



Computational Physics: Project 3

Variational Monte Carlo project

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1 Introduction

Quantum computing today is an important research field, which requires qubits. Quantum dots as they are treated in this report are regarded as possible qubits. Furthermore, they might be agents for medical imaging and are therefore worth analysing. In this report we will consider systems of two and six electrons in a harmonic oscillator potential with and without electron-electron repulsion.

For solving the two dimensional quantum mechanical eigenvalue problem of the ground state energy we will use the Variational Monte Carlo method (VMC), proposing trial wavefunctions, that contain variational parameters, to calculate the energy. Optimization of these parameters will lead to a wave function, that represents the actual wave function including just small errors and that will give us the opportunity to compute the ground state energy of these systems.

The physical background is explained in section 2, where we focus first on the unperturbed case in order to move on the interacting particles. The VMC method as basis of our simulation is then treated in section 3.1. To obtain optimized results we will also introduce importance sampling to the simulation in 3.4. The calculations, especially those involving derivatives, will be done both numerically and analytically (see section 3.6 and 4.4 for analytical calculations).

Testing the simulation we first place emphasis on the case of two electrons in section 4.1 and then move on to six electrons 4.2, where the virial-theorem is verified as well. The computed energies are compared to those found by Høgberget (2013).

Finally the outcome is shortly presented in section 5.

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 2π , c is the speed of light, e is the elementary charge and m_e is the electron mass. The unit of energy than becomes atomic units, denoted as a.u. For reasons of simplicity we will not write the units explicitly in the report, so please note, that all energies are in a.u., as well as all distances and frequencies. The unit of the variational parameters α und β , that will be introduced later, are inverse 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 as quantum dots. In order to study such system, 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 than 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, ω 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 $r_{ij} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$.

2.1 Unperturbed wave functions

First we will take a good at the simpler case of unperturbed particles, not intercating with each other. A case, that is also called a pure harmonic oscillator, because there are no other potential terms in the Hamiltonian, than the oscillator's potential.

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 repell 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:

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

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. This lead to an overall spin of zero. Despite this they are indistinguishable, which means both states are possible.

Regarding the wave function we will now simplificate it by a separational ansatz:

$$\psi(\mathbf{r}_1, \sigma_1, \mathbf{r}_2, \sigma_2) = \phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2), \quad (9)$$

which is also known as the Hartree product. Considering fermions, this is not an appropriate way to represent the wave function, because it does not obey the Pauli exclusion principle, which yields to antisymmetric wave functions. To solve this problem, we can use a linear combination of such wave functions $\phi_{1,2}$:

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} (\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) - \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_1)), \quad (10)$$

This can also be displayed as a determinant:

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_1(\mathbf{r}_2) \\ \phi_2(\mathbf{r}_1) & \phi_2(\mathbf{r}_2) \end{vmatrix} \quad (11)$$

Since we are going to analyse systems of up to six electrons as well, we will generalize this method introducing the Slater determinant \mathbf{S} for N electrons:

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} |\mathbf{S}| = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \dots & \phi_1(r_N) \\ \phi_2(r_1) & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \phi_N(r_1) & \dots & \dots & \phi_N(r_N) \end{vmatrix} \quad (12)$$

For the calculation, it is convenient to reexpress the Slater determinant in terms of 3×3 -determinants according to Cramer's rule:

$$\begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \dots & \phi_1(r_6) \\ \phi_2(r_1) & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \phi_6(r_1) & \dots & \dots & \phi_6(r_6) \end{vmatrix} \propto \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \phi_1(r_3) \\ \phi_3(r_1) & \phi_3(r_2) & \phi_3(r_3) \\ \phi_5(r_1) & \phi_5(r_2) & \phi_5(r_3) \end{vmatrix} \cdot \begin{vmatrix} \phi_2(r_4) & \phi_2(r_5) & \phi_2(r_6) \\ \phi_4(r_4) & \phi_4(r_5) & \phi_4(r_6) \\ \phi_6(r_4) & \phi_6(r_5) & \phi_6(r_6) \end{vmatrix} \quad (13)$$

and to compute their determinants afterwards. What we then get is:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_6) = |\mathbf{S} \uparrow \uparrow \mathbf{S} \downarrow \downarrow|. \quad (14)$$

The arrows indicate whether we are looking at spin-up or spin-down particles. We are free to choose which three particles should have spin up and which have spin down. The important thing is, that the overall spin is zero and that two electrons fill up the lowest energy state at $E = 1\omega$ (with spin zero) and the other four electrons fill up the second lowest energy state at $E = 2\omega$ again with overall spin zero. For six electrons in a pure harmonic oscillator the ground state energy should be at

$$E = 2 \cdot 1\omega + 4 \cdot 2\omega = 10\omega. \quad (15)$$

2.2 Perturbed wave functions

Furthermore, we are interested at interactions between the electrons: Because of their charge there is a repulsive force between the electrons represented by \hat{H}_1 in the Hamiltonian. This must also be considered in the wave function and makes it not analytically solvable. Further explanation on this will be given in 3.1.

