FYS3150 Project 5

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Abstract

In this investigation, we approximate the ground state energy and particle separation of a three-dimensional system of two electrons in a harmonic oscillator potential, using a variational Monte Carlo simulation in conjunction with the Metropolis algorithm. Two trial wave functions, ψ_{T1} and ψ_{T2} are investigated. For both, grid searches were performed to find variational parameters that minimized the average local trial energy, and a novel, simple closed form expression was developed for the maximum step size used in the Metropolis algorithm. This step size was found to give an acceptance rate in the region of 0.56-0.59 for all investigated harmonic oscillator frequencies, and variational parameters. For ψ_{T1} particle-particle interactions were ignored, and the optimal parameter α was found to be 0.88, resulting in a trial energy of 3.77 a.u.for a harmonic oscillator frequency of $\omega = 1.0$. For the same oscillator frequency, the second trial wave function, which took particle interaction into account through the addition of a Jastrow factor, achieved a minimum average trial energy of 3.7302, and also a lower energy variance. Both results were found to agree with other findings in the literature, with ψ_{T2} giving the best ground state energy approximation for greater harmonic oscillator frequencies. In addition, it was found that in the non-interacting case, for ψ_{T1}, the system obeyed the virial theorem, with a ratio of average kinetic to potential energy of ≈ 1. When interactions were included, this was not the case, and the ratio was closer to 0.6 for large values of ω.

1 Introduction

Recently, Google announced that they had achieved so-called quantum supremacy[1]. Using what is put forth as a quantum computer, they completed a computation in 200 seconds, which would take a classical computer an estimated 10,000 years. While currently reserved for the very cutting edge of physics and science, this announcement suggests that quantum technology, and quantum-physics based computation might become an important part of our lives in the not-too-distant future. Until that time, we can still use classical computing to simulate many rich quantum systems, and gain valuable insights about the world at its smallest scales.

In this text, we consider the case of two electrons trapped in a three-dimensional harmonic oscillator potential, constituting a system of *quantum dots*, the precise control of which can even allow for the creation of quantum circuits[2]. As quantum particles, the electrons obey the well-known Schrödinger equation, but the electron-electron repulsion seems to make it impossible to find exact solutions for this system [3]. Luckily, we can use numerical methods to find approximate solutions, and for this investigation we will use Monte Carlo simulation in conjunction with the *variational principle* to do so. Specifically, we will look into the expected separation between the two particles, the expected ground state energy of the system, as well as the expected kinetic and potential energy.

To begin, we will attempt to explain the variational principle, and how we might apply it to our system, before moving on to the more quantum mechanical aspects of this problem. While doing so, we will also establish some useful analytical results for a similar, non-interacting case. Thereafter, we will consider how we can investigate this system numerically, through Monte Carlo simulations. Finally, we will attempt to establish an algorithm for actually computing quantities of interest, using the so-called Metropolis algorithm as a foundation.

2 Theory & Algorithm

2.1 The Variational Principle

In quantum mechanics, there are only a precious few exactly solvable systems, which means that we often need to resort to numerical methods in order to investigate more complex cases. Many times, we are interested in the energy levels of these systems, and of great interest is the ground state, or lowest energy state, as these are often the easiest to study experimentally. While it is not generally easy to find the ground state energy, the variational principle comes to our aid, by allowing a very simple method for determining an upper bound on the ground state energy. Stated using Dirac notation, the variational principle says that

$$E_{gs} \leq \langle\psi|\hat{H}|\psi\rangle, \tag{1}$$

where E_{gs} is the energy of the ground state, while $\hat{H}$ is the Hamiltonian of the system, while $|\psi\rangle$ can be *any* (time-independent) quantum state, assuming it has been properly normalized. (1) is actually the expectation value of the system's energy, $\langle H\rangle$, if it could be in the state $|\psi\rangle$. While it may sound remarkable that we can find an upper bound on the ground state energy using whatever state we wish, the proof is actually surprisingly simple: The actual energy eigenstates of the Hamiltonian constitute a complete set, spanning the Hilbert space in which the system can be said to live. If we, for example, have N such eigenstates, any possible state $|\psi\rangle$ can be expressed in terms of these, or in other words

$$|\psi\rangle = \sum_{i=0}^{N} c_i|E_i\rangle, \tag{2}$$

where c_i is some appropriate constant, and $|E_i\rangle$ is an energy eigenstate with energy E_i. If the spectrum is non-degenerate, we can also say that E_0 corresponds to the ground state energy, E_1 to the first excited state, and so on. If we allow the Hamiltonian to act on (2), each state, by definition, simply gives its corresponding energy. To find the expectation value $\langle H\rangle = \langle\psi|\hat{H}|\psi\rangle$, we simply take the inner product with the state ψ:

$$\langle\psi|\hat{H}|\psi\rangle = \sum_{i'=0}^{N}\sum_{i=0}^{N} E_i c_{i'}^* c_i\langle E_{i'}|E_i\rangle = \sum_{i=0}^{N}|c_i|^2 E_i,$$

where we have used that the eigenstates are (or can be made to be) orthonormal. Finally, we note that the ground state energy is, by definition, the lowest possible energy of the system, so adding a weighted sum of all energies, must be greater than, or equal to the ground state energy, as we wanted to show. For a more thorough introduction to this subject, see for example [3].

2.2 Quantum Dots

Our system of quantum dots, will as mentioned contain two electrons in a harmonic oscillator potential. To simplify things somewhat, we only consider the time-independent case, in all three spatial dimensions. For a harmonic oscillator with frequency ω, the Hamiltonian of this system is

$$\hat{H} = \sum_{i=1}^{2}\left(-\frac{\hbar^2}{2m_e}\nabla_i^2 + \frac{1}{2}m_e\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_{ij}},$$

where $\hbar$ is the reduced Planck constant, m_e is the electron mass, ∇_i^2 the Laplace operator for particle i. The second sum is the contribution from the Coulomb potential, due to the electron-electron repulsion, with e being the elementary charge, and ε_0 the vacuum permittivity. $r_{ij} = |\mathbf{r}_1 - \mathbf{r}_2|$ is just the distance between particles 1 and 2, and the summation over $i < j$ indicates that we do not count a mutual interaction twice.

