Project 5: Quantum Monte Carlo of Confined Electrons in a Quantum Dot

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In this project we have studied a Quantum dot in three dimensions, containing two electrons with a harmonic oscillator potential and a repulsive Coulomb interaction potential. The ground state energy of the system was approximated using the variational method to find an upper bound limit, and in order to numerically obtain the most accurate limit we implemented the Monte Carlo based Metropolis algorithm. Two trial wave functions was considered, both with the Jastrow factor, ψ_{T2}, and without, ψ_{T1}, and by running the Monte Carlo simulation for ψ_{T1} we estimated that the system reached equilibrium by 10^5 cycles. With ψ_{T1} for the Hamiltonian without perturbation, we arrived at the exact analytical ground state energy of $\langle E \rangle = 3.0$ a.u for the angular frequency $\omega = 1$, with zero variance and $\alpha = 1$. Furthermore, for the same trial function with the Coulomb potential added to the Hamiltonian, the resulting minimum value was 3.77 ± 0.5a.u for $\alpha = 0.85$. The analytical value by M.Taut[8] of 3.558a.u. was within the large confidence bound of obtained value, thus $\langle E \rangle = 3.77 \pm 0.5$a.u served its purpose of being an upper bound for this value. For ψ_{T2}, the average energy of the system was computed as function of the parameters α and β, resulting in a minimum value of $\langle E \rangle = 3.73$ a.u. with zero variance for $\omega = 1$. The deviation from the exact ground state energy was thus found to be 0.212 a.u. For other frequencies than $\omega = 1$, there are no analytical values of the mean energy. However, by comparing the energy with the ones calculated in Project 2[9], they differed with $\approx \pm 0.3$a.u. Additionally, the mean distance $\langle r_{12} \rangle$ between the electrons, for both the unperturbed Hamiltonian with ψ_{T1}, and for the perturbed Hamiltonian with both ψ_{T1} and ψ_{T2}, was found to decrease as ω increased, which was in total compliance with theory. For ψ_{T1} with the Hamiltonian without perturbation, a frequency $\omega = 1$ resulted in $\langle r_{12} \rangle = 1.60$, while for the Hamiltonian with perturbation it was $\langle r_{12} \rangle = 1.73$. Furthermore for ψ_{T2}, the distance increased even further to $\langle r_{12} \rangle = 1.81$. Moreover, testing with the virial theorem was a success, as the ratio $\langle T \rangle / \langle V \rangle \approx 1$ for the unperturbed Hamiltonian, except for some smaller fluctuations which most likely was due to numerical inaccuracies. This was once again a result in utter agreement with theory. For ψ_{T2} it was observed that the Coulomb interaction dominated the energies for lower frequencies, thus not complying with the virial theorem, but we expected that if tested for sufficiently high ωs, $\langle T \rangle / \langle V \rangle$ would in this case also approach 1 as the harmonic oscillator potential starts dominating.

I. INTRODUCTION

Quantum entanglement is the phenomenon where two particles are entangled in the sense that they are dependent on each others quantum mechanical properties, such as spin and polarization. Erwin Schrödinger stated in 1935 [1] "I would not call [entanglement] one but rather the characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought." It is therefore of great interest to study this phenomenon as it is a pillar part of the world of quantum mechanics.

In this project we will study a quantum dot, QD, consisting of two electrons in three dimensions. Quantum dot is a central topic in nanotechnology and has a multitude of potential applications, such as in solar cell engineering, light emitting diodes (LEDs) and most interestingly, in quantum computing. QDs are therefore of special interest to modern science. The electrons in a QD are affected by an harmonic oscillator potential, and their quantum states are entangled. The energy states of the Hamiltonian for such a system has analytic solutions to the Schrödinger equation. However, in actuality there is an additional potential, as the electrons are interacting with each other by a repulsive Coulomb potential. Taking the interaction into account, the total potential will also have an analytic solution of the ground state energy with one specific angular frequency.

Our goal is to approximate the ground state energies, both with and without the Coulomb interaction considered, by the so-called variational method. This method is one of the most used methods for obtaining analytically unattainable wave functions and energies in quantum systems. Briefly explained, one can determine any trial wavefunction for the system investigated in which the Schrödinger equation has exact solutions to, and the resulting expectation value for the energy will always be equal to or larger than the actual ground state energy for the system.

Additionally, we will test our numerically obtained results with the virial theorem. The virial theorem a widely used theorem in physics, and is applicable to e.g. thermodynamics, quantum mechanics and astrophysics. It linearly relates the average kinetic energy to the potential energy. This relation will only hold for the simple harmonic oscillator Hamiltonian, that is without the Coulomb interaction. However, we will test for both cases and investigate the Coulomb interaction's effect on the virial theorem. By comparing the mean kinetic and

potential energy without the interaction potential, one can test the accuracy of the numerically obtained energy expectation value of the harmonic oscillator Hamiltonian.

In order to arrive at an approximation of the ground state energies of the electrons, we will use the Monte Carlo based Metropolis algorithm. The algorithm performs numerical integration in a randomized matter, and converges towards equilibrium when the number of Monte Carlo cycles proceed towards infinity. It is a broadly used method as it can be used to obtain probability distributions of complex systems without direct sampling. In this project, the algorithm will be used to compute the expectation value of the QD system's local ground state energy, both with and without the Coulomb interaction taken into account. The state of equilibrium will be the state at which the local energy equals the ground state energy, thus, with sufficient number of sampling cycles we can expect this method to provide reliable estimations to the analytical value for the ground state energy of the quantum system.

II. THEORY

Variational method

The variational method involves approximating energy states of quantum mechanical systems. In order to approximate the ground state energy, one would need to choose a trial wave function of the ground state, $\psi_{\text{trial}}(r)$. Where $r = \sqrt{x^2 + y^2 + z^2}$, and x, y and z are the three dimensional Cartesian coordinates of the particle. The Hamiltonian is an operator representing the total energy of the system. The associated ground state trial energy of the trial state will we obtained using the known Hamiltonian, $\hat{H}$, of the system. The variational method states

$$\int_{-\infty}^{\infty} dr \, \psi_{\text{trial}}(r)^* \hat{H} \psi_{\text{trial}}(r) = \langle E_{\text{trial}} \rangle \geq \langle E_0 \rangle. \quad (1)$$

Where $\langle E_0 \rangle$ is the exact solution of the expectation value of energy in the ground state. ψ_{trial} is the 'guessed' trial wave function and $\langle E_{\text{trial}} \rangle$ its corresponding expectation value of energy. The inequality is deviated by D.J. Griffiths [2]. Choosing the best fit trial wave function is key in order to arrive at a good approximation. Since the trial energy is always lower than the exact energy, one can guess a myriad of different wave functions. Since all energy states of the trial functions are lower than the actual ground state, one can choose the state corresponding to the lowest trial energy with a guessed variational parameter. Thus, when receiving the corresponding energies to the trial function with different variational parameters, the most accurate ground state energy will be the lowest.