3 The method

Solving quantum mechanical eigenvalue problems can be a hard task, especially when it involves particle interaction and when the number of particles increases. This is why we introduce the Variational Monte Carlo Method for estimating the energy and the wave function of the electron states. Using this method we will be able to consider different oscillator potentials and varying numbers of particles.

The repository to the program can be found under <https://github.com/Canadanja/Project-3.git>.

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:

$$\varphi_0 = \sum_{\lambda=0}^{\infty} c_{0\lambda} \psi_{\lambda}, \quad (16)$$

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

In quantum mechanics the energy is the expectation value

$$E = \frac{\langle \psi_0 | \hat{H} | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle}. \quad (17)$$

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

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

$$= \frac{\sum_{\alpha,\beta} c_{0\alpha}^* c_{0\beta} \int d\tau \psi_{\alpha}^*(\tau) \hat{H} \psi_{\beta}(\tau)}{\sum_{\alpha,\beta} c_{0\alpha}^* c_{0\beta} \int d\tau \psi_{\alpha}^*(\tau) \psi_{\beta}(\tau)} \quad (19)$$

$$= \frac{\sum_{\alpha} E_{\alpha} |c_{0\alpha}|^2}{\sum_{\alpha} |c_{0\alpha}|^2}, \quad (20)$$

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 φ_0 is not the eigenfunction ψ_0 we get an energy

$$E_0 \leq \frac{\langle \varphi_0 | \hat{H} | \varphi_0 \rangle}{\langle \varphi_0 | \varphi_0 \rangle}. \quad (21)$$

- If the expansion φ_0 corresponds exactly to the eigenfunction ψ_0 we get the exact energy

$$E_0 = \frac{\langle \varphi_0 | \hat{H} | \varphi_0 \rangle}{\langle \varphi_0 | \varphi_0 \rangle}. \quad (22)$$

In the second case the variance of the energy

$$\text{var}(E) = \langle H^2 \rangle - \langle H \rangle^2 = 0. \quad (23)$$

As expansion wave function φ_0 we use a trial wave function we will call $\psi_T(\mathbf{r}_1, \mathbf{r}_2, \alpha, \beta)$, with α and β being the variational parameters. In this report the trial wave function for two interacting electrons has the form:

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \alpha, \beta) = C \exp \left[-\alpha \frac{\omega}{2} (r_1^2 + r_2^2) \right] \exp \left[\frac{a_{12} r_{12}}{(1 + \beta r_{12})} \right] \quad (24)$$

with

$$a_{12} = \begin{cases} 1, & \text{for } \uparrow\downarrow \\ 1/3, & \text{for } \uparrow\uparrow, \downarrow\downarrow \end{cases} \quad (25)$$

and

$$r_{12} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}. \quad (26)$$

The factor $J = \exp\left[\frac{a_{12}r_{12}}{(1+\beta r_{12})}\right]$ is called the Jastrow factor. It introduces the repulsion terms between the particles. For the unperturbed wave function it becomes 1. In section 4.1.1 we will have a close look at the correlations introduced by this factor.

Corresponding to the wave function and the variational parameter α we can then define the local energy

$$E(\mathbf{r}_1, \mathbf{r}_2, \alpha, \beta) = \frac{1}{\psi_T} \hat{\mathbf{H}} \psi_T. \quad (27)$$

Inserting the Hamiltonian in the local energy calculation we get

$$E(\mathbf{r}_1, \mathbf{r}_2, \alpha, \beta) = \frac{1}{\psi_T} \left(-\frac{\hbar^2}{2m} \sum_{i=1}^2 \nabla_i^2 \right) \frac{1}{\psi_T} + V_1(\mathbf{r}_1) + V_2(\mathbf{r}_2) + V_{interaction}(|\mathbf{r}_1 - \mathbf{r}_2|), \quad (28)$$

with the harmonic oscillator potentials V_1 and V_2 .

This means, that we need the second derivative of the trial wavefunction. There are different ways to calculate this quantity. First we will approximate it by numerical brute force derivation

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}, \quad (29)$$

where $f(x)$ is a function evaluated at x and h is the step length for the derivation. This calculation is a very timeconsuming part of our computation. That is why later, in section 3.6 and 4.4, we will consider the analytical expressions of the derivative.