As a first approximation to solving this system, we can simply ignore the particle-particle interaction, meaning that we are looking for energy eigenfunctions ψ that satisfy

$$\left(\sum_{i=1}^{2} -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2\right)\psi = E\psi, \tag{3}$$

where E is some energy eigenvalue, and we have introduced atomic units $\hbar = c = e = m_e = 1$, with c being the speed of light. Without particle interaction, this problem admits separable solutions of the form $\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)$, where $\phi(\mathbf{r})$ is a single particle wave function given[2] by

$$\phi(\mathbf{r}) = Ah_{n_x}(x)h_{n_y}(y)h_{n_z}(z)e^{-\frac{\omega}{2}r^2}, \tag{4}$$

where h_n is a Hermite polynomial, while n_x, n_y and n_z can be all positive integers, including zero, and denote the energy level associated with the state ϕ, as the single particle energy (in atomic units) is given by

$$E = \omega\left(n_x + n_y + n_z + \frac{3}{2}\right).$$

As the total wave function is just the product of two single-particle wave functions, and there is no interaction between the two, the total energy is just the sum of the single-particle energies

$$E^{total} = E_1 + E_2 = \omega\left(n_{x,1} + n_{x,2} + n_{y,1} + n_{y,2} + n_{z,1} + n_{z,2} + 3\right), \tag{5}$$

where the added subscripts just indicate particles 1 and 2. However, as we are going to study only the ground state energy using the variational principle, we only really need to consider the case where $n_x = n_y = n_z = 0$ for both particles, and

$$E_{gs}^{total} = 3\omega.$$

The corresponding total ground state wave function is then, according to (4),

$$\psi_{gs}(\mathbf{r}_1, \mathbf{r}_2) = Ce^{-\frac{\omega}{2}(r_1^2 + r_2^2)}, \tag{6}$$

as the Hermite polynomial $h_0(x) = 1$. Note that C is a normalization constant. It is important to point out that this is only the *spatial* part of the wave function, and that the complete wave function would necessarily also have a spin component. Since we are considering a pair of electrons, that is a set of fermions, the Pauli exclusion principle tells us that the two electrons must occupy opposite spin states, as fermions cannot occupy the exact same quantum state, simultaneously. If they did, their wave functions would simply vanish, which means such a state is not only improbable, but impossible. More specifically, this is due to the fact that both our electrons are exactly identical, and indistinguishable. As we can see from (6), performing an interchange of particles, $\mathbf{r}_1 \leftrightarrow \mathbf{r}_2$ does not change the spatial part of the wave function, meaning it is symmetric under interchange. For fermions, their total wave functions *must* be antisymmetric under interchange, and so the spin part must be antisymmetric. As electrons are spin-$\frac{1}{2}$ particles, and the spin part of the wave function must be antisymmetric, we find that the total spin must be $\frac{1}{2} - \frac{1}{2} = 0$.

To recap (6) gives us the ground state wave function when we simply ignore any particle-particle interactions. While this might sound a bit simplistic, it does serve as a first approximation. If we allow for our harmonic oscillator potential to be quite weak, we could also use this as a test of our variational calculations, as the energy of the interacting system should tend toward the non-interacting case, when the separation between electrons is large. In other words, we should expect to find that also the interacting system should tend toward a ground state energy of 3ω, if our harmonic oscillator potential is weak and the separation between particles is large.

2.3 Trial Wave Functions & Local Energy

As mentioned previously, *any* normalized function can be the trial function used in (1), but as one might imagine, a trial function that is similar to the true ground state wave function, will also provide a more accurate upper bound on the ground state energy. Therefore, we want to select trial wave functions that we imagine behave similarly to the true ground state wave functions. In this investigation we will consider two trial functions,

$$\psi_{T1}(\mathbf{r}_1, \mathbf{r}_2) = Ce^{-\alpha\frac{\omega}{2}(r_1^2 + r_2^2)}, \tag{7}$$

as well as

$$\psi_{T2}(\mathbf{r}_1, \mathbf{r}_2) = Ce^{-\alpha\frac{\omega}{2}(r_1^2 + r_2^2)}e^{r_{12}/(2+2\beta r_{12}))}, \tag{8}$$

where α and β are both *variational parameters*; constants which we tune in order to determine the lowest possible trial energy (and closest upper bound on the ground state energy), given our choice of trial functions. r_{12} is simply the separation between electrons. It turns out that actually computing the expectation value of (1) can be extremely difficult, especially when the problem at hand is multidimensional. In our case, we are considering two particles, each in three spatial dimensions meaning that the inner product turns into a six-dimensional integral. Therefore, we are only going to consider the *local* energy for a trial function $\psi(\mathbf{r}_1, \mathbf{r}_2)$, defined as

$$E_L(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\psi_T(\mathbf{r}_1, \mathbf{r}_2)} \hat{H} \psi_T(\mathbf{r}_1, \mathbf{r}_2). \tag{9}$$

As we can see, the local energy, as the name suggests, depends on the position of both particles, and is not (necessarily) the energy eigenvalue of the system. However, if we investigate the expected value of E_L over all of space, we should find that its expected value, and the most likely energy of the system, is the lowest energy. If the trial wavefunction then resembles the true wavefunction, it should therefore tend towards the ground state energy. Said differently

$$\langle E_L \rangle = \int P(\mathbf{r}_1, \mathbf{r}_2) E_L(\mathbf{r}_1, \mathbf{r}_2) d^3\mathbf{r}_1 d^3\mathbf{r}_2, \tag{10}$$

where $P(\mathbf{r}_1, \mathbf{r}_2)$ is the probability of finding the particles at positions $\mathbf{r}_1$ and $\mathbf{r}_2$, which is given according to the Born rule as $|\psi(\mathbf{r}_1, \mathbf{r}_2)|^2$. This is, as one might figure, also a costly computation which we can, to some degree, avoid by means of a Monte Carlo simulation. By virtue of the law of large numbers, we know that if we sample the local energy a sufficient number of times, the average of the local energy will tend towards the expected value, which is an excellent starting point for a Monte Carlo (MC) simulation. Before we proceed with developing a Monte Carlo strategy, we can investigate our trial wave a bit further, to ensure that our choice of trial functions is a realistic one. As a simple check, we can see if our wave functions fulfill the so-called cusp condition for two electrons, which states[4] that

$$\mathcal{R} \propto e^{r_{12}/2}, \tag{11}$$

where $\mathcal{R}$ is the radial part of the wave function. Note that the above is only true when the spins of the electrons are anti-parallel, and in the limit where the electrons are very close, that is $r_{12} \to 0$. As our wave functions are purely radial, we can simply check whether the entire trial wave function ψ_T fulfills (11). We can immediately see that this is untrue for ψ_{T1}, as there is no explicit dependence on the particle separation. For ψ_{T2}, on the other hand, the second exponential factor carries an r_{12} dependence, and in the limit where $2 \gg 2\beta r_{12}$, this factor *is* proportional to $\exp(r_{12}/2)$. For very small r_{12}, we have that $r_1 \approx r_2$, and a small change in the position of both particles can cause them to be much closer, and so the leading dependency of ψ_{T2} is $\exp(r_{12}/2)$, and ψ_{T2} does satisfy the cusp condition.