The harmonic oscillator potential

The Hamiltonian, $\hat{H}_0$, of N non-interacting electrons in a harmonic oscillator potential is,

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{K}_i + \hat{U}_i = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m_e} + \frac{1}{2}\omega^2 \hat{r}_i^2. \quad (2)$$

Where ω is the angular frequency of the harmonic oscillator, and m_e the electron mass. $\hat{K}$ is the kinetic energy operator, and $\hat{U}$ the potential energy operator. $\hat{p}_i$ is the momentum operator and $\hat{r}_i$ the position operator of the i-th electron. In the position basis one can simply rewrite the momentum and position operators as vectors.

In atomic units, $m_e = c = \hbar = e = 1$, the Hamiltonian reads,

$$\hat{H}_0 = \sum_{N=1}^{N} -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2. \quad (3)$$

Since we have introduced radial position, as we are investigating the harmonic oscillator in three dimensions, it proves to be beneficial to change the basis of the ∇ operator from Cartesian to spherical coordinates. The spherical squared ∇ operator in spherical coordinates reads,

$$\frac{1}{r^2}\frac{\partial^2}{\partial r^2}r^2 + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2 \sin\theta}\frac{\partial^2}{\partial\phi^2} \quad (4)$$

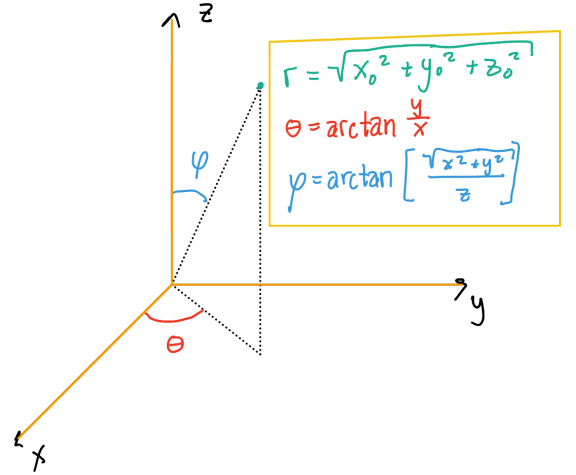Where the angles θ and ϕ is presented in figure 1.

Figure 1. The figure presents the connection between the spherical and Cartesian coordinates.

For two non-interacting electrons the corresponding radial wave function and energy states of the Hamiltonian have analytical solutions. The radial wave function is,

$$\psi_0(r_1, r_2) = Ce^{-\omega/2\cdot(r_1^2 + r_2^2)}. \quad (5)$$

Where C is a normalization constant, satisfying the condition $\int_{-\infty}^{\infty} |\psi_0(r_1, r_2)|^2 dr \equiv 1$. The exact wave function is deviated in reference [3] by D.J. Griffiths. Since the radial wave function is only dependent of r_1 and r_2, the angular factors of the derivation operator in 4 are zero.

The corresponding energy $\psi_0(r_1, r_2)$ in the ground state for one particle, also from reference [3] is,

$$E_0 = \frac{3}{2}\omega. \tag{6}$$

Since the two particles are identical, one can separate the wave function into two wave functions for the two electrons, as they evidently are identical. The resulting ground state energy deviated in Appendix B is,

$$E_{0,N=2} = \frac{3}{2}N\omega = 3\omega. \tag{7}$$

When introducing the angular dependent wave function $\Phi(\theta, \phi)$, the partial angular derivatives are the factors of the ∇ operator which act on the angular wave function. From source [4 - 3d] we can separate the radial and angular wave functions, so-called separation of variables, to the total wave function Ψ can be written as,

$$\Psi(r_1, r_2, \theta, \phi) = \psi(r_1, r_2)\phi(\theta, \phi). \tag{8}$$

In this report we will only focus on the radial wave function.

Spin

Spin is a fundamental part of quantum mechanics. All fermions, including electrons, have half integer spins, in either 'up' or 'down' direction. Electron have one-half spin. The notation of Pauli's exclusion principle states that two fermions cannot occupy the same state[page 204 griffiths]. Thus, electrons in the same same spacial state, must have anti-symmetric spin. Meaning one of the electron will have 'up'-spin, denoted $\uparrow$, and the other 'down', $\downarrow$. This is a very simplified explanation of the anti-symmetry of fermions. We will only simulate for two electrons in their ground state, such that the total spin of the system is 0.

Interacting electrons

In actual fact, the electrons are repulsively interacting with each other with a so-called Coulomb interaction. The interaction of the electrons is repulsive due to their equal charge. In order to arrive at the total Hamiltonian one would need to add a term to the unperturbed Hamiltonian, $\hat{H}_0$ in equation 2. The repulsive term of the Hamiltonian for two electrons, given by ref. [oppgavetekst], is

$$\hat{H}' = \sum_{i>j} \frac{1}{\sqrt{r_i - r_j}} = \sum_{i>j} \frac{1}{r_{ij}}. \tag{9}$$

Naturally, the perturbed Hamiltonian is in atomic units. It goes without saying that new Hamiltonian will result in a higher ground state energy the connecting energy of the unperturbed Hamiltonian.

Virial theorem

The virial theorem is broadly used in quantum mechanics. It relates the mean kinetic energy to the potential energy in a bound state consisting of N particles. The definition of bound states are states in which the particles are bound to a potential, meaning they cannot escape the potential, and are to a certain degree localized. Reference [5] states that if the potential energy satisfies $r\frac{\partial V}{\partial r} = nV$, the quantum state is bound. For an harmonic oscillator potential this relation is satisfied,

$$r\frac{\partial V}{\partial r} = \omega^2 r^2 = 2V. \tag{10}$$

Meaning that $n = 2$ for the harmonic oscillator potential.

The virial theorem states that the relation between the mean kinetic energy, $\langle T \rangle$, and mean potential energy, $\langle V \rangle$, is

$$\langle T \rangle = \frac{n}{2}\langle V \rangle. \tag{11}$$

This is also deviated in [5].

Hence, the virial theorem of a quantum harmonic oscillator is,

$$\langle T \rangle = \langle V \rangle. \tag{12}$$

III. ALGORITHM

The Metropolis algorithm

The local energy E_L is the total (kinetic and potential) mechanical energy of the two particle system, which is obtained using the time-independent Schrödinger equation 13. It reads;

$$E_L \psi_T(r_1, r_2) = \hat{H}\psi_T(r_1, r_2). \tag{13}$$

The different trial functions we wish to test for, ψ_T, will naturally have different local energies. These trial functions and their resulting expressions for the local energy are dependent on several variational parameters. In order to find the minimum for the expectation value of the system's energy, calculations of said expectation value must be carried out for numerous variations of

these parameters. Here, the Metropolis algorithm proves to be very beneficial.

