

Quantum Monte Carlo of confined electrons

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Abstract

In this project we use variational Monte Carlo to find an upper bound on the ground state energy of two quantum dots in a harmonic oscillator potential, with a repulsive Coulomb interaction. Two different trial wave functions are used; first a general exponential function based on the ground state without any repulsion, and then an improved function where the first approximation is multiplied by a Jastrow factor. The expectation value of the energy is minimized with respect to α and β (the parameters of the improved trial wave function): We find upper bounds of, e.g., $\langle E_{min} \rangle = 3.73012(2)$ for harmonic oscillator frequency $\omega = 1$, $\langle E_{min} \rangle = 2.00198(5)$ for $\omega = 0.5$ and $\langle E_{min} \rangle = 0.51364(6)$ for $\omega = 0.1$, all in pretty good agreement with the theory (in particular for the last two). We also examine the ratio $\langle T \rangle / \langle U \rangle$ (T and U are kinetic and potential energies, respectively) for different oscillator frequencies, and find that it is constant for a pure harmonic oscillator potential as expected; when the repulsion is taken into account it is no longer constant, but it approaches the same value as the oscillator frequency increases.

All programs used to produce and plot these results, as well as output files containing the results referred to in this text, can be seen at <https://github.com/Krissvang/Computational-Physics-group>.



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1 Introduction

In a non-conductive or semiconducting material there is a band gap that is an avoid energy gap for the electron energies in the material. We say that electrons with a smaller energy than the band gap are in the valence band. If they have a bigger energy they are in the conduction band. Quantum dots are nano-crystals sized typically in the range $(2, 10)nm$. They are formed by the inclusion of a semiconducting material with a certain band gap in a material with a bigger band gap. This structure generates a three dimensional potential well that encloses electrons and holes in a small region. In this region the energy levels are discrete. Quantum dots are a central topic in nanotechnology since they do have many practical applications as in solar cells, quantum computing

and nano-medicine.

The aim of this project is to study a quantum dot with two electrons in three dimensions. In order to do this we model the quantum dot as a system of two electrons, confined in a isotropic three dimensional harmonic oscillator potential. We want to evaluate in particular the ground state energy, the average relative distance between the electrons and the expectation value of the potential and kinetic energies of the system. To achieve this results we apply the variational Monte Carlo (VMC) method on the model [1]. The variational principle states that the expectation value of a system's Hamiltonian is greater than or equal to the ground state energy. This means that we can estimate an upper limit for the ground state energy with some trial functions (or test functions) that approximate the ground state wave function. The trial functions depend on the positions of the particles in the system and on α that is the variational parameter we want to optimize. The aim is to find the best approximation of the ground state wave function by varying α . We want to do this in order to get the best estimation for the ground state energy. We use the Metropolis algorithm in order to inspect the different configurations of the system, that consist different \vec{R} .

In this project we use two trial functions that are Ψ_{T1} and Ψ_{T2} . The first one does not takes into account the interaction between the electrons while the second does. This is done by introducing a new variational parameter in a term called Jastrow factor that allows us to get a better approximation of the electron-electron interaction.

In this text we firstly describe the variational Monte Carlo Method, we motivate the choice of the two trial functions and we describe the algorithm. After that we show the result we get for both the trials functions. In the end we use our result to check the virial theorem.

If the reader is not familiar with the Metropolis algorithm and the Monte Carlo method could be useful to read other two projects [2, 3] written by the same authors that deal with this topics. The reader is assumed to have a basic knowledge of quantum mechanics.

2 Methods

In this section are described the methods used in this project. The focus is not on the Monte Carlo and Metropolis algorithms; for a more detailed discussion of these subjects see [3]. Here we describe the variational principle and its application at our system through two trial functions. Moreover is presented the virial theorem.

2.1 Variational principle

This principle allows us to evaluate an upper limit for the ground state energy E_0 in a quantum system. The Hamiltonian function \hat{H} of the system defines a basis of energy eigenstate Ψ_i^E [4]. We can decompose every state of the system $\Psi_T(\vec{R})$ on the energy eigenstates

$$\Psi_T(\vec{R}) = \sum a_i \Psi_i^E, \quad (1)$$

where a_i are the decomposition coefficients. We can evaluate now the mean value of H on the state $\Psi_T(\vec{R})$

$$\langle \hat{H} \rangle = \frac{\int d\vec{R} \Psi_T^*(\vec{R}) \hat{H}(\vec{R}) \Psi_T(\vec{R})}{\int d\vec{R} \Psi_T^*(\vec{R}) \Psi_T(\vec{R})}. \quad (2)$$