In order to perform Monte Carlo (MC) simulations, we will need exact expressions for the local energy of each trial wave function. In Appendix: Local Energies, the local energy is derived for both ψ_{T1} and ψ_{T2}, according to (9), using the Hamiltonian in (3). For ψ_{T1}, we find that the local energy is

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

while for ψ_{T2} we end up with

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

2.4 Monte Carlo Simulation

We are going to consider a Monte Carlo simulation scheme in which we imagine the electrons to be two independent, random walkers. As random walkers, there should be no preference to move in any particular direction, and moving in any direction should be equiprobable. We do, however, need to set a maximum step size, Δr, which is taken to be the same in all directions. If we denote the collective positions of both particles, $(\mathbf{r}_1, \mathbf{r}_2)$ as just $\mathbf{R}$, we propose a new position $\mathbf{R}'$ according to

$$\mathbf{R}' = \mathbf{R} + (2\mathbf{u} - 1)\Delta r, \tag{13}$$

where Δr is the maximum length of the proposed step, and $\mathbf{u}$ a vector of random numbers between 0 and 1 drawn from the uniform distribution, with one component for each spatial coordinate. By moving $(2u-1)\Delta r$ in a given direction, all possible displacements are contained in the interval $[-\Delta r, \Delta r]$, as we desired.

To ensure that the random walkers move towards the most probable state, we will impose a sampling rule, based on the Metropolis algorithm, which is often used to simulate the Ising model from statistical physics. For our purposes, however, we are mainly interested in its clever central premise, namely that the transition probability is modelled as being proportional to the *ratio* of the probabilities of being in either state. If we denote the probability of being in a position state $\mathbf{R}$ as $P(\mathbf{R})$, then the transition probability is taken to be

$$w = \frac{P(\mathbf{R}')}{P(\mathbf{R})}. \tag{14}$$

We know from the Born rule of quantum mechanics that these probabilities (or more stringently, probability densities) are in fact just the squared magnitude of the particle wave function, i.e. $|\psi(\mathbf{r}_1, \mathbf{r}_2)|^2$. One very handy consequence of using the ratio of probabilites, rather than the probabilities themselves, is that the normalization factor C of the wave function is cancelled. Calculating C can be computationally expensive, or even unfeasible, which makes this fact a great advantage of the Metropolis algorithm. To find w we can then simply insert for our choice of trial wave function, and for $\psi_{T1}(\mathbf{R})$, we get

$$w_{T1} = \exp(-\alpha\omega(r_1'^2 + r_2'^2 - r_1^2 - r_2^2)).$$

In order to reject or accept the proposed move, we compare w to a random number between 0 and 1 drawn from a uniform distribution, and if $w > s$ we accept the proposed move, otherwise it is rejected. The reasoning behind this is quite simple, in that we by doing this automatically accept moves to more probable position states ($w > 1$), but we also allow for moves to *less* probable states. By doing so, we can prevent our simulation from getting stuck in local regions in position space which are highly probable, but might not actually give the global energy minimum. Another way of phrasing this, is to say that we wish that our system of random walkers can reach every possible position state, given a sufficiently long simulation. To be precise, we wish for our system to have the property of ergodicity. For a more detailed discussion of ergodicity, the Metropolis algorithm, and Markov chains, of which our simulation is actually an example of, see for example [5].

All that remains is to select a suitable maximum step size Δr. Since we are using a brute force approach, we want the acceptance rate to be approximately 50 %. Since the acceptance or rejection of a move is based on comparison with a uniformly distributed random number, one simple way of achieving a 50 % acceptance rate, is by simply looking for a step size Δr such that w, on average, is approximately 1/2. More strictly, we want a step size Δr, such that w is evenly distributed around 1/2, such that the acceptance rate must be close to 50 %. To find such a step, we can begin by inserting for the proposed moves in w:

$$w = \exp\left(\sum_{i=1}^{2}\sum_{j=1}^{3} -\alpha\omega(2x_{i,j}\cdot\Delta r(2u_{i,j}-1) + \Delta r^2(2u_{i,j}-1)^2)\right) = \exp(\gamma), \tag{15}$$

where i denotes the particle in question, while j signals the spatial coordinate, so that $x_{1,2}$ is the y-coordinate of the first particle, and so on. In order to find some useful value of Δr, we will perform the following trick: we will only consider the *average* behaviour of all involved terms. As stated previously, we want w to be evenly distributed around 1/2, or in other words

$$\bar{w} = \frac{1}{2} \rightarrow \bar{\gamma} = -\ln 2.$$

Which is not an attempt at a stringent definition, we simply seek values of Δr which center γ, on average, at $-\ln 2$ and therefore w at 1/2. Fortunately, (15) allows for such a value, as the random numbers $u_{i,j}$ and the particle coordinates should be uncorrelated, and both zero-centered, meaning that the average value of the cross term is zero. As for the Δr^2 term, the average value of Δr^2 is of course Δr^2, while $(2u_{i,j}-1)^2$ is a random number between 0 and 1. As $u_{i,j}$ is drawn from the uniform distribution, it is easily shown that the average, or indeed expected value of this factor is 1/3. Evaluating all these quantities at their central values and carrying out the sum, we find

$$\Delta r^2 \frac{6}{3} = \frac{\ln 2}{\alpha\omega},$$

or that

$$\Delta r = \sqrt{\frac{\ln 2}{2\alpha\omega}}, \tag{16}$$

where we have chosen the positive square root. Optimally, this step size would give decent results for all values of α, and also the harmonic oscillator frequency ω, but that might be hopeful for such a simple procedure.

For the second wave function, we can compute the transition probability w_{T2} in a similar manner as before, and find that

$$w_{T2} = w_{T1} \exp\left(\frac{r'_{12}}{1+\beta r'_{12}} - \frac{r_{12}}{1+\beta r_{12}}\right), \tag{17}$$

where r'_{12} is the particle separation at the proposed positions. The above follows quite simply from the Born rule, and the fact that ψ_{T1} and ψ_{T2} are identical, aside from the added r_{12}-dependent exponential factor, often dubbed the Jastrow factor.

3 Method

In order to determine the lowest ground state energy for each trial wave function, the Monte Carlo simulation procedure outlined in the previous section was implemented in c++, for a 2-electron system of quantum dots. In order to produce a sufficient amount of pseudo-random numbers, the MT19937 Mersenne Twister random number generator (RNG) from the c++ standard library was used. For all simulations, the positions of both electrons were initialized randomly using the MT19937 RNG, inside a unit sphere centered about the origin.

As before, all calculations were performed using atomic units. At each simulation step, a move in the position of both electrons was proposed, and the updated step given by (13). At each simulation step, the proposed step length was determined by drawing six random uniform numbers between 0 and 1 using the MT19937 RNG, one for each spatial direction, for each electron. For both trial wave functions, the proposed move was either rejected or accepted, by calculating w, i.e. the ratio in (14) at each step and comparing the resulting value to a pseudo-random number s drawn from the uniform distribution. If $w > s$ the move was accepted, otherwise it was rejected. Upon acceptance, the position of both particles were updated, and their potential and kinetic energies were recorded. In effect the kinetic energy was just the contribution of the Lagrangian to the Hamiltonian, while the potential energy was computed as the harmonic oscillator potential. In order to investigate both non-interacting and interacting systems, the potential energy was recorded with and without any added Coulomb potential. In addition, the separation between particles, as well as squared energy was also logged. If a proposed move was rejected, all quantities were set equal to their value at the previous simulation step. At the end of a simulation, the average value of all recorded quantities was computed by taking the cumulative sum up to each simulation step, and dividing by the step number.