The calculation of the expectation value of the energy $\langle E_L \rangle$, and its square $\langle E_L^2 \rangle$, is carried out by the following algorithm;

> Fix number of Monte Carlo cycles $MCCs$
> Set variational parameters α, β and ω
> Set positions r, $\psi_{T,\alpha,\beta,\omega}(r)$
> Set $\langle E_L \rangle, \langle E_L^2 \rangle = 0$
>
> **for** $n \in MCCs$ **do**
>   **for** particle $\in \{1, number\ of\ particles\}$ **do**
>
>   **for** dimension $\in \{1, total\ dimensions\}$ **do**
> R = random variable $\in \{0, 1\}$
> $r_{\text{trial}} = r + (R - 0.5) \cdot$step
>   **end for**
>
>   **if** $R < P(r_{trial})/P(r)$ **then**
> $r = r_{trial}$
> $\psi_{T,\alpha,\beta,\omega}(r) = \psi_{T,\alpha,\beta,\omega}(r_{trial})$
>   **end if**
>
>   **end for**
>   calculate ΔE_L as function of α, β, ω
> $\Sigma E_L = \Sigma E_L + \Delta E_L$
> $\Sigma E_L^2 = \Sigma E_L^2 + \Delta E_L^2$
> **end for**
> $\langle E_L \rangle = \Sigma E_L / MCCs$
> $\langle E_L^2 \rangle = \Sigma E_L^2 / MCCs$

Here, the fraction $P(r_{\text{trial}})/P(r)$ is the relative probability of the attempted change in the electrons positions to occur.

Random number generator

In our program we will use the Mersenne Twister random number generator, which has a period of 2^{19937}-1. This implies that this generator provides seemingly fully random numbers for programs with a lower period than than 2^{19937}-1. The maximum amount of random numbers this projects requires that we generate in one go is $4 \cdot 10^{11}$. Since the Mersenne RNG period is that much larger, it will be more than sufficient for this purpose.

Parallel computing

In order to speed up some of the more time consuming computations performed in this project we utilize parallelization of our code. For this, the library OpenMP is used, which enable all threads to share memory and data. The section of the code that is to be executed in parallel is marked by a special directive # *pragma omp parallel.*

Reference [6] states that when the calculations are performed, each thread will execute its assigned section of the code independently.

IV. METHOD

The variational method of the unperturbed Hamiltonian

We start by using the metropolis algorithm in order to compute the ground state energy of the unperturbed Hamiltonian in equation 2. This will serve as a benchmark for the algorithm, as the analytical solution is known. The trial wave function we will use is,

$$\psi_{T1}(r_1, r_2) = Ce^{-\alpha\omega/2 \cdot (r_1^2 + r_2^2)}. \tag{14}$$

Where α is the variational parameter. We will loop over many different αs, and the best fit parameter is the one who results the smallest energy. With $\alpha = 1$ the analytical wave function in equation 5 is equal to the trial function. With the variational parameter, we assume the trial wave function is suitable in order to arrive at the analytical solution numerically.

The corresponding energy of the trial wave function is deviated in Appendix A and reads,

$$E_{T1} = \frac{1}{2}\omega^2(r_1^2 + r_2^2)(1 - \alpha^2) + 3\alpha\omega. \tag{15}$$

It is apparent that for $\alpha = 1$, the energy and wave function satisfies the analytical ones. Equation 15 is derived in Appendix A.

Setting $\omega = 1$ the exact energy of the unperturbed Hamiltonian is 3a.u. This value will be tested against the ones obtained by the Metropolis algorithm.

Variational method of the perturbed Hamiltonian

In order to approximate the ground state energy of the harmonic oscillator with the repulsive Coulomb interaction, we will use two trial wave functions. The first being equal to equation 14, with a new term to the corresponding energy in equation 15,

$$E'_{T1} = \frac{1}{r_{12}}. \tag{16}$$

The added term is also derived in Appendix A. E'_{T1} does not have a variational parameter connected to the repulsive term of the energy, such that it would not be possible to minimize the total energy with respect to the Coulomb interaction term. One can therefore argue that equation 14 is not sufficient in order to arrive at a good approximation of the ground state energy with the perturbed term to the Hamiltonian. Thus, we will use another trial

function in order to arrive at a ground state energy of higher quality. The new trial wave function, given by reference [oppg.tekst], is

$$\psi_{T2}(r_1, r_2) = Ce^{-\alpha\omega/2\cdot(r_1^2+r_2^2)} \cdot e^{\frac{r_{12}}{2(1+\beta r_{12})}}. \qquad (17)$$

Where β, in addition to α, is a variational parameter. The factor added to the other trial function in equation 17 is called the Jastrow factor. We assume that the factor will result in a better approximation of the ground state energy. The factor weights the probability distribution, $|\psi_{T1}(r_1, r_2)|^2$, and is in favor of larger distances between the electrons, which is intuitive as the Coulomb interaction potential is lower for larger distances. When $r_{12} \to \infty$ the Jastrow factor converges to $e^{\frac{1}{2\beta}}$, whereas the the first factor approaches 1.

For the second trial wave function's corresponding energy, stated by M.J. Jensen in reference [7], is

$$E_{T2} = E_{T1} + E_{T1}' + \frac{1}{2(1+\beta r_{12})^2} \times \qquad (18)$$

$$\left(\alpha\omega r_{12} - \frac{1}{2(1+\beta r_{12})^2} - \frac{2}{r_{12}} - \frac{2\beta}{1+\beta r_{12}}\right) = \qquad (19)$$

$$E_{T1} + E_{T1}' + E_{T2}'. \qquad (20)$$

Here the unperturbed ground state energy has an added term which is dependent on the two variational parameters. Hence, we can minimize the perturbed term with respect to α and β. The two singularities in E_{T2} when $r_{12} \to 0$ cancel each other. This due to $\frac{1}{2(1+\beta r_{12})} \to \frac{1}{2\beta}$ such that $\frac{1}{r_{12}}$ and $\frac{2}{r_{12}}$ cancel each other out, and we are left with only the harmonic oscillator energy.

Deviated by M.Taut[8] the exact ground state energy is 3.558a.u for the perturbed Hamiltonian when $\omega = 1$. We can therefore test the accuracy of our algorithm by comparing our numerical values to the exact value.