By using equation (1) the last equation becomes

$$\langle \hat{H} \rangle = \frac{\sum_{mn} a_m^* a_n \int d\vec{R} \Psi_m^{E*}(\vec{R}) \hat{H}(\vec{R}) \Psi_n^E(\vec{R})}{\sum_{mn} a_m^* a_n \int d\vec{R} \Psi_m^*(\vec{R}) \Psi_n(\vec{R})} = \frac{\sum_{mn} a_m^* a_n \int d\vec{R} \Psi_m^{E*}(\vec{R}) E_n \Psi_n^E(\vec{R})}{\sum_{mn} a_m^* a_n}, \quad (3)$$

where E_n is the eigenvalue associated with the energy eigenstate $\Psi_n^E(\vec{R})$. We can rewrite it as

$$E_0 \leq \frac{\sum_n a_n^2 E_n}{\sum_n a_n^2}. \quad (4)$$

Usually in order to evaluate the upper bound for the ground state energy with this principle we need to construct the trial wave function $\Psi_T(\vec{R}, \alpha)$. Here the vector $\vec{R} = (\vec{r}_1, \dots, \vec{r}_n)$ contains the positions of the particles in the system and α in the most general case is a vector made by the variational parameters $\alpha = (\alpha_1, \dots, \alpha_m)$. If the trial wave function is the ground state eigenstate of the system, then equation (4) becomes an inequality. If not, then we get only an approximation for the ground state energy. When the trial wave function is a good approximation for the ground state function the upper bound for the ground state energy is close to the expected value. For this reason we need the trial function to be really similar to the ground state function. In order to optimize the trial function and find a reliable estimation for the ground state energy we vary the parameters a . We calculate the upper bound to the ground state energy with equation (2), therefore we have to evaluate multi dimensional integrals on the variable \vec{R} . In our case we have two electrons in three dimension that results in six dimensional integrals. For this reason the Monte Carlo method is the most effective as is shown in [2].

2.2 Variational Monte Carlo

In Monte Carlo integration, the integral of a function on a domain is approximated as the mean value of the function at N randomly selected points within this area. If we use the importance sampling then we get

$$\int_{domain} d\vec{R} p(\vec{R}) f(\vec{R}) \approx \frac{1}{N} \sum_{i=1}^N f(\vec{R}_i), \quad (5)$$

where N is the number of Monte Carlo samples and $p(\vec{R})$ is a probability distribution. From now on we neglect the trial function dependence from the variational parametre α . In order to make equation (2) similar to equation (5) we define

$$p(\vec{R}) = \frac{|\Psi_T(\vec{R})|^2}{\int d\vec{R} |\Psi_T(\vec{R})|^2}. \quad (6)$$

We define also the local energy E_L as

$$\hat{E}_L(\vec{R}) = \frac{1}{\Psi_T(\vec{R})} \hat{H} \Psi_T(\vec{R}). \quad (7)$$

Now we can rewrite equation (2) as

$$\langle \hat{H} \rangle = E_L = \int d\vec{R} p(\vec{R}) \hat{E}_L(\vec{R}) \quad (8)$$

This last equation is written in the right form to be solved by the Monte Carlo integration method.

This is implemented almost identically as for the Ising model, see [3] (with energies and probabilities replaced by E_L and p as given above), except that the local energies and probability ratios $p_{\text{new}}/p_{\text{old}}$ cannot be pre-calculated; they must be calculated explicitly for each new proposed step. The ratio between the new and old is simply given by the ratio of the squared trial wave functions. Furthermore, steps are proposed by making changes in the position; thus for each of the six coordinates (3 for each particle) we make the transformation

$$r'_i = r_i + h\Delta r_i \quad (9)$$

where Δr_i is a random number, drawn from a uniform distribution in $[-0.5, 0.5]$, and h is the step size. The ratio of the probabilities for the proposed state and the current one is calculated; if it is greater than one the move is accepted, if not the probability for accepting the move is equal to the aforementioned ratio. h is chosen so that about 50% of all the proposed moves are accepted (to do this, we ran the algorithm for varying step sizes until the number of accepted moves divided by the number of Monte Carlo cycles was sufficiently close to 0.5). At the end of every Monte Carlo cycle (regardless of whether the proposed move was accepted) new values for the total, kinetic and potential energies and the distance between the particles, and their squares, are calculated. Finally, these are averaged to calculate the mean values and variances of the different quantities.