For the first trial wave function, ψ_{T1}, the maximum step size Δr was taken to be equal to that found in (16), for all values of ω and α. In order to determine an optimal variational parameter for ψ_{T1}, a grid search was performed for values of $\alpha \in [0.1, 5.0]$, for a total of 500 simulations, each consisting of 10^6 Monte Carlo cycles. Searches were performed for different harmonic oscillator frequencies, $\hbar\omega = 0.01, 0.50$ and 1.00, and the results logged with and without the electron-electron repulsion. Furthermore, the average local energy for a given α, $\langle E_{T1}(\alpha)\rangle$, was selected to be the final calculated value of the average energy. The optimal value of α was taken to be that which minimized the final average local trial energy.

For ψ_{T2}, all simulations were also performed with a step size as in (16), and the simulation procedure was generally the same. The transition probability was however computed using (17). In order to find a suitable upper bound on the ground state energy of the system using ψ_{T2}, a grid-search was performed for values of both α and β for a harmonic oscillator frequency of $\omega = 1.00$. For this search, a 200×200 grid of values of α and β was used, with both variational parameters in the interval $[0.1, 1.1]$ and a parameter step of 0.005. For each of the 40000 simulations, the number of Monte Carlo cycles (MC cycles) was $2 \cdot 10^6$. To speed up calculations, this grid search was parallelized using the OpenMPI Message Passing Interface library, with each process handling a unique α/β combination. Upon identifying the set of α and β-values that yielded the lowest ground state energy ($\alpha = 1.000, \beta = 0.270$), simulations were performed using these

values, and the resulting energy, particle separation, and energy variance was recorded and compared with results for ψ_{T1}.

Finally, the virial theorem was investigated, by computing the ratio $\langle T\rangle/\langle V\rangle$, i.e. the ratio of kinetic to potential energy of the system, for 200 evenly spaced harmonic oscillator frequencies between 0 and 1 with and without particle interaction. For the interacting case, ψ_{T2} was used, with the computed optimal values of α and β at $\omega = 1.00$, that is $\alpha = 1.000$ and $\beta = 0.270$. For the non-interacting case, the kinetic and potential energy of the first trial wave function was used, and the optimal, non-interacting value of $\alpha = 1.00$ found using the grid search was used. Note that for the non-interacting case, the potential energy did not include the Coulomb potential.

4 Results

Fig. 1 shows the computed average local energy $\langle E\rangle$ for both trial wave functions, as a function of the number of MC cycles n, for $\omega = 0.01, 0.5$ and 1.00. For ψ_{T1}, the Coulomb potential was included, and the variational parameter $\alpha = 0.88$. For ψ_{T2}, the variational parameters were set to $\alpha = 1.000$ and $\beta = 0.270$, in keeping with the previous result. As we can tell, both wave function settle into an equilibrium quickly for a weak harmonic oscillator potential, requiring less than 1000 MC cycles for $\omega = 0.01$. For $\omega = 0.5$, however, we can clearly tell that ψ_{T2} settles more readily into an equilibrium state than ψ_{T1}, with the first taking approximately 1000 MC cycles to do so, while the latter required 2000-3000 MC cycles to do the same. This trend appears to hold true for $\omega = 1.00$, and we can tell that a stronger oscillator potential requires a longer equilibration time, especially for ψ_{T1}.

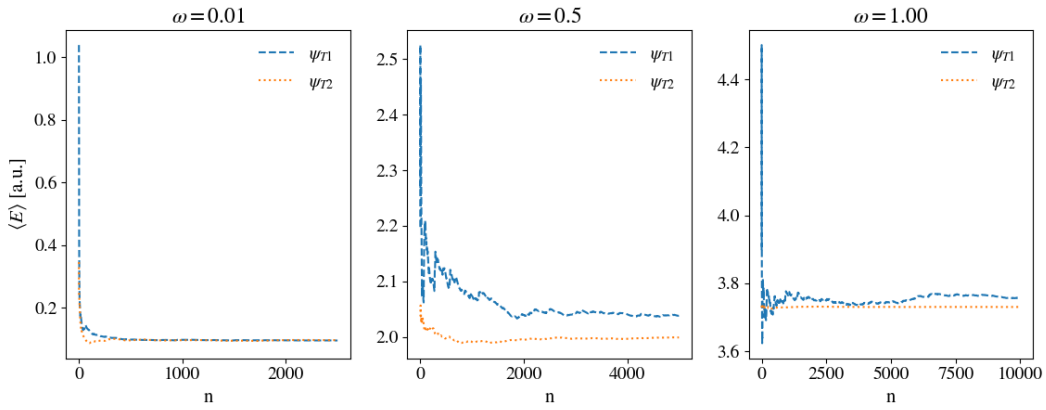

Figure 1: The final local average energy of both trial wave functions, simulated for harmonic oscillator frequencies $\omega = 0.01, 0.5$ and 1.00, shown as functions of the number of Monte Carlo cycles. For the first trial wave function ψ_{T1}, the variational parameter was set to $\alpha = 0.88$, while for ψ_{T2} the variational parameters used where $\alpha = 1.00$ and $\beta = 0.270$.

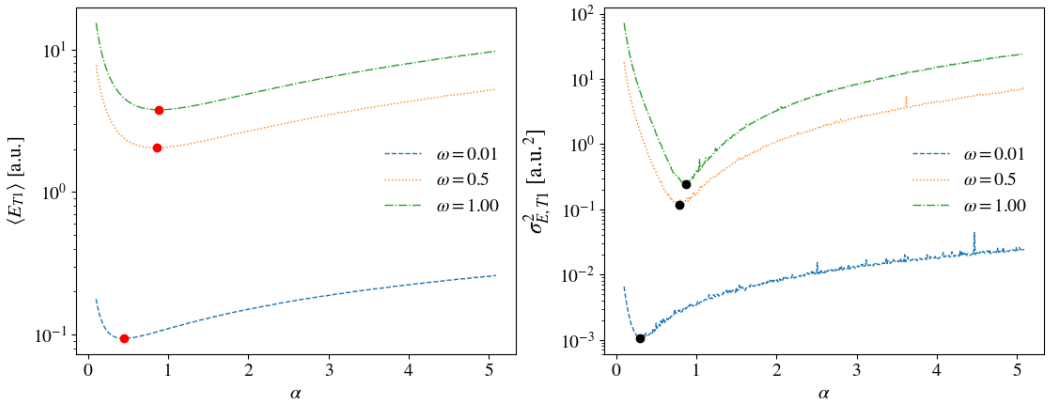

Figure 2: Grid search of the variational parameter α for the first trial wave function ψ_{T1}, with the Coulomb potential included. Shown on the left hand side is the final value of the local average energy, computed using 10^6 Monte Carlo cycles, for different harmonic oscillator frequencies ω. The right hand side shows the computed variance in energy for the same grid search. For all quantities, the measured minimum value is indicated by a marker. For each frequency, simulations were performed for a total of 500 different values of α.