When numerically obtaining the ground state energy we will sample over 100 numbers each of the two variational parameters. We will leap over $\beta \in \{0.2, 1.2\}$ and $\alpha \in \{0.6, 1.6\}$ respectively.

Equilibrium

We will now go on to benchmark our algorithm for the first trial function with and without the perturbation. That is, we will study the behaviour of the variance in and the expectation value of the energy when increasing the number of Monte Carlo cycles. We can thereby study the sufficient number of MCCs in order to reach equilibrium. I.e. when the variances and expectation values are stable for a further increase of MCCs.

Variational method for different ground state oscillator energies

We will use the Metropolis algorithm in order to simulate for different angular frequencies ω for the perturbed Hamiltonian. We choose to simulate for $\omega \in \{0.01, 1\}$ with a step size of $\Delta\omega = 0.01$. We will use the values of β and α which resulted in the lowest energy in equation 20. We will use the values of β and α which resulted in the lowest energy in equation 20.

We can compare our results of the unit less energy (in atomic units) with the results of the eigenvalues, λ, in Project 2[9]. The eigenvalues are for the perturbed Hamiltonian. In order to achieve the same units of E and λ, we will need to scale the eigenvalues from Project 2. The scaling results in $E = \frac{\lambda}{2} + 1.5 \cdot \omega_r$. It is interesting to compare the numerical eigenvaules from Project 2 with our new computed eigenvalues, as the eigenvalues do not have analytical solutions for varying frequencies (only for $\omega = 1$).

Testing with the virial theorem

By testing the mean kinetic and potential energy against the virial theorem we can investigate the reliability of our algorithm. The linear relation in equation 12 is true when ignoring the Coulomb interaction potential. Thus, we will expect the relation between the two energies for the perturbed Hamiltonian will not be stable at 1. We will test the relation both with and without the Coulomb potential with varying frequencies. Needless to say, we expect that the two mean energies will comply more with the virial theorem without the Coulomb potential. Comparing the mean energies with the virial theorem without the repulsive interaction will test the accuracy of our algorithm. Additionally, by testing for different ωs we can observe which values produce the highest compliance with the virial theorem. Again, we will use the number of MCCs in which the equilibrium is reached, in order to have stable energies.

Additionally we can observe the effect of the different ωs have on the virial theorem.

Optimal step length

The step length δ is the length of which the position of the particles are attempted shifted by each Monte Carlo cycle. The optimal value of this entity is obtained when the step length results in an acceptance rate of $\approx 50\%$ for the trial positions. By testing various step lengths for eight different values of α, running the Monte Carlo simulation for 10^6 cycles, we will study the number of accepted changes to the particles' position with respect to total number of attempts, and by this approximate the relation between the parameters α and δ.

Parallel computing

The numerical operations we intend to perform is costly for the number of sampling points which we intend to simulate. When using the Metropolis algorithm

in order to arrive at the numerical value of the ground state energy of the second trial functions we will sample over 200×200 numbers of α and β, with 10^7 MCCs. Thus, it proves necessary to use parallelization in our simulations in order to decrease the run-time.

V. RESULTS

The first trial function

The figures 2 and 4 display the expectation value of the local energies with and without the Coulomb interaction as functions of number of Monte Carlo cycles. It is apparent that without the Coulomb interaction for $\alpha = 1$, the expectation value is stable at 3.00 for every Monte Carlo cycle. In comparison, for different values of α the expectation values appear chaotic in equal matter to the expectation values with Coulomb interaction. However, with the Coulomb interaction all the curves with different values of the variational parameter is chaotic. In both of the figures the curves seem to stabilize at different energies at $\approx 10^4$ MCCs.

The variance in the local energies with and without the Coulomb interaction as functions of number of Monte Carlo cycles are viewble in figures 3 and 5. In figure 3, the variance appears stable at $\sigma^2 = 0$, for all numbers of MCCs for psi_{T1} with $\alpha = 1$. For $\alpha \neq 1$, the same trend is not apparent, but the variance seem to stabilize at certain values after $\approx 10^5$ MCCs when the system reaches equilibrium. The highest variance of energy is observed to be for $\alpha = 0.6$. In figure 5 the variances stabilize after $\approx 10^6$ MCCs for the trial function with Coulomb interaction. For $\alpha = 1$, the variance appears stable at approximately $\sigma^2 = 0.25$. As for the non-interacting trial function it is apparent that $\alpha = 0.6$ gives the highest variance in energy.

From figure 6 the expectation value of the energy without Coulomb interaction taken into account appears to be at its minimum for $\alpha \approx 1.0$. With Coulomb interaction the minimum appears to be between 0.5 and 1.0. For both curves the expectation value of the local energy decreases rapidly for the lower values of α. Past the minimal points, the curves are observed to increase less rapidly than for the lower values of the parameter. Additionally, the local energy minimum with the Coulomb interaction is higher than for the unperturbed Hamiltonian. From table I, we see that the energy E_{L1} without the Coulomb term has its minimum at $\langle E_{L1} \rangle = 3.00$ with $\alpha = 3$. With interaction the minimum appears at $\langle E_{L1} \rangle = 3.77$ with $\alpha = 0.85$.

Figure 7 displays the variance of the local energy with and without Coulomb interaction. We see that for the Hamiltonian without Coulomb interaction the minimum value of the variance is $\sigma^2 = 0$ for $\alpha = 1$, as presented

in table I. From the same table, the variance for the Hamiltonian with Coulomb interaction has its minimum at $\sigma^2 = 0.24$ for $\alpha = 0.85$, which can also be observed from the corresponding figure. As for the expectation value of the energy figure, the curves increase less expeditiously after the minimum of α, than they decrease before this value has been reached.
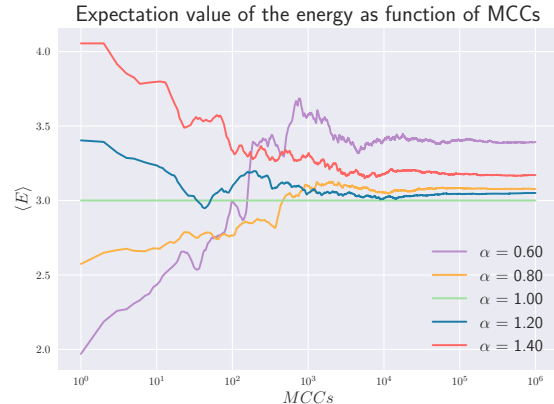

