

**Computational Physics: Project 3**

**Variational Monte Carlo project**

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## 1 Introduction

In this report we will be using natural units:

$$\begin{aligned}\hbar = c = e = m_e &= 1 \\ \Rightarrow [E] &= \text{a.u.},\end{aligned}$$

where  $\hbar$  is the Planck constants divided by  $2\pi$ ,  $c$  is the speed of light,  $e$  is the elementary charge and  $m_e$  is the electron mass. The unit of energy then becomes atomic units, denoted as a.u.

## 2 The physical problem

Quantum dots are nanoscopic crystals usually from semiconducting materials being of a size to exhibit quantum mechanical properties. In this report we will look at systems of electrons confined in a harmonic oscillator, which acts like a trap. These systems can be considered quantum dots. In order to study such systems, we have to look at the Hamiltonian, which consists of two parts:

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad (1)$$

where  $\hat{H}_0$  describes the standard harmonic oscillator and  $\hat{H}_1$  the repulsive term between the charged particles (in this case electrons). We can then write

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

The quantity  $N$  denotes the number of charged particles,  $\omega$  is the oscillator frequency,  $r_i$  is the position of particle  $i$  given by  $r_i = \sqrt{r_{ix}^2 + r_{iy}^2}$  and the distance between two particles is referred to as  $r_{ij} = \sqrt{\mathbf{r}_i - \mathbf{r}_j}$ . From quantum mechanics we know, that the wave function corresponding to this Hamiltonian for one electron in two dimensions  $(x, y)$  is

$$\phi_{n_x, n_y}(x, y) = A H_{n_x}(\sqrt{\omega}x) H_{n_y}(\sqrt{\omega}y) \exp \left[ -\frac{\omega}{2}(x^2 + y^2) \right]. \quad (3)$$

In this equation the Hermite polynomials  $H_{n_x}(\sqrt{\omega}x)$  appear as well as a constant  $A$  responsible for the normalization.

To get the energy  $E$ , we have to consider the Eigenvalue equation

$$\hat{H}\phi_\lambda = E\phi_\lambda, \quad (4)$$

which leads to the energy

$$E_{n_x, n_y} = \omega(n_x + n_y + 1) \quad (5)$$

Looking at the lowest energy state we have  $E_{(1)} = \omega$ .

Advancing now to the case of two electrons who do not repel each other we have two independent Hamiltonians, one for each electron, and as a result two independent eigenvalue problems as in equation 4. This leads to the same energy as before, but this time the energy must be taken into account twice. So we get:

$$E_{(2)} = E_{(1)} + E_{(1)} = 2E_{(1)}. \quad (6)$$

The corresponding wave function is then given by

$$\Phi(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left[ -\frac{\omega}{2}(r_1^2 + r_2^2) \right]. \quad (7)$$

As in equation 3  $C$  is the normalization constant.

Since the particles we are considering are fermions, we must regard the spin as well. The overall spin must be zero, because according to the Pauli principle two fermions cannot have the same quantum numbers. The electrons we are looking at have exactly the same energy of  $E = \omega$ , so their only way of obeying the principle is to have different spins. There are two possible states:

$$|\uparrow\downarrow\rangle \text{ and } |\downarrow\uparrow\rangle \quad (8)$$

Hence one of the electrons has spin  $1/2$  and the other one has spin  $-1/2$ . Despite this they are indistinguishable, which means both states are possible.

Regarding the wave function we will now make an separational ansatz for its simplification:

$$\psi(\mathbf{r}_1, \sigma_1, \mathbf{r}_2, \sigma_2) = R(\mathbf{r}_1, \mathbf{r}_2)X(\sigma_1, \sigma_2) \quad (9)$$

with

$$R(\mathbf{r}_1, \mathbf{r}_2) = \varphi_{n_{x_1} n_{y_1}}(x_1, y_1) \varphi_{n_{x_2} n_{y_2}}(x_2, y_2) \quad (10)$$

In this ansatz  $R(\mathbf{r}_1, \mathbf{r}_2)$  is the part of the wave function depending on the positions and  $X(\sigma_1, \sigma_2)$  is the spin-depending part, the matrices  $\sigma_1$  and  $\sigma_2$  are the spin matrices for particle 1 and 2.