2.3 Trial functions

The system we are considering is composed by two electrons confined in a three dimensional isotropic harmonic oscillator potential. Thus the Hamiltonian of this system is

$$\hat{H} = \sum_{i=1}^2 \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right) + \frac{1}{|\vec{r}_1 - \vec{r}_2|}, \quad (10)$$

where ω is the oscillator frequency. The Hamiltonian is written in natural units ($\hbar = c = e = m_e = 1$) and all the energies are expressed in atomic units (*a.u.*). We refer to the term with the sum in the Hamiltonian as unperturbed Hamiltonian and we call it \hat{H}_0 . This term represents both the kinetic and the harmonic oscillator potential energy. The second term is the perturbation one and we call it \hat{H}_1 . This represents the electron-electron repulsion. We call $r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}$ and $r_{12} = |\vec{r}_1 - \vec{r}_2|$.

The energy eigenvalues for one electron in a isotropic three dimensional oscillator are given by

$$E_{\vec{n}} = \omega \left(n_x + n_y + n_z + \frac{3}{2} \right). \quad (11)$$

The electron is in the ground state when $n_x = n_y = n_z = 0$, thus the ground state energy is $E_0 = 3/2\omega$. As a consequence, if we consider only the unperturbed Hamiltonian \hat{H}_0 for a two electrons system the ground state energy results to be the sum of the energies for two non-interacting electrons that is $E_0 = 3\omega$.

The wave functions of the system are composed by a positional part and a spin part. Positional part is the solution of the equation $\hat{H}\Psi = E_L\Psi$.

2.3.1 First approximation

The first trial function for the positional part we look at is the solution for the unperturbed part of the Hamiltonian

$$\Psi_{T1}(\vec{r}_1, \vec{r}_2) = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2), \quad (12)$$

where C is a normalization constant which is irrelevant to the calculations, as we are only interested in ratios of squared wave functions. This is on the same form as the solution of the unperturbed system (i.e. without \hat{H}_1), but with an extra factor α in the exponent to account for the perturbation (this means that without the interaction term, the ground state is given exactly by Ψ_{T1} with $\alpha = 1$).

We focus now on the spin component of the wave function. Each electron has got spin $s_1 = s_2 = 1/2$. We have to sum those with the quantum mechanics rules for the momenta sum to compute the total spin of the system [4]. In this case we get four different spin states with total spin $s = 0, 1$. Three states corresponds to the case $s = 1$ and one state to the case $s = 0$.

Electrons are fermions and due to the Pauli exclusion principle, the total wave function that is composed by the positional part and total spin part must be antisymmetric under exchange of particles. As visible from the trial functions (12) we have a symmetrical positional part. Thus the total spin component has to be antisymmetrical. The only state that fulfill this requirement is the $s = 0$ state. Thus the electrons have to be in a singlet spin state with total spin equal to zero.

To find the analytical expression for the local energy, we need to solve the eigenvalue equation $\hat{H}_0\Psi_{T1} = E_{L1}\Psi_{T1}$. Where the Hamiltonian is given by

$$\hat{H}_0 = \sum_{i=1}^2 \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right) \quad (13)$$

where ∇_i^2 is the Laplacian acting on r_i , it is therefore useful to use the spherical representation of $\nabla_i^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \varphi}$. We can now easily see that

$$-\frac{1}{2} \nabla_i^2 \Psi_{T1} = -\frac{1}{2} \frac{\partial^2 \Psi_{T1}}{\partial r_i^2} - \frac{1}{r_i} \frac{\partial \Psi_{T1}}{\partial r_i}$$

Where we have used that Ψ_{T1} is independent of θ and φ . Now we can use that

$$\frac{\partial \Psi_{T1}}{\partial r_i} = \frac{\partial}{\partial r_i} C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) = -\alpha\omega r_i \Psi_{T1}$$

$$\frac{\partial^2 \Psi_{T1}}{\partial r_i^2} = \frac{\partial}{\partial r_i} (-\alpha\omega r_i \Psi_{T1}) = -\alpha\omega \Psi_{T1} + (\alpha\omega r_i)^2 \Psi_{T1}$$

This gives us

$$-\frac{1}{2} \nabla_i^2 \Psi_{T1} = \left[\frac{3}{2} \alpha\omega - \frac{1}{2} (\alpha\omega r_i)^2 \right] \Psi_{T1}$$

The eigenvalue equation becomes

$$\begin{aligned}\hat{H}_0\Psi_{T1} &= \left(-\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}(\omega^2(r_1^2 + r_2^2))\right)\Psi_{T1} = \left[(3\alpha\omega) - \frac{1}{2}(\alpha^2\omega^2(r_1^2 + r_2^2)) + \frac{1}{2}(\omega^2(r_1^2 + r_2^2))\right]\Psi_{T1} \\ &= \left[\frac{1}{2}\omega^2(r_1^2 + r_2^2)(1 - \alpha^2) + 3\alpha\omega\right]\Psi_{T1}\end{aligned}$$