Figure 2. The figure displays the expectation values of the local energy E_{L1} without the Coulomb term as a function of number of MCCs, for ψ_{T1} with different values of the parameter α.
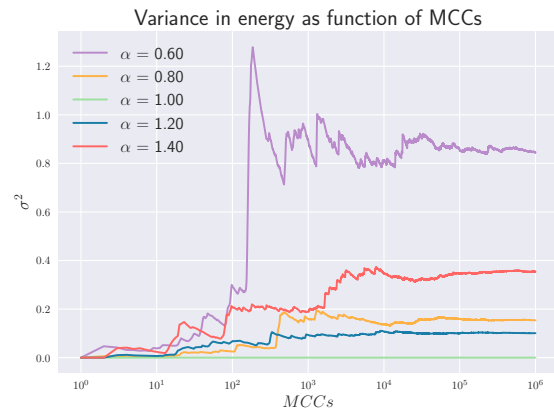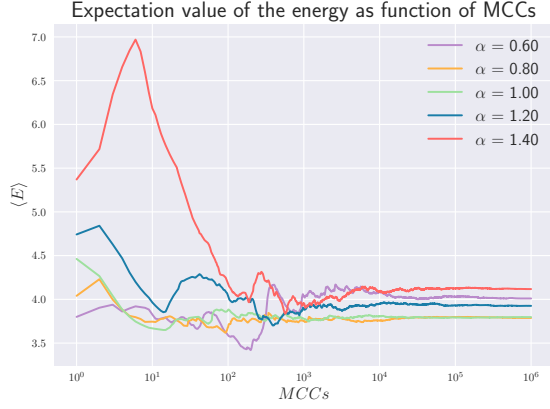

Figure 3. The figure displays the variance in the local energy E_{L1} without the Coulomb term as a function of number of MCCs, for ψ_{T1} with different values of the parameter α.

Table I. The table displays the minima of the expectation value of the local energy and the variance for ψ_{T1} with and without Coulomb interaction.

	$\langle E_{L1} \rangle$	σ^2	α
Non-interacting	3.00	0.00	1.00
Interacting	3.77	0.24	0.85

Figure 8 shows the number of accepted Monte Carlo moves in percentage as function of the step length δ. We

Figure 4. The figure displays the expectation values of the local energy E_{L1} with the Coulomb term as a function of number of MCCs, for ψ_{T1} with different values of the parameter α.
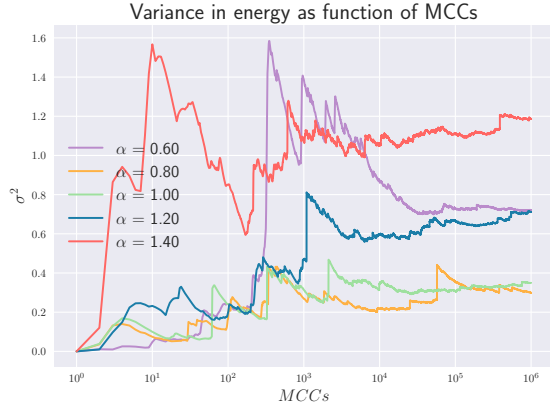

Figure 6. The figure displays energies of with and without the Coulomb interaction as a function of the variational parameter α, for number of MCCs $= 10^6$.

Figure 5. The figure displays the variance in the local energy E_{L1} with the Coulomb term as a function of number of MCCs, for ψ_{T1} with different values of the parameter α.

Figure 7. The figure displays variance of the energy with and without the Coulomb interaction as a function of the variational parameter α, for number of MCCs $= 10^6$.

see that the optimal step length, where roughly 50% of the suggested moves is accepted, varies for different values of α. We have used the intercepts between the 50%-line and the curves for the different values of α to calculate values for the step length resulting in 50% acceptance of suggested moves. Using linear regression of the logarithmic values of the step length δ we have presented the optimal step length as function of α in figure 9. The best fit curve between the data points we found to be $\delta = e^{-0.518\alpha + 0.982}$, which will provide acceptance rates in the range $45\% - 60\%$ for the values of α considered in this project. We observe that the optimal step length decreases for increasing values of α.

From table II the mean distance at the energy minimum between the two electrons decrease with increasing value of ω. The expectation value of the distance is smallest for $\omega = 1.0$ for the Hamiltonian both with the Coulomb term and without. Furthermore, we see that
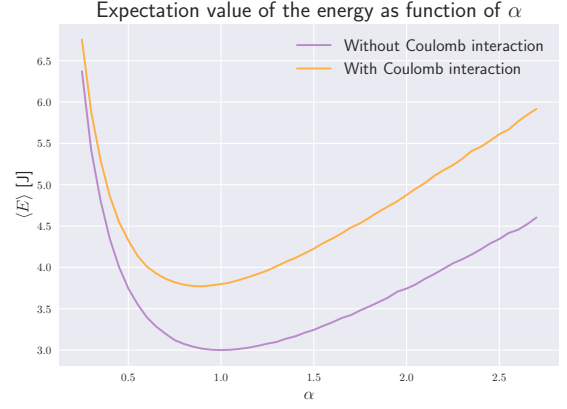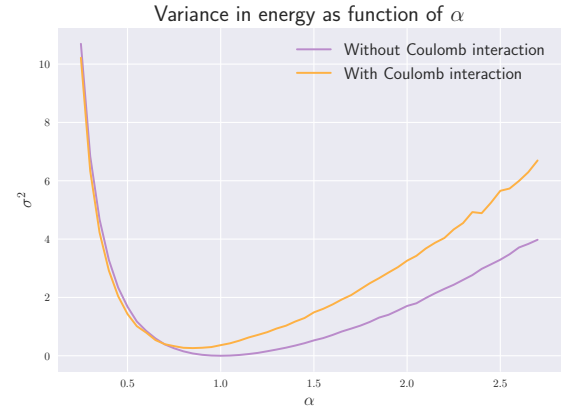
the expectation values appear to be slightly higher for the system whose Hamiltonian include the perturbation, than for the system without.

Table II. The table displays the expectation value of the mean distance at the energy minimum $r_{12} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$ between the two electrons for the optimal set of the variational parameters, $\omega = 0.01$, $\omega = 0.50$ and $\omega = 1.00$. The values of the mean distances are for the first trial function, ψ_{T1}.