According to this ansatz we can focus on the position-based part of the wave function for the following analysis of two electrons.

## 2.1 Many-body problems

Furthermore we are going to focus on many-body problem by considering up to six electrons. In this case, the wave function can be written as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_6) = \det(\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \dots, \phi_6(\mathbf{r}_6)) \prod_{i < j}^6 \exp \left[ \frac{ar_{ij}}{(1 + \beta r_{ij})} \right], \quad (11)$$

where again the  $\phi_i(r_i)$  refer to single particle wave functions as in equation 3.

The determinant is also known to be called Slater determinant. Although it is the determinant of a  $6 \times 6$ -matrix, it can be reexpressed in terms of  $3 \times 3$ -determinants according to Cramer's rule.

$$\begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \cdots & \phi_1(r_6) \\ \phi_2(r_1) & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \phi_6(r_1) & \cdots & \cdots & \phi_6(r_6) \end{vmatrix} \propto \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \phi_1(r_3) \\ \phi_3(r_1) & \phi_3(r_2) & \phi_3(r_3) \\ \phi_5(r_1) & \phi_5(r_2) & \phi_5(r_3) \end{vmatrix} \cdot \begin{vmatrix} \phi_2(r_4) & \phi_2(r_5) & \phi_2(r_6) \\ \phi_4(r_4) & \phi_4(r_5) & \phi_4(r_6) \\ \phi_6(r_4) & \phi_6(r_5) & \phi_6(r_6) \end{vmatrix} \quad (12)$$

### 3 The method

As presented in the previous section the eigenvalue problem of two electrons in a harmonic oscillator without any interaction terms can be easily solved. Looking at electrons in a quantum dot this calculation gains complexity. This is why we introduce the Variational Monte Carlo Method for estimating the electron states.

#### 3.1 Variational Monte Carlo method

In the Variational principle, we take the eigenvalue problem from equation 4 and expand the wave function as following:

$$\varphi_0 = \sum_{\lambda=0}^{\infty} c_{0\lambda} \psi_{\lambda}, \quad (13)$$

where  $c_{0\lambda}$  are coefficients.

In quantum mechanics the energy is the expectation value

$$E = \frac{\langle \psi_0 | \hat{H} | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} \quad (14)$$

So when we apply the expansion to this, we get:

$$\frac{\langle \varphi_0 | \hat{H} | \varphi_0 \rangle}{\langle \varphi_0 | \varphi_0 \rangle} \quad (15)$$

$$= \frac{\sum_{\alpha,\beta} c_{0\alpha}^* c_{0\beta} \int d\tau \psi_{\alpha}^*(\tau) \hat{H} \psi_{\beta}(\tau)}{\sum_{\alpha,\beta} c_{0\alpha}^* c_{0\beta} \int d\tau \psi_{\alpha}^*(\tau) \psi_{\beta}(\tau)} \quad (16)$$

$$= \frac{\sum_{\alpha} E_{\alpha} |c_{0\alpha}|^2}{\sum_{\alpha} |c_{0\alpha}|^2}, \quad (17)$$

because by construction  $\langle \psi_{\alpha} | \psi_{\beta} \rangle = \delta_{\alpha\beta}$  for eigenfunctions  $\psi_{\alpha}, \psi_{\beta}$ .

We have to consider two cases now:

- If the expansion  $\varphi_0$  is not the eigenfunction  $\psi_0$  we get the an energy

$$E_0 \leq \frac{\langle \varphi_0 | \hat{H} | \varphi_0 \rangle}{\langle \varphi_0 | \varphi_0 \rangle}. \quad (18)$$

- If the expansion  $\varphi_0$  corresponds exactly to the eigenfunction  $\psi_0$  we get the exact energy

$$E_0 = \frac{\langle \varphi_0 | \hat{H} | \varphi_0 \rangle}{\langle \varphi_0 | \varphi_0 \rangle}. \quad (19)$$