This means that the analytical expression for the local energy given by

$$E_{L1U} = \frac{1}{2}\omega^2(r_1^2 + r_2^2)(1 - \alpha^2) + 3\alpha\omega. \quad (14)$$

Remember that this expression has been computed considering only the unperturbed part of the Hamiltonian. If we want to consider the electron-electron repulsion we should add the extra term $1/r_{12}$.

$$E_{L1P} = E_{L1U} + \frac{1}{r_{12}}. \quad (15)$$

We found the expectation value of the energy for several different values of α ; the one that gave the lowest energy was used as a starting point for finding an even lower upper bound with an improved trial wave function.

2.3.2 Improved trial wave function

The second trial function we consider is

$$\Psi_{T2}(\vec{r}_1, \vec{r}_2) = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \exp\left(\frac{r_{12}}{2(1 + \beta r_{12})}\right). \quad (16)$$

In this case α and β are the variational parameters. The factor we have introduced here is called Jastrow factor and takes into account the electron-electron repulsion. Another task of this term is to handle the infinities that could arise during the calculation of the expectation values. Indeed in the perturbed Hamiltonian (10) the perturbation term diverges when $r_{12} \rightarrow 0$.

With this trial wave function, the local energy is given by [5]

$$E_{L2} = E_{L1P} + \frac{1}{2(1 + \beta r_{12})^2} \left\{ \alpha r_{12} - \frac{1}{2(1 + \beta r_{12})^2} - \frac{2}{r_{12}} + \frac{2\beta}{1 + \beta r_{12}} \right\} \quad (17)$$

We ran the VMC algorithm again for this trial wave function and local energy, varying α and β to find the combination that gave the lowest possible upper bound for the ground state energy.

2.4 Virial theorem

This theorem provide a tool to inspect the relationship between the mean kinetic energy $\langle T \rangle$ and the mean potential energy $\langle U \rangle$ for a system in a state of equilibrium. The theorem states that

$$\langle T \rangle = \frac{1}{2} \langle \vec{r} \cdot \nabla U \rangle, \quad (18)$$

where \vec{r} is the directional distance and ∇U is the opposite of the force. This relation holds for both a classical and quantum system. A theoretical demonstration for this theorem could be found at [6]. For a simple harmonic oscillator the equation (18) reduces to

$$\langle T \rangle = \langle U \rangle. \quad (19)$$

3 Implementation

In this section are described the steps of the algorithm we implemented and the test we have done on the code to check its functioning.

3.1 Algorithm

The Monte Carlo evaluation of a integral with the Metropolis algorithm goes as follows:

- Given a number of Monte Carlo steps and parameters (α , β , ω and h .) Calculate $|\psi_T|^2$.
- Initialise the energy and variance.
- Start the loop over Monte Carlo cycles
 1. Calculate the trial position $r'_i = r_i + h\Delta r_i$, where Δr_i is a random number from the uniform distribution of the interval $[-0.5, 0.5]$.
 2. Use the Metropolis algorithm to accept or reject this move by calculating the ratio

$$w = \frac{P(\vec{R}_{new})}{P(\vec{R}_{old})}$$

If $w \geq s$, where s is a random number from the uniform distribution of the interval $[0, 1]$, the new position is accepted, else it is rejected and we let the new position be the old position.

3. Update the local energy and local variance
- When looped over all Monte Carlo samplings, calculate the mean energy and mean variance and print to file.

The step-length h is found by looping over the given number of Monte Carlo steps while varying a local step-length h_{local} . When the acceptance ratio is 50% we set $h = h_{local}$.

The variational procedure in VMC is then to loop over a given parameter, e.g. α or β , and finding the minimum energy. The way we found the minimum is to first find the minimum energy for the first trial wave function with the energy E_{L1P} . Using the α at this minimum we use improved trial wave function and varied β to look for a lower minimum. Using this β we then varied α again and so forth.

3.2 Unit tests

We made several tests that the programs had to pass, in order to ensure that the algorithms had been implemented correctly. As mentioned previously, the first approximation of the trial wave function with $\alpha = 1$ is exactly the ground state of the unperturbed system. Thus the VMC algorithm should reproduce exactly $\langle E \rangle = 3$ (i.e. with $\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \approx 0$) for $\alpha = \omega = 1$. We also tested the function for finding the optimal step size h , by requiring the rate of accepted moves versus the number of Monte Carlo cycles to be in the range $[0.45, 0.55]$.