In order to find the wave function and its corresponding energy, 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.

3.1.1 Many-body problems

Furthermore we are going to focus on a many-body problem by considering up to six electrons. In this case, the wave function can be written as in section 2.1

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_6) = |\mathbf{S} \uparrow(\alpha)||\mathbf{S} \downarrow(\alpha)| \prod_{i < j}^6 J(\beta). \quad (30)$$

Sure we want to calculate the local energy for six electron as well. For this purpose, we will generalize equation 28 as following for 6 electrons:

$$E(\mathbf{R}, \alpha, \beta) = \frac{1}{\psi_T} \left(-\frac{\hbar^2}{2m} \sum_{i=1}^6 \nabla_i^2 \right) \frac{1}{\psi_T} + \sum_{i=1}^6 V_{oneparticle}(r_i) + \sum_{i < j}^6 V_{interaction}(|r_i - r_j|) \quad (31)$$

In this case, we refer to the particles positions as $(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, \mathbf{r}_5, \mathbf{r}_6) = \mathbf{R}$.

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 `ran1` and `ran2` and are provided by the lib-package of the computational physics course.

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 loose the overview of the function we are evaluating.
- Jumping to numbers far away from the initial value, where the distribution is negligible, for example to r_k in figure 1.

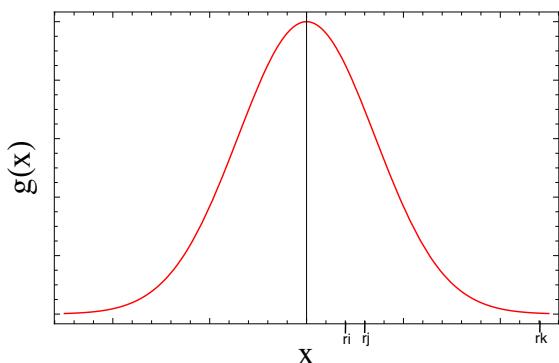


Figure 1: Gaussian distribution showing problems in selection of random states

Preventing the simulation in creating biased averages and imprecise 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.

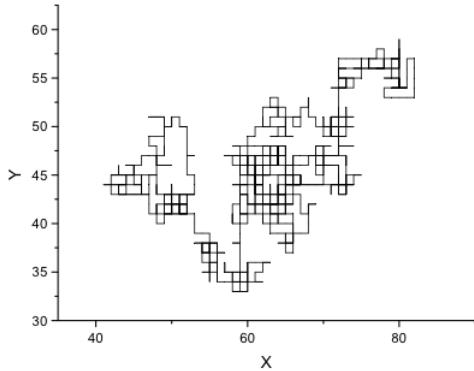


Figure 2: Brownian random walk of 100 steps in x - y -plane and step length 1

In this report we have implemented the Metropolis test as following:

```
// ----- metropolis test ----- //
if (ran2(&idum) <= wfnew*wfnew/wfold/wfold){
    for (j = 0; j < dimension; j++){
        r_old(i,j) = r_new(i,j);
    }
    wfold = wfnew;
    accept = accept + 1;
}
}
```

where `wfnew` and `wfold` are the wave functions $\psi(r_{old})$ and $\psi(r_{new})$ and `ran2()` generates random numbers.

This means, that we test whether the random number is smaller, than the squared wave function at the new position divided by the squared wave function at the old position:

$$\text{ran2}(\&idum) \leq q(r_{old}, r_{new}) = \frac{|\psi_T(r_{new})|^2}{|\psi_T(r_{old})|^2} \quad (32)$$

3.4 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 and explained by Hjorth-Jensen (2014, p.486ff.).

The 'old' and 'new' positions in space can be calculated by

$$r_{old} = \eta \quad (33)$$

$$r_{new} = r_{old} + \eta + \delta t D F_{old}, \quad (34)$$

where η denotes a gaussian distributed random variable, δt 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 η 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 probability of moving would be the same for all directions. The quantum force is

$$\mathbf{F} = 2 \frac{1}{\psi_T} \nabla \psi_T \quad (35)$$

$$= 2 \left[|\mathbf{S} \uparrow(\alpha)| |\mathbf{S} \downarrow(\alpha)| \prod_{i < j}^N J(\beta) \right]^{-1} \nabla \left(|\mathbf{S} \uparrow(\alpha)| |\mathbf{S} \downarrow(\alpha)| \prod_{i < j}^N J(\beta) \right). \quad (36)$$