In the second case the variance of the energy

$$\text{var}(E) = \langle H^2 \rangle - \langle H \rangle^2 = 0. \quad (20)$$

As expansion wave function  $\varphi_0$  we use a trial wave function we will call  $\psi_T(\mathbf{r}_1, \mathbf{r}_2, \alpha, \beta)$ , with  $\alpha$  and  $\beta$  being the variational parameters. In this report the trial wave function for two electrons has the form:

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left[ -\alpha \frac{\omega}{2} (r_1^2 + r_2^2) \right] \exp \left[ \frac{a_{12} r_{12}}{(1 + \beta r_{12})} \right] \quad (21)$$

with

$$a_{12} = \begin{cases} 1, & \text{for } \uparrow\downarrow \\ 1/3, & \text{for } \uparrow\uparrow, \downarrow\downarrow \end{cases} \quad (22)$$

and

$$r_{12} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}. \quad (23)$$

The factor  $J = \exp \left[ \frac{a_{12} r_{12}}{(1 + \beta r_{12})} \right]$  is called the Jastrow factor, which we will refer to later.

In order to find the wave function and its corresponding energy to the case we are considering, we compute the expectation value  $E(\alpha, \beta)$  and find its minimum or alternatively the minimum of its variance  $\text{var}(E(\alpha, \beta))$ . This procedure is used in section 4. For the six electron case, the variational wave function becomes as in equation 11 and we can again search the minimum energy.

## 3.2 Monte Carlo methods

The basis of the method explained above are the Monte Carlo methods, which can be referred to as statistical simulation methods. The central building block of these methods is the probability distribution function (PDF), which is used to describe and characterize the physical problem. This does not restrict the method to statistical problems, but by displaying the desired solution in terms of PDF's, non-stochastic problems can be handled as well. During a Monte-Carlo simulation, random numbers must be generated covering an interval uniformly. Using these numbers, many random samples are taken from the PDF. In order to get the desired result the average of all samples is computed. According to this, the precision of the simulation rises with the amount of samples. The error has to be estimated to get an impression of the simulation's precision.

On the contrary of statistical random number-based methods, in standard mathematical modelling, the problem would be discretized and solved by a numerical approach.

### 3.2.1 Pseudo-random number generation

As a main ingredient, random numbers play an important role in Monte-Carlo simulations and therefore have to be 'as random as possible'. The generation of truly random numbers is practically not possible, this is why the random numbers we work with are pseudo-random, generated by an algorithm fulfilling the criteria of

- generating equally distributed numbers in a given interval (usually  $[0,1]$ )
- repeating random number sequences seldom
- being fast
- generating insignificantly correlated numbers

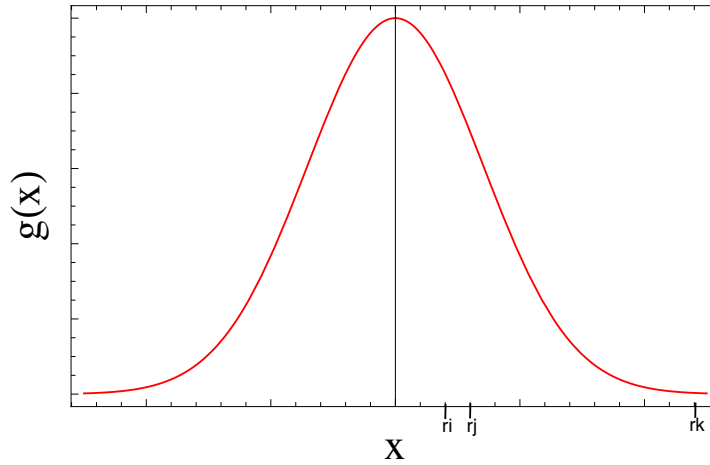
In this report, we use random number generators explained in Press et al. (1999), that are called **ran0** and **ran1**.

Furthermore, we generate random gaussian distributed random numbers using **gaussian**.