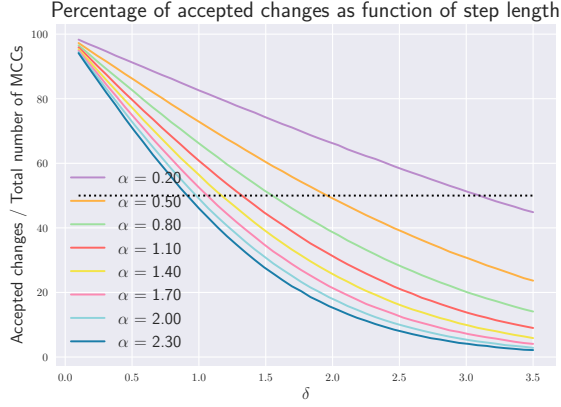| ω	$\langle r_{12} \rangle$ without interaction	$\langle r_{12} \rangle$ with interaction
0.01	16.1	17.4
0.50	2.25	2.44
1.00	1.60	1.73

Figure 8. The figure presents the accepted number of changes in percent as function of step length δ, for number of MCCs $=10^6$.
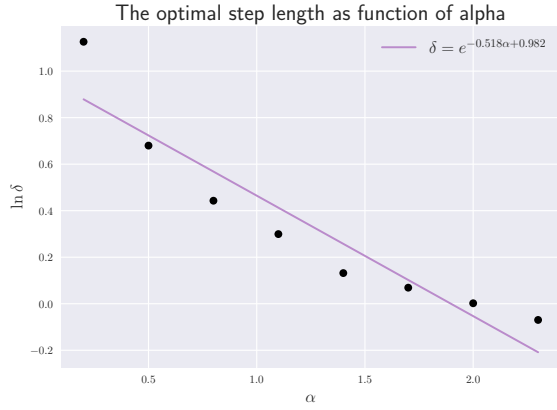

Figure 9. The figure displays the optimal step length δ as function of the variational parameter α.

The trial function with the Jastrow factor

From figure 10 we see how different sets of the variational parameters α and β affects the expectation value of the energy for trial function ψ_{T2}. Moreover, we found that the expectation value has its minimum for $\alpha = 0.995$ and $\beta = 0.290$, with the minimum value being 3.730.

In table III the mean distance of the two electrons as well as the system's mean local energy is displayed for three different frequencies, $\omega = 0.01, 0.50$ and 1.00. These values are computed with the optimal values of $\alpha = 0.995$ and $\beta = 0.290$. The expectation values calculated with the variational method and in Project 2[9] are of the same magnitude, but differ with a factor of $\approx \pm 0.3$. It is noted that the analytical value for the expectation value of the local energy for $\omega = 1$, equal to 3.558 [8], is in more agreement with the result from Project 2 than the

results obtained using the variational method. We observe the deviation from the analytic value of the ground state energy for $\omega = 1.00$ for the second trial function to be 0.212 a.u. The mean distances displayed is observed to decrease rapidly from $\omega = 0.01$ to $\omega = 0.50$, just as seen for the first trial function in table II.

Table III. The table displays the expectation value of the energy and the variance for the second trial wave function. It is calculated with the optimal parameters for the ground state wave function, using $\omega = 0.01$, $\omega = 0.50$ and $\omega = 1.00$. The table also shows the mean distance at the energy minimum $r_{12} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$ between the two electrons for the same parameters. In addition the table display the obtained mean energy values, $\langle E_{\text{project 2}} \rangle$, of different ωs.

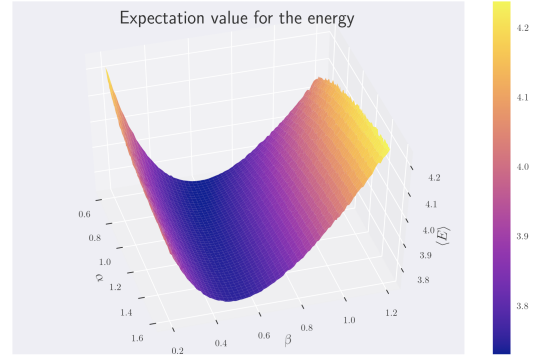| ω	$\langle E \rangle$	σ^2	$\langle r_{12} \rangle$	$\langle E_{\text{project 2}} \rangle$
0.01	0.10	0.00	17.45	0.314
0.50	2.00	0.00	2.58	2.27
1.00	3.73	0.00	1.81	3.56

Figure 10. The figure displays the expectation value of the energy as function of the variational parameters α and β for the second trial function ψ_{T2}.

The virial theorem

Figure 11 displays the energy ratio between the kinetic and potential energy as function of frequencies. For the non-interacting curve, the ratio appears somewhat stable around 1 for all values of ωs. For the case of the perturbed Hamiltonian with the optimal value of α in the first trial function the curve is constantly increasing with an increasing ω.
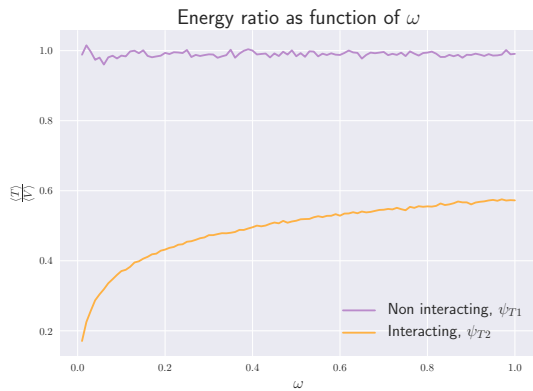
Figure 11. The figure shows the ratio between the kinetic energy $\langle T \rangle$ and the potential energy $\langle V \rangle$ as function of frequencies ω for the optimal values of α and β.

VI. DISCUSSION

Reaching equilibrium

As seen in figure 2, for $\alpha = 1$ the expectation value of the energy is constant at 3.0 for every Monte Carlo cycle. This is as expected, as for $\alpha = 1$ the local energy E_{L1} is equal to the analytical ground state energy for a system of two electrons in a harmonic oscillator potential, neglecting the Coulomb interaction between the electrons. The stability of the expectation value of the energy for $\alpha = 1$ is further confirmed by figure 3, where the variance remains stable at 0 for all cycles.

In the figures 2 and 3 it appears that after 10^5 number of MCCs, the system has reached its equilibrium state for the unperturbed Hamiltonian as the expectation value and the variance becomes stable. For the expectation value and variance of energy of the perturbed Hamiltonian in figures 4 and 5 appear more chaotic for every value of α. In the figure displaying the variance of energy as a function of MCCs it appears that the equilibrium is almost reached after at least 10^6 MCCs, however in the expectation value figure, the equilibration seem to be met at 10^5 MCCs. One would expect these graphs to stabilize at the same time, as the variance is totally dependent of the expectation value of the energy and its square, and the reason they're not approaching equilibrium at the same time we're unsure of. Due to the fact that it seems to require 10^6 MCCs to reach equilibrium in figure 5, it could have been beneficial to start the sampling for MCCs not lower than 10^6 in the remaining computations. However, for the most part the figures indicated that the equilibration of the system occurred at 10^5, and as a higher number of MCCs makes the computations much more time costly, we decided to perform the sampling after 10^5 MCCs in the further calculations. This is something we can expect to slightly decrease the

precision of our calculations, all though making the computations less troublesome in the sense that they don't require to much time to be performed.