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

$$q(r_{old}, r_{new}) = \frac{|\psi_T(r_{new})|^2}{|\psi_T(r_{old})|^2} \quad (37)$$

by

$$q(r_{old}, r_{new}) = \frac{G(r_{old}, r_{new}, \delta t) |\psi_T(r_{new})|^2}{G(r_{new}, r_{old}, \delta t) |\psi_T(r_{old})|^2}, \quad (38)$$

where the quantity G refers to the Greensfunction

$$G(y, x, \delta t) = \frac{1}{(4\pi D \delta t)^{3N/2}} \exp \left[-(y - x - D \delta t F(x))^2 \frac{1}{4D \delta t} \right] \quad (39)$$

In the source code this looks like:

```
// ----- metropolis test ----- //  
if (ran2(&idum) <= greensfunction*wfnew*wfnew/wfold/wfold){  
    for (j = 0; j < dimension; j++){  
        r_old(i,j) = r_new(i,j);  
        qforce_old(i,j) = qforce_new(i,j);  
    }  
    wfold = wfnew;  
    accept = accept + 1;  
}  
}
```

Compared to the source code in section 3.3 we have just added two things: the additional `greensfunction` and the line, where we set `qforce.old` to be `qforce.new`. This is equivalent to what happens in equation 38, just that `Greensfunction` is the ratio of the Greensfunctions $G(r_{old}, r_{new}, \delta t)$ and $G(r_{new}, r_{old}, \delta t)$.

3.5 Parallelization

The code is parallelized with shared memory and realized through OpenMP. Every core goes thereby through the whole Monte-Carlo simulation and at the end the mean of the energies are taken.

3.6 Closed form solutions

The quantum force (eq. 35) and the kinetic energy part in equation 28 are until now calculated by a brute force derivation. A disadvantage of this method is, that the wavefunction has to be evaluated multiple times at different positions $r + h$, $r - h$ respectively. In order to optimize this step one can implement

the analytical expressions. These are derived for example in Høgberget (2013). The quantum force can thereby be expressed by

$$\mathbf{F}_i = 2 \left(\frac{\nabla_i |\mathbf{S} \uparrow|}{|\mathbf{S} \uparrow|} + \frac{\nabla_i J}{J} \right). \quad (40)$$

The first part of the right side denotes the gradient of the Slater determinant, the second one the gradient of the Jastrow factor. It has to be payed attention that this is the expression for only one particle with index i moved with spin up. Considering a spin down particle the $|\mathbf{S} \uparrow|$ becomes $|\mathbf{S} \downarrow|$. Further the kinetic part of the local energy arises as a result of

$$\frac{\nabla_i^2 \psi_T}{\psi_T} = \frac{\nabla_i^2 |\mathbf{S} \uparrow|}{|\mathbf{S} \uparrow|} + \frac{\nabla_i^2 J}{J} + 2 \left(\frac{\nabla_i |\mathbf{S} \uparrow|}{|\mathbf{S} \uparrow|} \cdot \frac{\nabla_i J}{J} \right), \quad (41)$$

again assuming a spin up particle.

The missing expressions can be obtained by deriving the trial wavefunction 30. This is also done in Høgberget (2013) and reveals

$$\frac{\nabla_i J}{J} = \sum_{k \neq i=1}^N \frac{a_{ik}}{r_{ik}} \frac{\mathbf{r}_i - \mathbf{r}_k}{(1 + \beta r_{ik})^2} \quad (42)$$

for the gradient and

$$\frac{\nabla_i^2 J}{J} = \left| \frac{\nabla_i J}{J} \right| - \sum_{k \neq i=1}^N a_{ik} \frac{\beta r_{ik} - 1}{r_{ik} (1 + \beta r_{ik})^3} \quad (43)$$

for the Laplacian of the Jastrow-factor. The derivations of the Slater determinants can be calculated to

$$\frac{\nabla_i |\mathbf{S}|}{|\mathbf{S}|} = \sum_k (\nabla_i \phi_k(\mathbf{r}_i)) (\mathbf{S}_{ki}^{-1}) \quad (44)$$

for the gradient and

$$\frac{\nabla_i^2 |\mathbf{S}|}{|\mathbf{S}|} = \sum_k^{N/2} (\nabla_i^2 \phi_k(\mathbf{r}_i)) (\mathbf{S}_{ki}^{-1}) \quad (45)$$

for the Laplacian. For the first part on the right side of eqs. 44 and 45 exists analytical expressions which can be determined by applying the operands on the single particle equation 3. These can also be found in tabulated form in Høgberget (2013, app. D). The last term \mathbf{S}_{ki}^{-1} is the transpose of the inverse Slater matrix.