Fig. 2 shows the result of the grid search for the variational parameter α, for the first trial wave function, with the Coulomb interaction included, and both the average final local energy, as well as energy variance for different harmonic oscillator frequencies, ω is indicated. Initially, we can tell that the average energy is lower for a weak harmonic oscillator potential, at approximately $\langle E \rangle = 0.1$ a.u. for $\omega = 0.01$, versus 3.77 a.u. for $\omega = 1.00$. We can also tell that energy variance follows the same trend, with lower variance for a lower energy. Importantly, we find that the measured optimal value of α at the energy minimum $\langle E \rangle = 3.77$ a.u. is $\alpha = 0.88$ in the interacting case, for $\omega = 1.0$. We can also tell that this value of α appears to be almost the same for $\omega = 0.5$, but lower, at approximately 0.45, for $\omega = 0.01$. We see a similar effect for the energy variance σ^2_E, but we can see that the shifting of the optimal parameter is slightly more pronounced. In addition, the energy variance minima and energy minima do not quite coincide in terms of α. The minimum variance is found at $\alpha = 0.87, 0.76$ and 0.28, for $\omega = 0.01, 0.5$ and 1.0, respectively, while the comparable energy minima are found at $\alpha = 0.88, 0.83$, and 0.43.

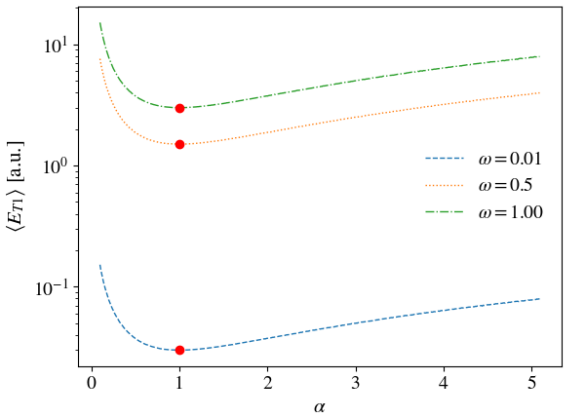

Figure 3: Grid search of the variational parameter α for the first trial wave function ψ_{T1} in the non-interacting case, for different values of the harmonic oscillator frequency ω. Shown is the final value of the local average energy, computed using 10^6 Monte Carlo cycles. For each frequency, the measured minimum in energy is indicated by a marker, corresponding to the optimal value of α.

Fig. 3 shows the result of the grid search for the parameter α, in terms of the final average energy for the first trial wave function, in the non-interacting case. As with the interacting case, we can tell that lower harmonic oscillator frequencies, and weaker potentials, lead to a lower average local energy. However, unlike before, it appears that the optimal value of ω is centered much closer to unity for all the investigated values of ω, suggesting we set $\alpha = 1.00$ in the non-interacting case. For $\omega = 1.00$, the minimum average energy is 3.0, which matches the exact result found in the theory section.

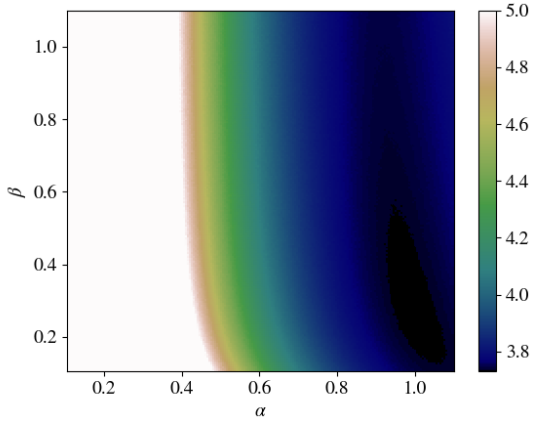

Figure 4: 2D grid search of the variational parameters α and β for the second trial wave function ψ_{T2}. The actual grid consisted of 200×200 combinations of α and β, both contained in the interval $[0.1, 1.1]$. The actual color value of the map corresponds the to the final average local energy of a given combination of α and β, each simulated using $2 \cdot 10^6$ Monte Carlo cycles. Note that color values are capped at 5.0 to better increase contrast in low-energy regions, and that the white-saturated region necessarily only carries $\langle E \rangle > 5.0$ a.u..

Fig. 4 shows the result of the grid search for the variational parameters α and β for the second trial wave function, in terms of the final average local energy, which is coded in the colour value. As we can tell from the colour map, the energy grows exceedingly large for low values of α, irrespective of β, while for $\alpha \approx 0.9 - 1.0$, we can observe an energy valley for all values of β. However, closer inspection reveals that

the minimum average energy, $\langle E \rangle = 3.73$ is found for $\alpha = 1.00$ and $\beta = 0.270$, suggesting we set these as the optimal variational parameters, at least for ψ_{T2} at $\omega = 1.0$.

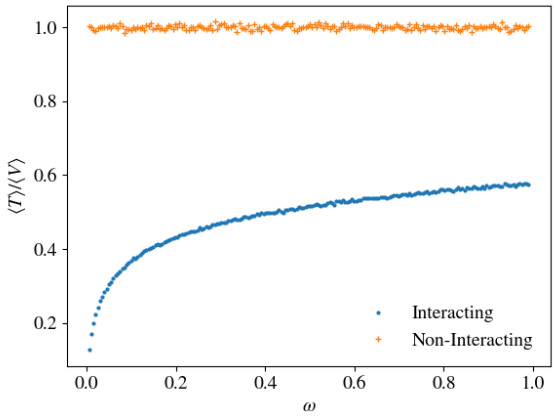

Figure 5: Computed ratio of the final average local kinetic to potential energy, $\langle T \rangle / \langle V \rangle$ in the non-interacting and interacting case, for 200 different values of the harmonic oscillator frequency ω. For the non-interacting case, the first trial wave function was used, and the Coulomb potential was ignored while the variational parameter was set to $\alpha = 1.00$ for each simulation. For the interacting case, the second wave function, ψ_{T2} was used, and the variational parameters were set to $\alpha = 1.00$ and $\beta = 0.270$ for all simulations. Note that in all cases, the simulation length was 10^6 Monte Carlo cycles.