The first trial wave function

The minimum of the energy expectation value is as seen in figure 6 reached at $\alpha = 1.0$ for the Hamiltonian without the Coulomb interaction, computed with 10^6 number of MCCs. The minimum value was found to be 3.0, which is in total compliance with theory. This is more apparent in table I, whereas the variation, σ^2, is zero. With this in mind, our implemented algorithm gives the impression of providing viable results for the unperturbed Hamiltonian, thus boosting our confidence in the further computations.

With the Coulomb interaction taken into account, the lowest expectation value of energy is at 3.7 at $\alpha = 0.85$. This also seem to comply with our expectations, as the Coulomb interaction potential results in higher energies than the simple harmonic oscillator potential. The analytical value of the ground state energy for this Hamiltonian is 3.558 from reference [8]. Using the standard deviation, $\sigma \approx 0.5$, as the confidence bound the analytic expectation value of the ground state energy is found to be within the numerically obtained value's bound. However, the confidence bound is exceedingly large. Thus, the precision of the resulting energy with the perturbed Hamiltonian is certainly of less caliber than for the Hamiltonian without the perturbation. With that being said, as it was highly unlikely that we would be able to estimate this result precisely, the result is as anticipated.

Obtaining the optimal step length

From figure 8 it is observed that the optimal step length, providing roughly 50% accepted alterations to the electrons' positions, vary for different values of α, and we used linear regression to approximate an expression for this optimal step length as function of the parameter. The data points do not entirely match the best fit line presented in figure 9 perfectly, especially for the case of the smallest value of α as it deviates quite strongly. However, the other data points seem to be in larger agreement with the model we made. As a result of the somewhat unperfect model, we do expect some smaller inaccuracies in the further calculations due to the choice of model. As the model determines a step size slightly smaller than preferred for some αs while slightly larger for others, providing acceptance rates in the range $45\% - 60\%$, we do it will affect the expectation value of the energy to some degree, such that it will require a somewhat higher number of MC cycles for the system to stabilize in comparison to the case with the true optimal step length.

Mean distance at the energy minimum

When studying the expectation value of the distance at the energy minimum as function of α between the two electrons, for the Hamiltonian both with and without the perturbation and the first trial function, we found that the mean distance decreased as the frequency increased. As the potential energy is proportional to $\omega^2 r^2$, 12, these findings are in total compliance with what one would expect. In other words when the potential becomes steeper, the distance between the electrons decreases. Likewise, when the potential incline decreases, the electrons are more likely to be positioned further apart.

Furthermore, the mean distance is observed to be higher for the Hamiltonian with the perturbation than without. This, of course, is quite satisfying, as we would expect the mean distance between the two electrons to increase, when taking their repulsive forces into account. For both cases, with the Hamiltonian with and without the perturbation term, there are no analytical values to compare the mean distances to. Therefore, we cannot be certain of the reliability of these results. Nonetheless, the trend we do observe are in total agreement with our expectations and we are therefore confident that these are in fact reliable results.

The trial wave function with the Jastrow factor

The figure 10 displays how the average energy changes for different values of the variational parameters α and β. It is not as deceptive as to which specific values of α and β produces the lowest mean energy, but it does give us some insight to how the the mean energy roughly is affected by the parameters. It is not surprising that the energy increases rapidly from its lowest point with a different β than the one producing the lowest mean energy, as the trial function's mean energy is weighed by $\frac{1}{\beta}$. It is furthermore apparent that the implications α has on the expectation value is of somewhat less significance compared to β, as the expectation value seems to not vary quite as much for varying values of this parameter as for the other.

From table III the average energies both calculated with the variational method and from Project 2[9] are displayed. The associated entities of the second trial function are computed with our obtained optimal values of the variational parameters $\alpha = 0.995$ and $\beta = 0.290$. These values and the values from Project 2 are of the same magnitude, but especially for $omega = 0.01$ the relative deviation is clear. Since the obtained variances of the average energies were found to be 0 with three leading digits, the results can be said to not comply with the ones from Project 2. The computed variance of 0 is not easily explainable, as we initially would expect

it to be higher as our computations are not flawless. If the computational precision had been higher, our results would have been able to be described by a higher number of digits thus leading to a higher accuracy, and we would then have expected our results to resemble the Project 2 results somewhat more. It should be mentioned that as the variational method only provides an upper bound limit for the true ground state energy, the deviations are expected, and as anticipated the computed mean energies in this project are certainly higher than both the analytical value and the results from Project 2.

When further comparing the result from Project 2 and the results obtained in this project, the expectation value of the energy for $\omega = 1.0$ from Project 2 is found to be in a much higher agreement with the analytical value of $\langle E \rangle = 3.558$ from M.Taut[8] than the upper bound estimates found in this project. One could expect that this is true for the other values of $\omega = 0.01$ and 0.5. However, since we do not have any analytic results to compare the values with (for $\omega \neq 1$) we cannot say whether or not this is true.

The table III also displays the mean distances between the electrons for different values of ω. The values are larger, but not substantially, than the associated values for the first trial function with the perturbed Hamiltonian in table II. This can indicate that with the Jastrow factor the repulsive interaction plays a bigger role in where the electrons' prefer to stay, as a larger mean distance demonstrates that the perturbation term of the Hamiltonian is more dominant. We further note that the mean distance decreases for increased values of ω, which is anticipated as when the harmonic oscillator potential becomes steeper, the electrons will be more likely to be near each other. This is due to the fact that it would require more energy for the electrons to move far apart.

The virial theorem

When testing the virial theorem we found that the energy ratio between the kinetic and potential energies, for the wave function without the Coulomb interaction taken into account fluctuated around 1.0. The fluctuations apparent in figure 11 we assume to be a consequence of numerical inaccuracies. With this being said, the trend is still clear. Roughly spoken, we can therefore say that the kinetic and potential energy seem to be more or less equal for all values of ω. This is as anticipated for the pure harmonic oscillator potential's relation with the mean kinetic energy in equation 12. In other words, the first trial function, with $\alpha = 1$, gives the true ground state for the pure harmonic oscillator system. We can therefore say that the test with the virial theorem has succeeded.

Considering the second trial function for the system described by the Hamiltonian with Coulomb interaction, we note that the contribution from the Coulomb interaction dominates for small values of ω, thus the deviation from the virial theorem is apparent for these ωs. However, as the frequency increases, the contribution from the harmonic oscillator potential becomes more and more significant. All though this is not shown in figure 11, we do expect that the energy ratio for the perturbed Hamiltonian will approach 1.0 as ω becomes sufficiently large. However, this will require a very steep Harmonic Oscillator potential. For such a potential, it is safe to say that the effect from the added term proportional to $\frac{1}{r_{12}}$ will become negligible. This in alignment with theory, as with an increasing angular frequency the harmonic oscillator potential increases (in equation 2)), whereas the Coulomb potential is independent of ω.