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 perform a Variational Monte Carlo simulation and use the Metropolis algorithm explained in section 3.3 to find the energy of the ground state. Therefor we use numerical derivation. We will later introduce analytical calculations based on closed-form expressions as well (section 4.4). Besides, we put emphasis on the correlations introduced by the Jastrow 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 δt .

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 Lohne et al. (2011) the corresponding energy is at $E = 3$ a.u. (atomic units). For the computation we use the variational wave function

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left[-\alpha \frac{\omega}{2} (r_1^2 + r_2^2) \right] \exp \left[\frac{a_{12} r_{12}}{(1 + \beta r_{12})} \right], \quad (46)$$

where we start by considering a wide range of $\alpha \in [0.7, 1.3]$ and $\beta \in [0.2, 0.6]$ first and perform a more precise simulation afterwards. The goal is to find the variational parameters α and β , 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 α and β . The 3D-plot results in a bended plane resembling to the shape of a valley. For increasing α the corresponding β at minimal energy is decreasing. The minimum energy calculated is

$$E = 3.0003 \quad (47)$$

at

$$\alpha = 0.9867, \quad (48)$$

$$\beta = 0.4033 \quad (49)$$

and at a mean distance of

$$r_{12} = 1.607 \quad (50)$$

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 α -dependency for different β . Consistent with figure 3 this figure reveals, that β is shifted depending on α and that α 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 α and β . In figure 5 we also show the energy minimum dependent on β . In this plot, the errors seem to be larger, but in order to find the minimum, we had to look at a very small energy scale. Overall there are not many cases, where the error is significantly high, so we consider our results to be of sufficient accuracy.

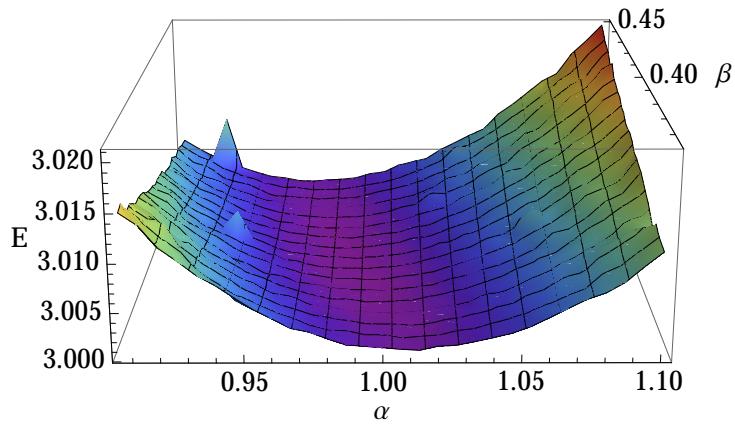


Figure 3: Plot of α - and β -dependencies of the ground state energy for two interacting electrons at the ground state based on a simulation involving 12 000 000 Metropolis cycles

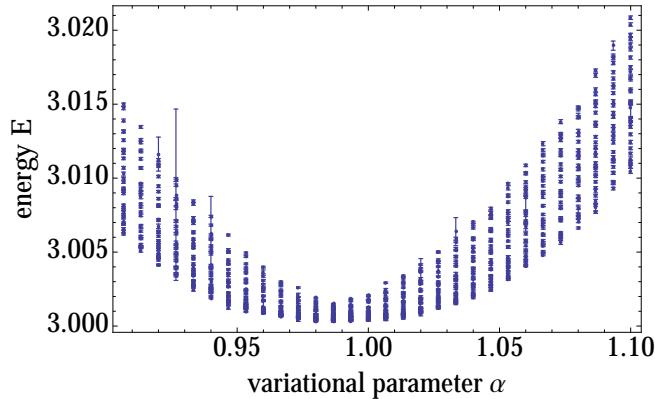


Figure 4: Plot of α -dependency of the ground state energy for two interacting electrons at the ground state for different β based on a simulation involving 12 000 000 Metropolis cycles

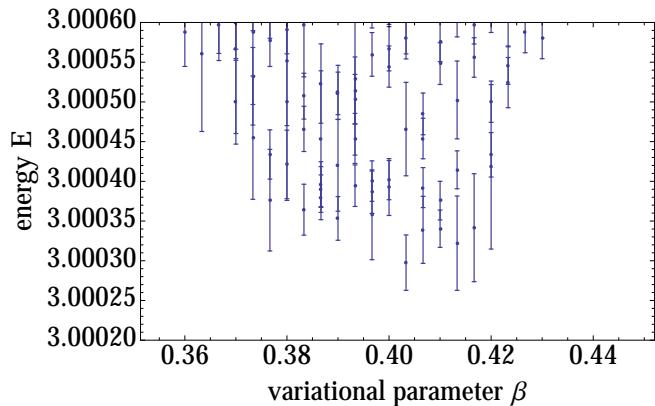


Figure 5: Plot of β -dependency of the ground state energy for two interacting electrons at the ground state for different α based on a simulation involving 12 000 000 Metropolis cycles