Finally, we made tests for the functions `r_squared` and `r_12`, which calculate $r_1^2 + r_2^2$ and $r_{12} = |\vec{r}_1 - \vec{r}_2|$ for a given set of positions \vec{r}_1, \vec{r}_2 , respectively, both of which are used in both the local energies and trial wave functions. We tested some very simple cases; specifically, that `r_squared` returns 25 and `r_12` returns 5 when $\vec{r}_1 = (3, 0, 0)$ and $\vec{r}_2 = (0, 0, 4)$, and that they return 0.91 and $\sqrt{0.43}$ respectively when $\vec{r}_1 = (0.1, -0.2, 0.3)$ and $\vec{r}_2 = (-0.4, -0.5, 0.6)$.

4 Results

4.1 First approximation

First we studied the stability of our calculations as a function of Monte Carlo cycles. We calculated the energy for the first trial function without repulsion for 10 to 10^6 Monte Carlo cycles for different α , which is shown in Fig. 1. The step length is found from an algorithm such that it gives 50% acceptance ratio.

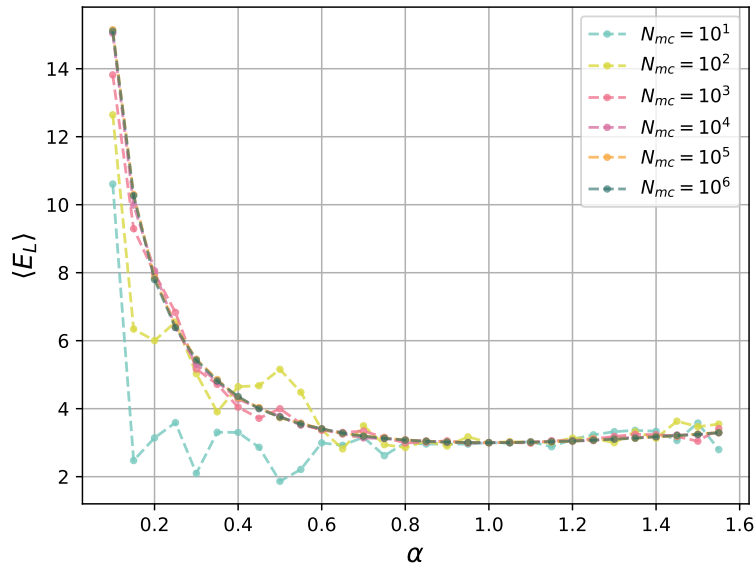


Fig. 1. Local energy $\langle E_L \rangle$ as a function of α for different Monte Carlo cycles.

We see that the VMC computations start to become reliable after about 10^4 Monte Carlo cycles. We thus chose to use 10^6 Monte Carlo cycles in order to get a satisfying result numerically and for computational efficiency.

We then calculated the energy of the first trial wave function for different α as shown in Fig. 2.

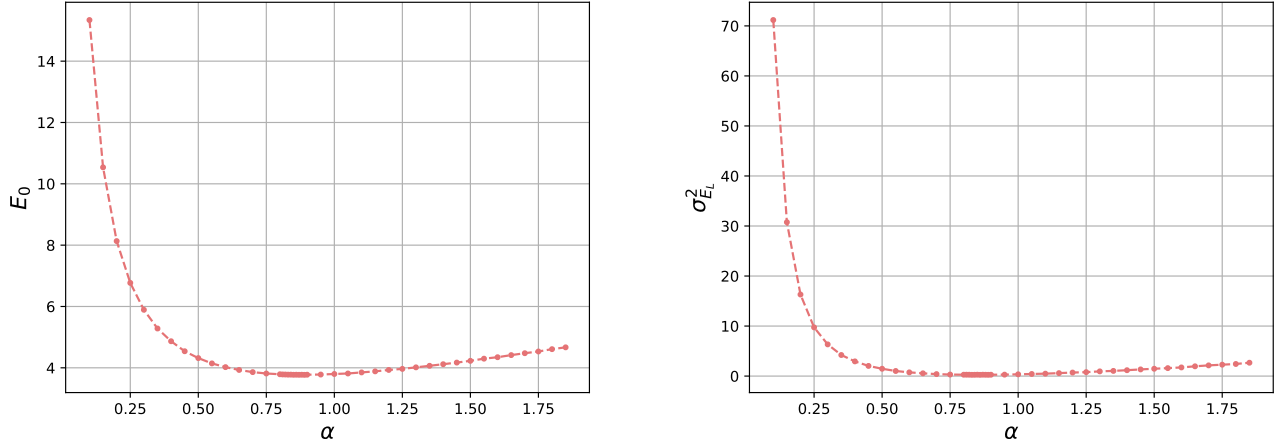


Fig. 2. Local energy $\langle E_L \rangle$ (left) and variance $\sigma_{E_L}^2$ (right) for different of α , calculated with 10^6 Monte Carlo cycles.