## 3.3 Metropolis algorithm

The difficult part of Monte-Carlo simulations is the selection rule for random states. One must find a method when to reject and when to accept the generated state. Precision and efficiency strongly depend on this rule. Supposing we have a distribution such as the one shown in figure 1 and we have already picked an initial random variable at  $r_i$ . Since we are performing the simulation on many samples, we now have to pick a new random number keeping in mind, that there are two cases, which must be avoided:

- Choosing repeatedly numbers very close to the initial value such as  $r_j$  in figure 1. We would then 'get stuck' around the interval of  $r_i$  and therefore lose the overview of the function we are evaluating.



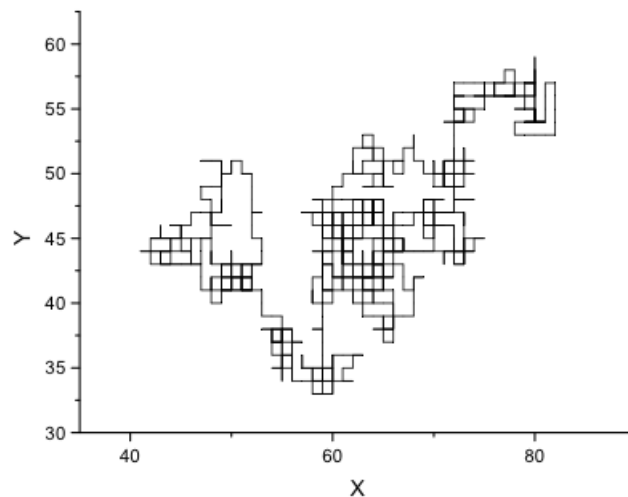
**Figure 1:** Gaussian distribution showing problems in selection of random states

- Jumping to numbers far away from the initial value, where the distribution is negligible, for example to  $r_k$  in figure 1.

Preventing the simulation in creating biased averages and unprecise results is possible by using the Metropolis algorithm, which is a Markov process, satisfying both ergodicity and detailed balance.

Ergodicity in random processes means, that the time average of a sequence of events has to be the same as the average of all possible states, the so-called ensemble-average. In order to obey detailed balance, the process must follow a distribution, where the transition probability from state  $i$  to state  $j$  is the same as from state  $j$  to state  $i$  at equilibrium. This is also called reversibility.

Markov chains are referred to as random walks with selected probability to make a move, which is independent of the previous step. An example of this movement is the Brownian random walk shown in figure 2, where a particle moves in the  $x$ - $y$ -plane with step length 1 performing hundred steps. The probability of moving is the same for every direction. Using Markov processes, we can generate new random states and reach the most likely state (equilibrium) after a certain time.



**Figure 2:** Brownian random walk of 100 steps in  $x$ - $y$ -plane and step length 1



### 3.3.1 Importance sampling

There are lots of examples in science, where biasing is disturbing and should be avoided. One example are the required unbiased uncorrelated random numbers in section 3.2.1. In Monte-carlo methods, biasing can be a tool to increase the simulation's efficiency by performing a Metropolis walk biased by the trial wave function. Since our problem is somewhat similar to a diffusion process in one dimension for one particle, we may use an approach based on the Fokker-Planck and the Langevin equation. The 'old' and 'new' positions in space can be calculated by

$$r_{old} = \eta \quad (24)$$

$$r_{new} = r_{old} + \eta + \delta t D F_{old}, \quad (25)$$

where  $\eta$  denotes a gaussian distributed random variable,  $\delta t$  refers to the time step,  $D$  is the diffusion constant, which is in our case set to  $D = 0.5$  and  $F_{old}$  is the quantum force at position  $r_{old}$ . Note, that  $\eta$  are different random numbers.

The term responsible for biasing the walk in space  $x$  is the quantum force, which leads the walk to regions with large trial wave function. In a brute force Metropolis algorithm, the propability of moving would be the same for all directions. The quantum force is

$$\mathbf{F} = 2 \frac{1}{\psi_T} \nabla \psi_T \quad (26)$$

In order to include this biasing in the Metropolis algorithm, we will replace

$$q(r_{old}, r_{new}) = \frac{|\psi_T(r_{new})|^2}{|\psi_T(r_{old})|^2} \quad (27)$$

by

$$q(r_{old}, r_{new}) = \frac{G(r_{old}, r_{new}, \delta t) |\psi_T(r_{new})|^2}{G(r_{new}, r_{old}, \delta t) |\psi_T(r_{old})|^2}, \quad (28)$$

where the quantity  $G$  refers to the Greensfunction

$$G(y, x, \delta t) = \frac{1}{(4\pi D \delta t)^{3N/2}} \exp \left[ -(y - x - D \delta t F(x))^2 \frac{1}{4D \delta t} \right]. \quad (29)$$