VII.   CONCLUSION

We have studied a quantum dot consisting of two electrons in three dimensions, and our goal was to approximate the system's ground state energy by the variation method, which gives an upper bound limit to the ground state energy. This has been done both with and without the Coulomb interaction potential considered, with two different trial wavefunctions with and without the Jastrow factor. In order to arrive at an approximation of the ground state energies of the electrons, we have used a Monte Carlo based Metropolis algorithm. By studying the expectation value of the Hamiltonian both with and without the perturbation for the first trial function, we found that the number of MCCs resulting in equilibrium was $\approx 10^5$, which we used in further calculations.

We further studied both Hamiltonians' expectation values as functions of the variational parameter α with the first trial function, by which we found the resulting expectation value of the local energy to be perfectly in alignment with theory for the Hamiltonian without the Coulomb interaction potential for $\alpha = 1.0$, which served as a benchmark for the later calculations. For the first trial function with the Hamiltonian including the Coulomb interaction, the resulting minimum value of the expectation energy was found to be higher, which aligned with our initial expectations. Additionally, the analytical value or the ground state energy for this system was within the large confidence bound of our expectation value. We also modeled the relation between the optimal step length δ and the variational parameter α, which all though not flawless, we presumed would provide reasonable results moving forward. For this first wavefunction without the Jastrow factor, the ratio between the expectation value of kinetic and potential energy also complied with the virial theorem as it seemed to be ≈ 1 for angular frequencies between 0.01 and 1. However, small fluctuations was observed to occur, which we assumed were due to smaller numerical inaccuracies, i.e. the unperfect model of the optimal step length as function of the parameter α, or the decision of equilibration time by which we started the sampling.

Furthermore we considered the second wavefunction with the Jastrow factor, and found the optimal values of α and β which provided the lowest upper bound estimate for the ground state energy of the system, Coulomb interaction considered. With these we further evaluated the resulting expectation value of the local energy for different angular frequencies, and all though the resulting expectational values of the energy seemed to not exactly outshine the corresponding results from Project 2, they still as far as we know are able to serve as good upper bound estimates for the exact ground state energy, as was intended. For this trial function, the ratio between the average kinetic and potential energy was found to be dominated by the Coulomb repulsion for lower frequencies, as expected, while we for higher frequencies do expect the steep Harmonic Oscillator contribution to the potential to take over, thus letting the ratio approach 1.

The mean distance between the electrons was further found to decrease rapidly as the frequency increased, and more over, all though not quite as apparent, the mean distance was observed to increase when taking the Coulomb repulsion into account. This was in total agreement with theory and what we anticipated initially. To sum things up, this project is considered to be quite a success as all results are satisfactory in the sense that they were either expected or that their deviations from theory are relatively small. As mentioned in the introduction, the Quantum Dot system has several applications to modern science, so one can imagine that it would be interesting to make further investigations. In hindsight, if we were to move on with our investigations of this type of system, we would probably first have perfected our computations by choosing a larger equilibration time for our computations, as well as experimented with other models for the optimal step length as function of α to increase the accuracy of our results. Still, without these perfectional adjustments this project accomplished what was intended, and for that we are pleased.

GITHUB

All data, code and plots are available at our GitHub page: https://github.com/hedvigborgen/fys3150. Follow the README.md file in order to run the codes.

VIII.   ACKNOWLEDGEMENTS

IX.   SOURCES

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Appendix A: Derivation of the corresponding energies of the trial wave functions

Unperturbed Hamiltonian

Firstly we will derive the corresponding energy to the trial wave function in 15 with the unperturbed Hamiltonian. The trial wave function is presented in equation 14. We will use the time independent Schrödinger equation of the unperturbed Hamiltonian,

$$\hat{H}_0 \psi_{T1} = E_0 \psi_{T1} =$$
$$\frac{1}{2}\Big[-(\nabla_1^2 + \nabla_2^2) + \omega^2 \big(r_1^2 + r_2^2\big)\Big]\psi_{T1} =$$
$$\Big[-\frac{1}{2}(-3 \cdot 2\alpha\omega + \alpha^2\omega^2(r_1^2 + r_2^2)$$
$$+\frac{1}{2}\omega^2\big(r_1^2 + r_2^2\big)\Big]\psi_{T1} =$$
$$\Big[\frac{1}{2}\omega^2(r_1^2 + r_2^2)(1 - \alpha^2) + 3\alpha\omega\Big]\psi_{T1}.$$

Thus the energy E_0 is equal to the energy in equation 15.

Perturbed Hamiltonian

The first trial function, in equation 14, with the perturbed Hamiltonian is obtained in the same matter as above.

$$(\hat{H} + \hat{H}')\psi_{T1} = E_0 \psi_{T1} =$$
$$\frac{1}{2}\Big[-(\nabla_1^2 + \nabla_2^2) + \omega^2\big(r_1^2 + r_2^2\big) + \frac{1}{r_{12}}\Big]\psi_{T1}.$$

Since the perturbed factor of the Hamiltonian is independent of the trial function, the resulting energy is simply,

$$E_{T1,\text{pert}} = E_{T1} + \frac{1}{r_{12}}. \tag{A1}$$

For the new trial function in equation 17, the deviation is much more strenuous, and so painful that we choose to not derive it here.

Appendix B: Ground state energy of two identical particles in an harmonic oscillator

Considering the Hamiltonian of the harmonic oscillator potential, the ground state energy of two identical

particles is obtainable. By using the time independent Schrödinger equation, we would need to guess on a wave function. The 'guessed' wave function is presented in equation 5 and the Hamiltonian of two particles in equation 2

$$\hat{H}_0\psi_0(r_1, r_2) = \sum_{i=1}^{2} -\frac{1}{2}\nabla_i + \frac{1}{2}\omega^2 r_i^2$$

$$Ce^{-\omega/2\cdot(r_1^2+r_2^2)}$$

From Johannes Skaar lecture notes in FYS3110 at UiO [10] we can rewrite the wave function of two electrons to,

$$\psi_0(r_1, r_2) = \psi_0(r_1)\psi_0(r_2). \tag{B1}$$

And the total energy,

$$E_{\text{tot}} = E(r_1) + E(r_2) = 3\omega. \tag{B2}$$

The energies $E(r_1)$ and $E(r_2)$ are both equal to $\frac{3}{2}\omega$, such that the total ground state energy is 3ω.

Appendix C: Meme - Optional

VIII. SOURCES

- [1] 'Quantum Mechanics - second edition' (2017), D. J. Griffiths, page 40-47 - The Harmonic Oscillator.

Figure 12. DJ Griffiths