Fig. 5 shows the computed ratio of the final average local kinetic and potential energy of the quantum dot system, in the interacting as well as non-interacting cases for different frequencies of the harmonic oscillator potential. The non-interacting case was taken to be that of the first trial wave function, with the optimal, non-interacting variational parameter $\alpha = 1.00$. The interacting case was that of ψ_{T2}, with variational parameters $\alpha = 1.00$ and $\beta = 0.270$. We can immediately deduce that the non-interacting case adheres to the virial theorem, as the computed ratio is ≈ 1 for all ω, and hence $\langle T \rangle \approx \langle V \rangle$, as we would expect [2]. The interacting case is however more interesting, as the ratio is not fixed, but rather appears to shift from near-zero at $\omega = 0.01$, to $\langle T \rangle / \langle V \rangle \approx 0.6$ near $\omega = 1.0$.

Table 1: Results of the variational Monte Carlo simulation of the 3D, two-electron quantum dot system. Inset is the final average particle separation r_{12}, average energy $\langle E \rangle$, and energy variance σ_E^2, for simulations of length 10^6 MC cycles. For each quantity, results are indicated for both trial wave functions, ψ_{T1} and ψ_{T2}. For ψ_{T1}, the variational parameter α was set to 0.88, and the Coulomb interaction included. For the second trial wave function, the variational parameters were $\alpha = 1.00$ and $\beta = 0.270$, and the Coulomb potential was included.

	r_{12}		$\langle E \rangle$ [a.u.]		σ_E^2 [a.u.^{2}]	
ω	ψ_{T1}	ψ_{T2}	ψ_{T1}	ψ_{T2}	ψ_{T1}	ψ_{T2}
0.01	23.75	17.66	0.094	0.098	0.0014	0.0010
0.50	2.43	2.60	2.04	2.00	0.13	0.002
1.00	1.70	1.82	3.77	3.7302	0.28	0.0003

Table 1 shows the results of the variational MC simulation of the quantum dot system, using both trial wave functions, using their respective optimal parameters ($\psi_{T1} : \alpha = 0.88, \psi_{T2} : \alpha = 1.00, \beta = 0.270$), in the interacting case. We can note particularly that the average particle separation r_{12} is actually greater for ψ_{T1} for $\omega = 0.01$, but for $\omega = 0.5$ and $\omega = 1.00$, ψ_{T2} carries the greater particle separation. As for the energy, we see that the first trial wave function has a slightly lower minimum energy for $\omega = 0.01$, but this role is also reversed for $\omega = 0.5$ and $\omega = 1.0$. Interestingly, the energy variance is always lower for ψ_{T2}, and almost

three order of magnitude smaller at $\omega = 1.00$, even though the difference in energy between the two trial functions is relatively small, at 0.04a.u.. As for the energies themselves, both ψ_{T1} and ψ_{T2} come close to the actual ground state energy, which is 3.558 a.u. [2] for $\omega = 1.0$, but as we can tell, ψ_{T2} gives us the lowest upper bound on this energy. These findings are also in agreement with findings made in [6], in which the ground state energy was calculated using an eigenvalue solver method, and the resulting energy eigenvalue for $\omega = 1.00$ was found to be approximately 3.5 a.u.. For $\omega = 0.5$, the reported ground state energy was 1.87 a.u., indicating that our current results are slightly higher than those found in [6].

5 Discussion

As we can tell from Fig. 1, the developed MC algorithm appears to converge to an equilibrium state for all investigated values of ω, but convergence appears slower for ψ_{T1} than ψ_{T2} in all cases, but for $\omega = 0.01$, the difference is hardly noticable. It should be pointed out that the current method of determining equilibrium is quite unsatisfactory, as it relies on simple visual inspection. On this note, it could be worth mentioning that the $\omega = 1.00$ case for ψ_{T1} can be argued to appears somewhat unstable, even after the 5000 MC cycle mark. On the other hand, this might possibly be expected, as the Couloumb repulsion becomes much more apparent at greater harmonic oscillator frequencies, as the particles on average should be brought close together. This implies that a wave function which takes particle separation into account (ψ_{T2} in our case) should perform better. Stated simply, the Jastrow factor in ψ_{T2} goes to zero around $r_{12} = 0$, and so the wave function, and the probability of finding the particles close, is smaller, as we would expect. Regardless, a more rigorous future investigation would require for example time auto-correlation analysis, in which time is represented by the number of MC cycles. However, for the purposes of simply checking stability, visual inspection is more or less adequate.

While not reported as an explicit result, it was found that the acceptance rate for *all* investigated wave functions, values of ω, α and β were approximately in the region of $(0.56, 0.59)$ using only the expression in (16) for the maximum proposed step. While this is slightly above the desired acceptance rate of 0.5, it is interesting that such a simple procedure produces such a stable acceptance ratio for both wave functions. For ψ_{T1} this is almost to be expected, as (16) was derived with this function in mind. For ψ_{T2}, the reason this step size works, could be that the Jastrow factor follows a distribution that is either distributed in a fashion similar to ψ_{T1}, or that its contribution to the exponential is, on average, rather small. It was however found that the acceptance ratio was slightly higher for ψ_{T2} than ψ_{T1} (the first often being close to $0.58 - 59$ while the latter remained stable near 0.56). This observation was confirmed for both wave functions for various oscillator frequencies between 0 and 1, but only for the optimal set of parameters for each wave function, and a rigorous analysis of this step size and the acceptance rate could be an interesting case for future studies, as it provides a computationally efficient way of determining a step size for a brute force Monte Carlo simulation.

As for the minimal energies in Fig. 2 and 3, it is interesting to see that the non-interacting case appears more consistent in terms of the variational parameter $\alpha \approx 1.00$. The fact that the non-interacting case for $\omega = 1.0$ determined the ground state energy to be 3.0 a.u., matching the exact result, is an important verification of our implementation and model. The same can also be said for the interacting case, which at $\langle E \rangle = 3.77$ a.u. is quite close to the actual ground state energy 3.558 a.u., albeit slightly higher, which we would expect when using variational wave functions, as the can only give us an upper bound on the ground state energy. It could however have been useful to perform an interpolation of the average energy/α curve, and possibly determine an even better value of α. As for the variance in energy, we can see that it follows the behaviour of the average energy, as we would expect, but that it is not exactly minimized at the same value of α as the average energy. The reason for this is not fully understood, but is likely due to the fact that we are not dealing with the actual wave function of the system, but rather a variational one. Regarding the stability of these simulations, it would appear from the crude analysis performed for Fig. 1, that the 10^6 MC cycles used for these simulations is more than sufficient.

The 2D grid search shown in Fig. 4 tells us quite clearly that the energy is minimized for ψ_{T2} in only a small region of parameter space, in the region of $\alpha \approx 1.00$ or slightly less. However, this search was only performed for $\omega = 1.00$, and it would be interesting to do new grid searches for different harmonic oscillator frequencies also, similar to the search performed for ψ_{T1}. However, the $\omega = 1.00$ case could be compared to

other findings, making it an attractive case for which to find the minimum average local energy. It should also be worth mentioning that the search could be expanded in terms of α and β values, as there is no guarantee that $(\alpha = 1.00, \beta = 0.270)$ is a global minima. As with ψ_{T1}. it could also have been useful to perform interpolation of the results. Finally, it would be very interesting to replace the systematic grid search method, with a machine learning method, as one could conceivably train a neural network to minimize the trial energy, and thus finding values of α and β in what might be a more robust manner.