4.1.1 Jastrow factor

After computing the ground state energy we now analyse the change in energy arising from different oscillator potentials ω . The corresponding 3D-plots with the α - β -dependency of the energy can be found in A. The results for $\omega = \{1.00, 0.70, 0.50, 0.28, 0.01\}$ 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 ω the potential gets wider, but flatter as well. In this case, the electrons interact less with each other, because they are further apart. As a result, kinetic energy drops.

Table 1: Kinetic and potential energy depending on the oscillator frequency ω

ω	E_{kin}	E_{pot}	$E_{kin}(\%)$	E_{total}	$E(H\ddot{o}gberget, 2013)$
0.01	0.010	0.064	14	0.074	0.074
0.28	0.248	0.773	24	1.021	1.022
0.50	0.452	1.206	27	1.658	1.660
0.70	0.607	1.600	28	2.207	-
1.00	0.862	2.137	29	3.0003	3.0003

In the wave equation

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left[-\alpha \frac{\omega}{2} (r_1^2 + r_2^2) \right] \exp \left[\frac{a_{12} r_{12}}{(1 + \beta r_{12})} \right] \quad (51)$$

only the first exponential term is affected by the oscillator frequency ω , while the Jastrow factor does not contain the frequency.

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

$$\lim_{\omega \rightarrow 0} \psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left[\frac{a_{12} r_{12}}{(1 + \beta r_{12})} \right] = C J, \quad (52)$$

where J is the Jastrow factor. This means, that in this case the Jastrow factor adopts a more important role. The interaction potential is then compared to the oscillator potential at a higher value.

4.1.2 Importance sampling: δt -dependency

To obtain accurate results we also introduce important sampling and optimize the calculation of the energy by studying its time step dependency. We will refer to the time step as δt . The time step plays an important role in importance sampling, since it is the biasing when calculating new random numbers. For large δt the newly picked random numbers for the particle position can vary more, than for smaller δt . 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 3.4. In figure 6 we plotted the energy calculated for $\alpha = 0.98$ and $\beta = 0.40$ (according to 4.1) for diverse δt . 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 δt , it is obvious in figure 6, 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 δt -value. For large time steps, that are still smaller than $\delta t = 4$ the energy converges to $E = 3.002$. For even higher time steps, the calculated energy increases strongly and precise simulations become impossible.

For further simulations we will vary the time step depending on the oscillator frequency as well, because of the potential spread for small frequencies. In this case, we have to choose the time step to get stable importance sampling with enough accepted steps. Otherwise we might end up in as described in section 3.4 at the boundaries of our distribution or in a small interval at a certain point, producing biased data.

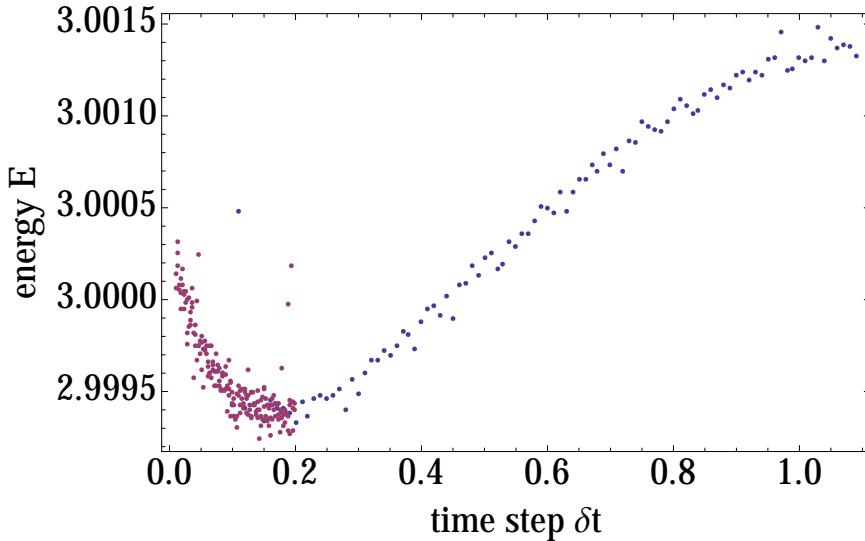


Figure 6: Results of energy calculation for varying time steps δt in the importance sampling. The blue dots refer to a wide-spaced simulation for $\delta t \in [0.1, 1]$ with step length $\Delta(\delta t) = 0.01$, whereas the violet dots refer to $\delta t \in [0.01, 0.2]$ with $\Delta(\delta t) = 0.001$