## 3.4 Analytical calculations

## 4 Results and discussion

We will now first take a look at the case of two electrons in a potential with different oscillator energies. In order to do so, we preform a Variational Monte Carlo simulation and use the Metropolis algorithm explained in section 3.3 to find the energy of the ground state. Therefore we use numerical derivation. We will later introduce analytical calculations based on closed-form expressions as well (section 4.3). Besides, we put emphasis on the correlations introduced by the Jastro factor by computing the kinetic and potential energy of the ground state for different oscillator frequencies. In addition we introduce importance sampling and analyse the dependency of the results to the time step  $\delta t$ .

### 4.1 Two electron case

Since it is the easiest case, we first look at two electrons in a quantum dot interacting with each other. According to ? the corresponding energy is at  $E = 3$  a.u. (atomic units). For the computation we use the variational wave function

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left[ -\alpha \frac{\omega}{2} (r_1^2 + r_2^2) \right] \exp \left[ \frac{a_{12} r_{12}}{(1 + \beta r_{12})} \right], \quad (30)$$

where we start by considering a wide range of  $\alpha \in [0.7, 1.3]$  and  $\beta \in [0.2, 0.6]$  first and preform a more precise simulation afterwards. The goal is to find the variational parameters  $\alpha$  and  $\beta$ , where the energy is at its minimum. After the first simulation we notice, that the minimum must be somewhere around  $\alpha \in [0.9, 1.1]$  and  $\beta \in [0.35, 0.45]$ . This is why we preform a simulation with these boundaries and use 3 000 000 Metropolis cycles to get an accurate result. In figure 3 the energy is plotted depending on both variational parameters  $\alpha$  and  $\beta$ . The 3D-plot results in a bended plane resembling to the shape of a valley. For increasing  $\alpha$  the corresponding  $\beta$  at minimal energy is decreasing. The minimum energy calculated is

