ground state energy at $\omega = 1.0$ indicates that neither numerical method provides a very good approximation. The VMC method is a better approximation for $\omega = 1$. The large error in the energy expectation value from the Jacobian method suggests that the wrong E_{COM} may have been added. The results from the unperturbed energy coincide with the Virial theorem, so Ψ_{T1} describes a pure harmonic oscillator. The perturbed case converges towards 1.7 for large ω 's, suggesting that the system is no longer a *pure* harmonic oscillator after the addition the Coulomb interaction.

Finally, some improvements that could have been done in our project include further optimization of trial functions and lowering of the variational parameter step length. The latter would provide a larger sample of values, opening for more accurate α, β . This was not done in our project due to the limited computational resources. A lower step length, h , for the differentiation used to find the local energy could also have been used, but was omitted due to the high computational cost.

A Hermite Polynomials

The Hermite polynomials are solutions of the differential equation

$$\frac{d^2 H(x)}{dx^2} - 2x \frac{dH(x)}{dx} + (\lambda - 1)H(x) = 0. \quad (21)$$

The first few polynomials are

$$H_0(x) = 1, \quad (22)$$

$$H_1(x) = 2x, \quad (23)$$

$$H_2(x) = 4x^2 - 2, \quad (24)$$

$$H_3(x) = 8x^3 - 12x. \quad (25)$$

$$(26)$$

They fulfill the orthogonality relation

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x)^2 dx = 2^n n! \sqrt{\pi}, \quad (27)$$

and the recursion relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x). \quad (28)$$

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