We find that the minimum local energy is given for $\alpha \simeq 0.87$ at $\langle E_L \rangle|_{\alpha=0.87} \simeq 3.7748(5)$ with a variance $\sigma^2 \simeq 0.28$. Even though this is the energy closest to the analytical value $E_0 = 3.558$ a.u. [5], it is not the energy with the lowest variance. The energy at $\alpha \simeq 0.86$ is $\langle E_L \rangle|_{\alpha=0.86} = 3.775$ with a variance $\sigma^2 = 0.25$. This comes from the fact that we are evaluating two different integrals. The expectation values of the mean distances $\langle r_{12} \rangle$ between the two electrons is plotted as the blue lines in Fig. 4. We see that as ω increases $\langle r_{12} \rangle$ decreases. This is because $\langle E_L \rangle \propto \omega$ as we see in Fig. 3, which mean that the electrons will have more kinetic energy and will travel closer to each other, resulting in lower $\langle r_{12} \rangle$.

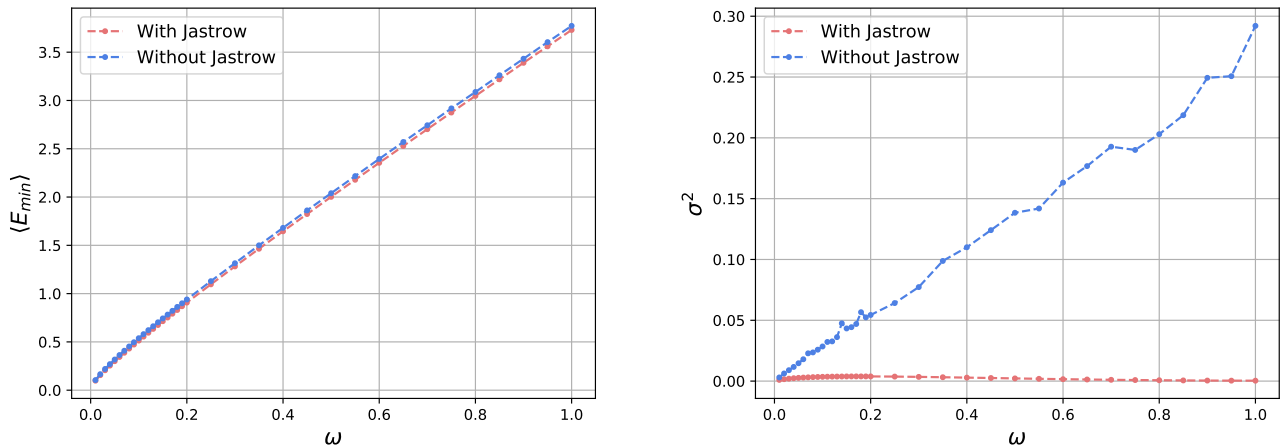


Fig. 3. Minimum energy $\langle E_{min} \rangle$ (left) and variance in the minimum energy (right) for the test wave functions with and without the Jastrow factor. Calculated for different ω , using $\alpha = 1.002$, $\beta = 0.276$ for the energies with the Jastrow factor and $\alpha = 0.87$ without the Jastrow factor. Run with 10^6 Monte Carlo cycles.