$$E = 3.0003 \text{ a.u.} \quad (31)$$

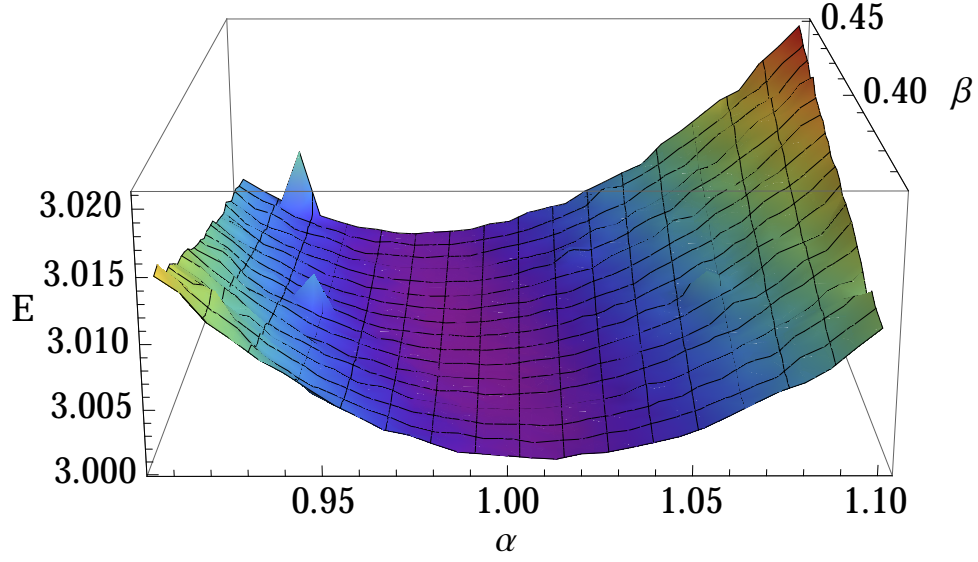
at

$$\alpha = 0.9867, \quad (32)$$

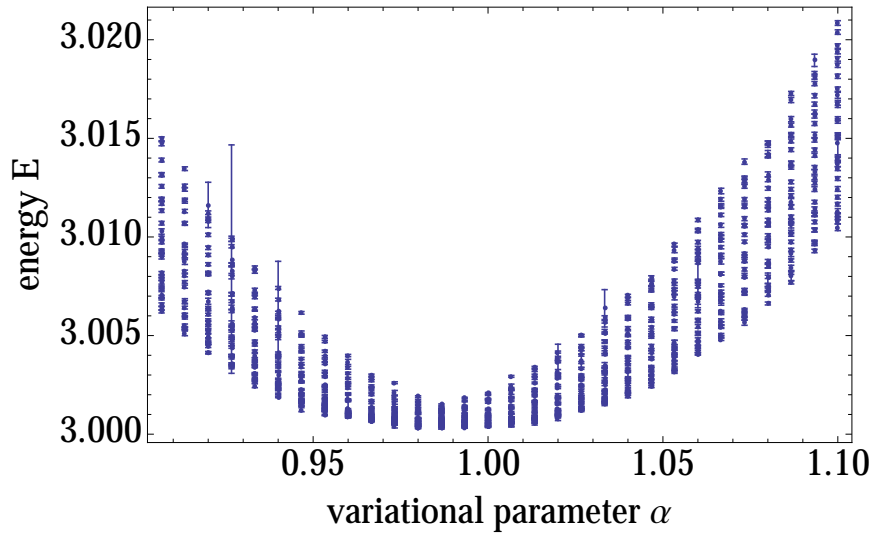
$$\beta = 0.4033. \quad (33)$$

As mentioned before we were expecting the energy to be at  $E = 3$  a.u., so the calculated value matches the expected one very well. In figure 3 there are some areas, where the plane is not as smooth as in others. We classify these small perturbations to the valley as numerical fluctuations and consider them to be strongly important.

To get a better understanding of the influence the parameters have on the calculated energy, figure 4 shows the energy's  $\alpha$ -dependency for different  $\beta$ . Consistent with figure 3 this figure reveals, that  $\beta$  is shifted depending on  $\alpha$  and that  $\alpha$  has a larger influence on the energy than the other variational parameter. The errors plotted in figure 4 are almost invisible, since they are very small compared to the energy fluctuations at varying  $\alpha$  and  $\beta$ . There are not many cases, where the error is significantly high, so we consider our results to be of sufficient accuracy.



**Figure 3:** Plot of  $\alpha$ - and  $\beta$ -dependencies of the ground state energy for two interacting electrons at the ground state based on a simulation involving 3 000 000 Metropolis cycles



**Figure 4:** Plot of  $\alpha$ -dependency of the ground state energy for two interacting electrons at the ground state for different  $\beta$  based on a simulation involving 3 000 000 Metropolis cycles

#### 4.1.1 Jastrow factor

After computing the ground state energy we now analyse the change in energy arising from different oscillator potentials  $\omega$ . The results for  $\omega = \{1, 0.28, 0.01\}$  are shown in table 1. It can be observed, that for small oscillator frequency the kinetic energy drops relative to the total energy of the system. The reason for this is, that for small  $\omega$  the potential gets wider, but flatter as well. In this case, the electrons interact less with each other, which results in decreasing kinetic energy.

**Table 1:** Kinetic and potential energy depending on the oscillator frequency  $\omega$

$\omega$	$E_{kin}(\text{a.u.})$	$E_{pot}(\text{a.u.})$	$E_{kin}/E(\%)$	$E_{kin}/E(\%)$
1.00	0.8891	2.111	29.6	70.4
0.28	0.2616	0.774	25.3	74.7
0.01	0.0106	0.096	9.9	90.1

In the wave equation

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left[ -\alpha \frac{\omega}{2} (r_1^2 + r_2^2) \right] \exp \left[ \frac{a_{12} r_{12}}{(1 + \beta r_{12})} \right] \quad (34)$$

only the first exponential term is affected by the oscillator frequency  $\omega$ , while the Jastro factor does not contain the frequency.