As for the results in Fig. 5, it is interesting to note that the non-interacting case very clearly follows the virial theorem, while the interacting case does not. However, for larger values of ω, the ratio $\langle T \rangle / \langle V \rangle$ appears to be almost linear, at around 0.6, and so it would be interesting to compute this ratio for even larger values of ω. It does however seem that the non-interacting case should be fundamentally different from the interacting one: Even though the virial theorem holds, and the kinetic/potential energy ratio is 1 for a pure harmonic oscillator [2], increasing the oscillator frequency would only serve to bring the electrons closer, increasing the Coulomb potential contribution, and would not necessarily move the system closer to being a pure harmonic oscillator.

For the results in Table 1, our most important observations might be that the system more or less behaves as we might expect: for large ω, the Jastrow factor becomes dominant, and ψ_{T2} carries the largest particle separation, but also the lowest trial energy, signifying that it most closely resembles the actual wave function. This is also confirmed by comparison with other findings. It is also interesting that the energy variance of ψ_{T2} is much lower at greater ω, indicating that the simulation not only provides a lower ground state energy approximation, but is also more stable, at higher ω. It would therefore appear that for a strong harmonic oscillator potential, ψ_{T2} is a better choice of variational wave function. On the other hand, it is more difficult to determine optimal, simultaneous values of α and β, and ψ_{T2} is also slightly more intricate than ψ_{T1}, and so ψ_{T1} might still serve as a simple, first approximation to investigating such a system.

Another point to be made is that it appears that the unit sphere position initialization appears to be somewhat close to the actual behaviour of the electrons in terms of position, as we can also tell from Table 1, at least for greater values of ω. For $\omega = 1.00$, for example, the particles are an average distance $r_{12} = 1.82$ apart in the case of ψ_{T2}. Assuming the particles are evenly distributed around the origin, this would imply that the particles are initialized very close to their most probable positions. However, it appears that a greater starting initialization radius in position could be more suitable for low values of ω, as $r_{12} = 17.66$ at $\omega = 0.01$.

6 Conclusion

In this investigation, we have used the variational principle, in conjunction with Monte Carlo simulation and the Metropolis algorithm, in order to study the ground state energy, as well as particle separation of a three-dimensional system of two electrons in a harmonic oscillator potential. By using two different trial wave functions, ψ_{T1} and ψ_{T2}, this system was studied with and without particle-particle interactions. For both wave functions, grid searches were performed to determine optimal values of the variational parameters α and β. For the first trial wave function, which did not take into account particle interactions, the optimal variational parameter α was found to be 0.88. For the second wave function, which did take particle interactions into account through the addition of a so-called Jastrow factor, the determined optimal variational parameters were $\alpha = 1.00$ and $\beta = 0.270$. As a proposed future development, one could possibly replace this grid searching method with a machine learning approach, in order to more efficiently search parameter space.

For the actual Metropolis algorithm implementation, a novel and simple expression for the maximum step size of an electron move was developed, in order to achieve an acceptance rate of approximately 50 % for the proposed moves of the Metropolis sampling. It was found that this maximum step size resulted in consistent acceptance rates of around 0.56-0.59 across a range of harmonic oscillator frequencies, for both trial wave functions. This was only investigated thoroughly for the optimal variational parameters listed above, and so a more rigorous analysis over a range of variational parameters would be an interesting case for future study.

Using these optimal parameters, the lowest average local energy of ψ_{T1} was found to be 3.77 a.u., while the corresponding energy for ψ_{T2} was 3.7302 a.u., both for a harmonic oscillator frequency of $\omega = 1.0$. These

results showed ample agreement with the corresponding exact value of 3.558 a.u., but results also agreed with a similar investigation performed by this author for a wider range of harmonic oscillator frequencies. While the results showed that all energies were slightly higher than other findings, this is to be expected for variational methods, and importantly, it was found ψ_{T2} provided the lowest upper bound on the ground state energy for larger values of ω, for which particle-particle interactions become significant. This was also reflected by the computed average particle separation r_{12}, which was typically slightly greater for ψ_{T2} than ψ_{T1} ($r_{12} = 1.70$ for ψ_{T1}, $r_{12} = 1.82$ for ψ_{T2} at $\omega = 1.0$). Taken together, these results indicate that ψ_{T2} provides a better estimate of the ground state wave function in the presence of a harmonic oscillator potential.

In addition, it was found that the quantum dot system obeys the virial theorem only in the non-interacing case, as the ratio of the average kinetic to potential energy was approximately 1 for all investigated values of ω, when the first trial wave function was used, and the Coulomb potential ignored. When particle-particle interaction was taken into account, this ratio increased with increasing ω, settling towards around $\langle T \rangle / \langle V \rangle \approx 0.6$ as ω approached unity, and it would be an interesting future development to investigate this ratio for greater values of ω, also.

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7 Appendix: Code

All code is freely available at: https://github.com/markusbp/fys3150/tree/master/project5

8 Appendix: Local Energies

Starting with the local energy expression

$$E_L(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\psi_T(\mathbf{r}_1, \mathbf{r}_2)} \hat{H} \psi_T(\mathbf{r}_1, \mathbf{r}_2), \tag{18}$$

which we can simplify, if we rewrite the Hamiltonian in terms of kinetic and potential energy contributions

$$\hat{H} = \left(\sum_{i=1}^{2} -\frac{1}{2} \nabla_i^2 \right) + \frac{1}{2} \omega^2 r_i^2 + \frac{1}{r_{12}} = \hat{T} + \hat{V},$$

where $\hat{T}$ contains the sum of Laplace operators, and $\hat{V}$ the remaining terms. The reasons we do this is simply that only $\hat{T}$ alters ψ_T, and therefore that

$$\begin{aligned} E_L &= \frac{1}{\psi_T(\mathbf{r}_1,\mathbf{r}_2)}\hat{T}\psi_T(\mathbf{r}_1,\mathbf{r}_2) + \hat{V}\frac{\psi_T(\mathbf{r}_1,\mathbf{r}_2)}{\psi_T(\mathbf{r}_1,\mathbf{r}_2)} \\ &= \frac{1}{\psi_T(\mathbf{r}_1,\mathbf{r}_2)}\hat{T}\psi_T(\mathbf{r}_1,\mathbf{r}_2) + \frac{1}{2}\omega^2(r_1^2+r_2^2) + \frac{1}{r_{12}}, \end{aligned}$$

and so our job is only to determine the action of $\hat{T}$ on the trial wavefunction ψ_T. We can begin by inserting the first trial wavefunction, ψ_{T1} from (7), and find that

$$E_{L1} = e^{\alpha\frac{\omega}{2}(r_1^2+r_2^2)}\left(\sum_{i=1}^{2} -\frac{1}{2}\nabla_i^2\right)e^{-\alpha\frac{\omega}{2}(r_1^2+r_2^2)} + \frac{1}{2}\omega^2(r_1^2+r_2^2) + \frac{1}{r_{12}},$$

which means that we are looking to determine the action of the Laplacian. In spherical coordinates, the action of the Laplacian on some function f can be written as