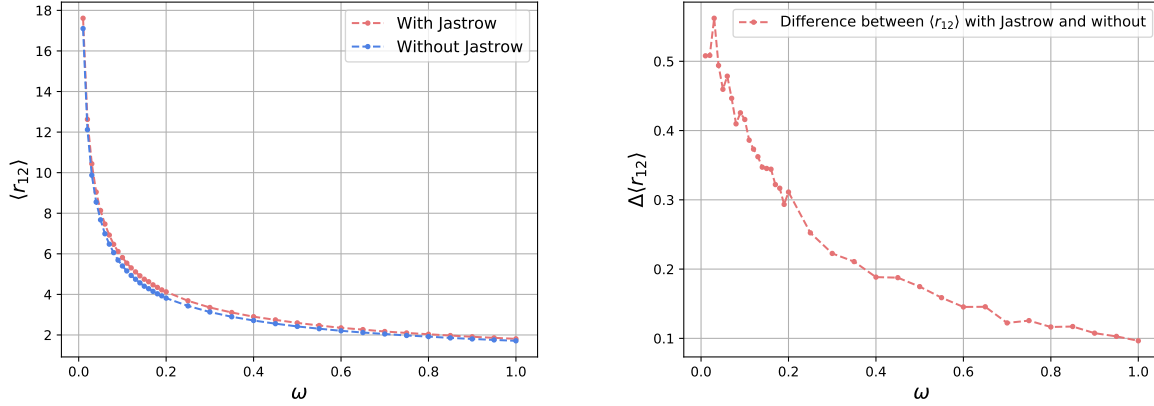


Fig. 4. Mean distance between the electrons $\langle r_{12} \rangle$ for the test wave functions with and without the Jastrow factor (left) and the differences between the mean distances (right). Calculated for different ω , using $\alpha = 1.002$, $\beta = 0.276$ for the energies with the Jastrow factor and $\alpha = 0.87$ without the Jastrow factor. Run with 10^6 Monte Carlo cycles.

4.2 Improved trial wave function

We found the optimal α and β for the improved trial wave function ψ_{T2} using the method described in section 3.1 to be $\alpha = 1.002$ and $\beta = 0.276$, with the corresponding energy and variance; $\langle E_{min} \rangle = 3.73012(2)$ and $\sigma^2 = 0.00035$. Comparing it to the energy found without the Jastrow factor:

$$\frac{E_{T1} - E_{T2}}{E_{analytic}} = \left| \frac{3.7748 - 3.73012}{3.558} \right| \simeq 1\%$$

we see that we get a 1% improvement. We see this trend for all $\omega \in [0.1, 1]$, see Fig. 3. While the variance for the first trial wave function increases linearly with ω , the variance for the improved trial wave function stays close to zero for all ω . This shows the importance of the Jastrow factor. We also see that the Jastrow factor impacts the distance between the two electrons (see Fig. 4), it increases the mean distance between them, especially for lower energies, i.e. lower ω . This is due to the fact that for lower energies, the repulsion force becomes more important, since the Coulomb force between the electrons have infinite range.

The results found here are fairly consistent with previous calculations of the same system, where the problem was re-stated as an eigenvalue problem and solved using the Jacobi method [2]. Here we calculated the ground state relative energy between the two particles for $\omega_r = 1/20$ (note that there is an error in the report here; the result should be given as 0.35, not 3.5) and $\omega_r = 1/4$, where in atomic units (all constants, e.g. \hbar and e , set to 1) $\omega_r = \omega/2$ (in these units the quantity λ which was calculated here corresponds exactly to the relative energy E_r). In both cases the computed results were identical to the theoretical ones up to four leading digits. The total ground state energy is found by adding the ground state center of mass(CM) energy E_R . The Schrödinger equation for the CM coordinates \vec{R} is [7]

$$\left[-\frac{1}{2} \nabla_{\vec{R}}^2 + \frac{1}{2} \omega_{\vec{R}}^2 \vec{R}^2 \right] \psi_{\vec{R}}(\vec{R}) = \eta' \psi_{\vec{R}}(\vec{R}) \quad (20)$$

where $\omega_{\vec{R}} = 2\omega$ and $\eta' = 2E_R$. Thus the ground state CM energy is given by $E_R^0 = \frac{3}{2}\omega$. The expected total energies from using the Jacobi methods are compared to the ones obtained in this report in table 1. Considering that the VMC method only gives an upper bound of the ground state energy, the agreement is pretty good,

meaning that our improved trial wave-function describes the system relatively well. An even better approximation (i.e. a lower upper bound for the ground state energy) could probably be achieved with increasingly complicated trial wave functions, with more variable parameters, but this would eventually become very time consuming.

Table 1. Comparison of the results obtained here with previous results obtained with the Jacobi eigenvalue method. The error is given by $\sigma = \sqrt{\sigma_E^2/N}$ where σ_E^2 is the variance of the energy and $N = 10^6$ is the number of Monte Carlo cycles.