4.2 Six electron case

In this part we introduce the six electron case. In order to do so we consider the more general trial wave function 30 which also can be reduced to the case of two electrons. The simulations are done like in section 4.1 but with 400000 cycles, because of higher computation times. These are divided on 4 threads. For the time-step of the importance sampling (eq. 35) we use the value $\delta t = 0.5$, because our code showed the best stability with a high amount of accepted steps.

4.2.1 Perturbed Case

For the perturbed six electron system the ground state energies are shown in table 2. Comparing the energies with Høgberget (2013) or alternatively with Lohne et al. (2011) we have a good agreement for the values. For increasing ω we have higher values of α and β . Figure 7 shows the dependencies in this case. It can be seen that there is no easy linear coherence, instead we made an arbitrarily chosen fit with a square-root function which seemed for us the best approximation and deals as a reference where to search for the energy minima for different ω .

All in all our code seems to calculate reliable and good energies. Nevertheless we had to struggle with rather seldom but randomly appearing negative kinetic energies in single cores when using importance sampling. Changing our initial guesses for the starting positions increased here the quality of the solution considerably. In Appendix A are shown some three-dimensional plots which show the problem, which results in high peaks for the energy.

Table 2: Ground state energies for six electrons in an oscillator well.

ω	α	β	E	$E_{(H\ddot{o}gberget, 2013)}$
0.01	0.700	0.08	0.6986	-
0.28	0.800	0.25	7.7360	7.6216
0.50	0.925	0.38	11.8047	11.8103
1.00	0.980	0.45	20.1850	20.1902

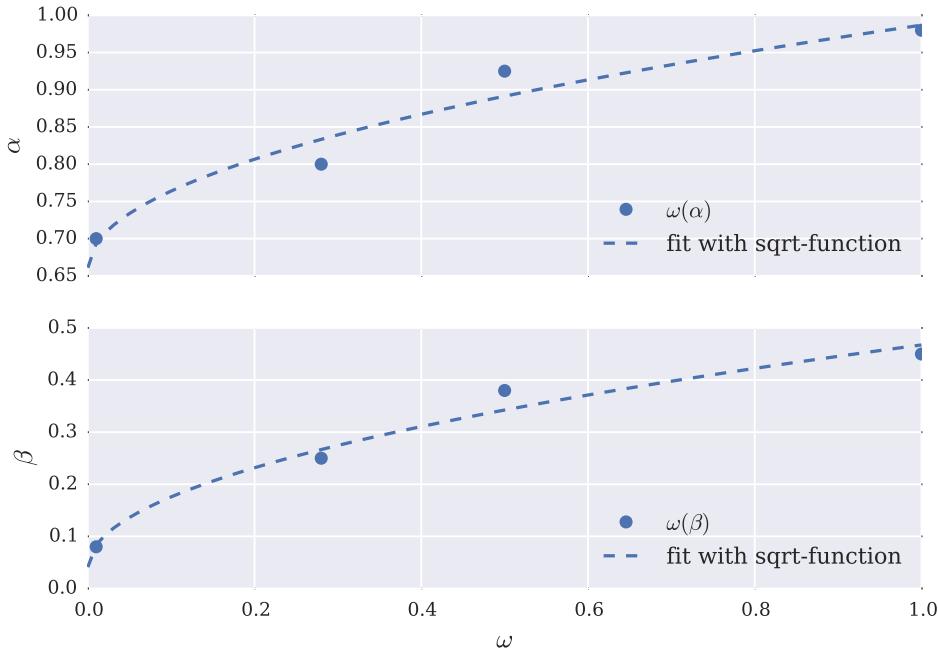


Figure 7: Shows the dependency between the locations of the energy minima and the variational parameter. The fit is arbitrary and just to have an orientation which values for α and β can be considered in order to reach the minimum.

4.2.2 Unperturbed Case

We know that with switched off electron-electron repulsion the lowest energy value should become 10ω , since we are observing six electrons. In figure 8 this relation is shown for different ω over α and it can be observed that our results fit very well to the theory.