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin^2\phi}\frac{\partial^2 f}{\partial\theta^2} + \frac{1}{r^2\sin\phi}\frac{\partial}{\partial\phi}\left(\sin\phi\frac{\partial f}{\partial\phi}\right),$$

where $\theta \in [0, 2\pi]$ is the azimuthal angle, and $\phi \in [0, \pi]$ the polar angle. For the local energy E_{L1}, we see that we only need to evaluate an expression of the form

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}e^{-\alpha\frac{\omega}{2}r^2}\right),$$

as the first trial wavefunction only carries a radial dependence. The kinetic energy contribution is then, for each particle

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(-\alpha\omega r^3 e^{-\alpha\frac{\omega}{2}r^2}\right) = \left(r^2\alpha^2\omega^2 - 3\alpha\omega\right)e^{-\alpha\frac{\omega}{2}r^2}.$$

Inserting this result into (8) for each particle, we find after some rearranging, that

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

For the second wavefunction, we will try a more direct approach, using the cartesian Laplacian

$$\nabla_i^2 = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2},$$

but since ψ_{T2} is symmetric in all spatial dimensions, it should be sufficient to determine

$$\frac{\partial\psi_{T2}}{\partial x_1^2},$$

and then argue from symmetry how all terms should contribute. Inserting, we find

$$\frac{\partial^2\psi_{T2}}{\partial x_1^2} = C\frac{\partial^2}{\partial x_1^2}e^{-\alpha\frac{\omega}{2}(r_1^2+r_2^2)}e^{1/(2/r_{12}+\beta)},$$

but r_2 has no x_1 dependence, and by noting that the exponentials are unchanged under differentiation, we get

$$\begin{aligned} \frac{\partial^2\psi_{T2}}{\partial x_1^2} &= \frac{\partial}{\partial x_1}\left(\psi_{T2}\left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_1}\right)\right) \\ &= \psi_{T2}\left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_1}\right)^2 + \psi_{T2}\left(\frac{\partial^2 u_1}{\partial^2 x_1^2} + \frac{\partial^2 u_2}{\partial x_1^2}\right) \end{aligned}$$

where

$$u_1 = -\alpha\frac{\omega}{2}r_1^2 \quad \text{and} \quad u_2 = \frac{r_{12}}{2+2\beta r_{12}}.$$

Starting with u_1, we find

$$\frac{\partial u_1}{\partial x_1} = -\alpha\omega x_1,$$

and

$$\frac{\partial^2 u_1}{\partial x_1^2} = -\alpha\omega,$$

as $r_1 = x_1^2 + y_1^2 + z_1^2$. u_2 is more tricky, as it contains $r_{12} = \sqrt{(x_1-x_2)^2 + (y_1-y_2)^2 + (z_1-z_2)^2}$, but we proceed in the same way:

$$\frac{\partial u_2}{\partial x_1} = \frac{(x_1-x_2)/r_{12}}{2(1+\beta r_{12})^2},$$

which is found using the chain rule for derivatives, and in a similar manner we find

$$\begin{aligned}\frac{\partial^2 u_2}{\partial x_1^2} &= \left(\frac{1}{r_{12}} - \frac{(x_1-x_2)^2}{r_{12}^3}\right)\frac{1}{2(1+\beta r_{12})^2} - \frac{x_1-x_2}{r_{12}}\cdot\frac{\beta(x_1-x_2)}{r_{12}(1+\beta r_{12})^3} \\ &= \left(\frac{1}{r_{12}} - \frac{(x_1-x_2)^2}{r_{12}^3}\right)\frac{1}{2(1+\beta r_{12})^2} - \frac{\beta(x_1-x_2)^2}{r_{12}^2(1+\beta r_{12})^3}.\end{aligned}$$

The x_1-contribution to the Laplacian is then

$$\begin{aligned}\frac{\partial^2 \psi_{T2}}{\partial x_1^2} &= \psi_{T2}\left(\alpha^2\omega^2 x_1^2 - \frac{\alpha\omega x_1(x_1-x_2)/r_{12}}{(1+\beta r_{12})^2} + \frac{(x_1-x_2)^2}{4r_{12}^2(1+\beta r_{12})^4} - \alpha\omega\right) \\ &\quad + \psi_{T2}\frac{1}{2(1+\beta r_{12})^2}\left(\frac{1}{r_{12}} - \frac{(x_1-x_2)^2}{r_{12}^3} - \frac{2\beta(x_1-x_2)^2}{r_{12}^2(1+\beta r_{12})}\right).\end{aligned}$$

Performing the same exercise for the y_1 and z_1 dependencies will give the same results, only with interchanged spatial variables. Therefore, we should have that

$$\nabla_1^2\psi_{T2} = \psi_{T2}\left(\alpha^2\omega^2 r_1^2 - 3\alpha\omega + \frac{1}{2(1+\beta r_{12})^2}\left(\frac{2}{r_{12}} - \frac{2\beta}{1+\beta r_{12}} + \frac{1}{2(1+\beta r_{12})^2} - \alpha\omega\frac{2}{r_{12}}\kappa\right)\right)$$

where $\kappa = x_1^2 + y_1^2 + z_1^2 - (x_1x_2 + y_1y_2 + z_1z_1)$ contains the cross terms we cannot cancel just yet. To do so, we can include the action of the Laplacian on both particles, which in effect only affects the cross terms, and the single-particle coordinates:

$$(\nabla_1^2 + \nabla_2^2)\psi_{T2} = \psi_{T2}\left(\alpha^2\omega^2(r_1^2 + r_2^2) - 6\alpha\omega + \frac{2}{2(1+\beta r_{12})^2}\left(\frac{2}{r_{12}} - \frac{2\beta}{1+\beta r_{12}} + \frac{1}{2(1+\beta r_{12})^2} - \alpha\omega r_{12}\right)\right),$$

since $x_1^2 + y_1^2 + z_1^2 + x_2^2 + y_2^2 + z_2^2 - 2(x_1x_2 + y_1y_2 + z_1z_1) = r_{12}^2$. We are now finally ready to find the local energy for the second trial wavefunction, but before doing so, we first recognize the first contributions as being exactly equal to those found for the first trial wave function, and upon inserting in the local energy expression, we find

$$E_{L2} = E_{L1} + \frac{1}{2(1+\beta r_{12})^2}\left(\frac{2\beta}{1+\beta r_{12}} - \frac{2}{r_{12}} - \frac{1}{2(1+\beta r_{12})^2} + \alpha\omega r_{12}\right), \tag{19}$$