ω [a.u.]	$\langle E_{\min} \rangle$ [a.u.] (Jacobi method)	$\langle E_{\min} \rangle$ [a.u.] (Variational Monte Carlo)
1/2	1.99998	2.00198(5)
1/10	0.5	0.51364(6)

4.3 Virial theorem

Plots of the ratio between the kinetic and potential energies (one where only the harmonic oscillator part of the potential is taken into account; another with the full potential, including the Coulomb repulsion) are shown in figure 5. For the pure harmonic oscillator potential, the simplified form of the virial theorem ($\langle T \rangle = \langle U \rangle$) roughly holds (the kinetic energy is about 20 percent too small, but the ratio is constant), while for the full potential it does not. This is as expected; for a more complicated potential, consisting of several parts, the relation between potential and kinetic energy is naturally not as simple. One can, however, see that as the oscillator frequency ω increases, the ratio seems to asymptotically approach that of the pure harmonic oscillator. This can be understood as the "strength" of the oscillator potential increasing compared to the Coulomb potential, so that the latter eventually becomes negligible.

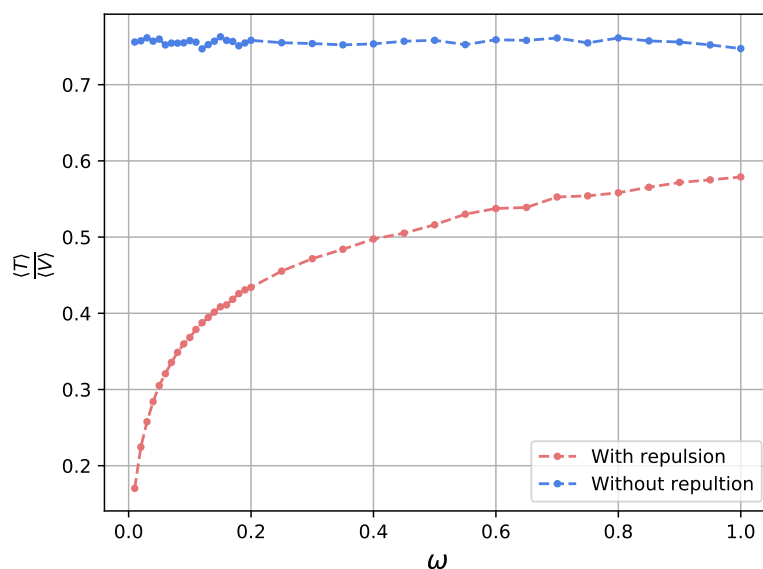


Fig. 5. Ratio of the expectation values of kinetic and potential energy, with and without Coulomb repulsion, as a function of the oscillator frequency.

5 Conclusion

By rewriting the expression for the expectation value of the energy for a quantum mechanical system, we have been able to solve a variational problem for a two-particle system using Markov Chain Monte Carlo methods. Specifically, we have examined two different trial wave functions for a system of two particles of identical charge in a harmonic oscillator potential, with Coulomb repulsion between them. First, we used a sort of generalized form of the unperturbed (no repulsion) ground state wave function with a variable parameter α , mainly to test the algorithm but also to get a starting point for a better approximation.

This was achieved by multiplying the first trial function by a Jastrow factor, containing another parameter β . The expectation value of the energy was minimized with respect to these two parameters, and we found a lowest upper bound of the ground state energy given for the oscillator frequency $\omega = 1$ by $\langle E_{min} \rangle = 3.73012(2)$, in decent agreement with the theoretical value $E_0 = 3.558$. Better agreement was achieved for other frequencies; for both $\omega = 1/10$ and $\omega = 1/2$ we found energies that were close to the theoretical ones.

Finally we tested the virial theorem for the system. Without taking Coulomb repulsion into account, we found that the expected relation $\langle T \rangle = \langle U \rangle$ did not hold exactly, but there was a constant ratio between the two. When the repulsion was included the relation no longer holds, as expected, but as the frequency increases, the ratio between the kinetic and potential energy approaches the same value as without repulsion.

Our results here are in good agreement with those obtained earlier, by reformulating the problem as an eigenvalue problem. This shows that there are several very different methods of solving the same problem. Which of them is preferable very much depends on the problem at hand; for the one discussed here one might argue that the eigenvalue solver is more effective, as it is able to find a fairly accurate estimate (not just an upper bound) of the ground state energy without having to find suitable trial wave functions. However the variational Monte Carlo method is usually simpler to implement; for example no rewriting of the problem in terms of polar coordinates, or relative and ground state energies, is necessary. This makes this method more generally applicable; apart from obtaining the analytical expressions for local energies (which can be done using symbolic calculator programs), increasing the complexity of the problem, e.g. by introducing more complicated potentials or more particles, introduces no further complications for this method. This would be interesting to look into in the future. This will quickly make the problem too complicated to solve using eigenvalue methods, however.

In conclusion, although the variational Monte Carlo method is not necessarily the most effective to use in this particular problem, we have demonstrated its usefulness in that it can easily be implemented for more complex systems.

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