For vanishing potential as for  $\omega = 0.01$  the wave function becomes:

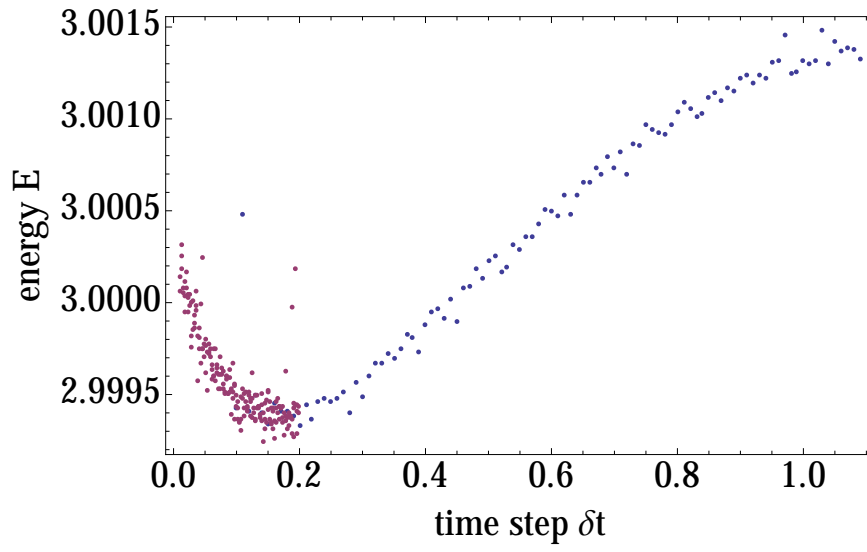
$$\lim_{\omega \rightarrow 0} \psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left[ \frac{a_{12} r_{12}}{(1 + \beta r_{12})} \right] = CJ, \quad (35)$$

where  $J$  is the Jastrow factor. This means, that in this case the Jastrow factor adopts a more important role. The correlations introduced by the Jastro factor ...

#### 4.1.2 Importance sampling: $\delta t$ -dependency

To obtain accurate results we also introduce importance sampling and optimize the calculation of the energy by studying its time step dependency. We will refer to the time step as  $\delta t$ . The time step plays an important role in importance sampling, since it the biasing when calculation new random numbers. For large  $\delta t$  the newly picked random numbers for the particle position can vary more, than for smaller  $\delta t$ . It is therefore relevant to use a reasonable time step to avoid jumping to far in the position or to get stuck in one place as explained previously in section 3.3.1. In figure 5 we plotted the energy calculated for  $\alpha = 0.98$  and  $\beta = 0.40$  (according to 4.1) for diverse  $\delta t$ . Comparing the results including importance sampling to those in section 4.1 we notice, that with importance sampling we can obtain a lot smaller energies, than when using a brute force Metropolis algorithm. This shows, that the importance sampling has an impact on the precision of the results, because we get energies very near the exact solution.

Concerning the optimal value of  $\delta t$ , it is obvious in figure 5, that it must be  $\delta t \in [0.1, 0.2]$ . Because of the statistical spread of the energy values, we cannot find the one and only perfect  $\delta t$ -value. For large time steps the energy converges to  $E = 3.0016$  ...



**Figure 5:** Results of energy calculation for varying time steps  $\delta t$  in the importance sampling. The blue dots refer to a wide-spaced simulation for  $\delta t \in [0.1, 1]$  with step length  $\Delta(\delta t) = 0.01$ , whereas the violet dots refer to  $\delta t \in [0.01, 0.2]$  with  $\Delta(\delta t) = 0.001$

## 4.2 Six electron case

### 4.2.1 Virial theorem

## 4.3 Analytical Calculations

## 5 Conclusion

## References

Press, W., Flannery, B., Teukolsky, S., and Vetterling, W. (1999). *Numerical Recipes in C++: The Art of Scientific Computing*. Cambridge University Press.