4.3 Virial theorem

The virial theorem states a relationship between the mean of the potential $\langle V \rangle$ and of the kinetic energy $\langle T \rangle$ of a closed system. This is described by

$$\gamma \langle V \rangle = 2 \langle T \rangle, \quad (53)$$

with γ the homogeneity of the potential V . This means for a harmonic oscillator which potential goes with the power of 2 that one can expect the relationship $\langle V \rangle = \langle T \rangle$. However if we consider the perturbed wavefunction we have additional terms which are stated by the repulsion of the electron and would reveal $\gamma = -1$. Hence, we can make the prediction that the perturbed wavefunction should yield to a smaller ratio

$$\left(\frac{\langle V \rangle}{\langle T \rangle} \right)_{\text{perturbed}} \leq \left(\frac{\langle V \rangle}{\langle T \rangle} \right)_{\text{unperturbed}}, \quad (54)$$

whereas the difference should be larger for smaller ω , because thereby the oscillator potential becomes less relevant. Meanwhile for different ω and the unperturbed case the ratio should not change and be unity.

In figure 9 this behaviour is shown and mostly consistent. Considering first the two electron case we can observe for the unperturbed wavefunction a ratio that is nearly one for all omega. The perturbed part indeed shows the predicted behaviour that it is firstly smaller and secondly it increases with increasing omega. For the six electron system the perturbed functions have the same dependencies as for two

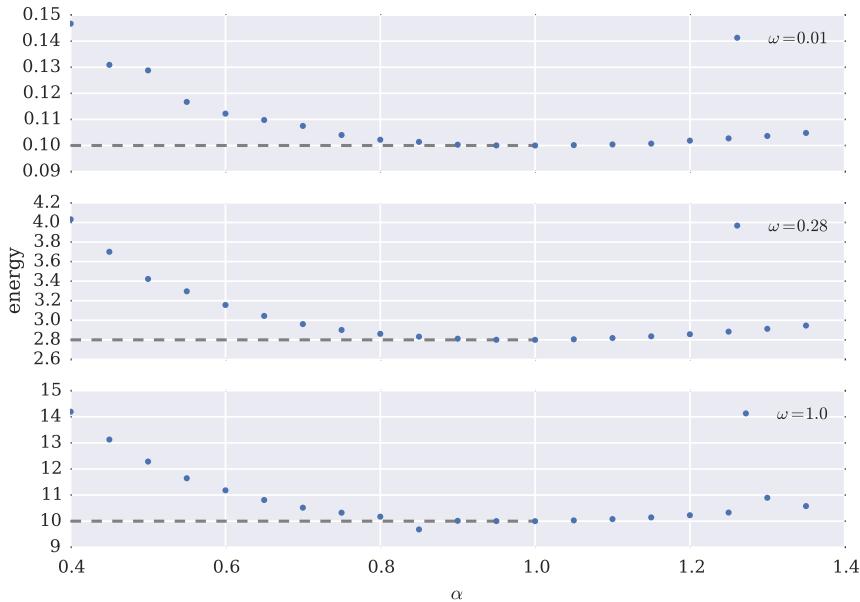


Figure 8: The figure shows the energy plotted over the variational parameter *alpha* assuming six electrons without the repulsive electron-electron forces. For different values of ω the minimum lies at 10ω which is coherent with the theoretical view.

electrons with even smaller ratios. This can be physically understood as a more important role for the electron-electron interactions in the six electron case which go with $\gamma = -1$. For the unperturbed part there is a small deviation to unity for larger omegas. This shouldn't be the case and reveals a potential problem in the code for multiple particles. Indeed the data shows that there might be an issue in the draft of the Slater matrix. However taking also in reference the known issues of section 4.2.1 it could also depend on the important sampling but still after extensive search we were not able to find a malfunction and all other calculations run reasonable which leads us to the conclusion that the energies that are produced by our code are reliable values.

4.4 Closed form solutions

Finally we still want to perform calculations with the closed form solutions described in section 3.6. For that reason the program was restructured in parts and new classes for the Jastrow-factor and the Slater-matrix including their derivations were introduced. This can be found at the separate branch `closed_form` at the provided git repository. The part is fully implemented but unfortunately we were not able to reproduce the solution of the brute force approximations. But still, because we implemented the full code, we are able to examine the time profiling. We thereby used no optimizations yet, like an improved calculation of the inverse slater matrix yet (see Høgberget (2013) for more details). An overview for the profiling is given in table 3. It was done by calculating 5 steps with 400000 cycles on 4 cores either for $N = 2$ or $N = 6$ electrons. The time is measured by the linux-command `time`.

Table 3: CPU-time comparison between closed-form and brute-force measurement

number of electrons	closed-form	brute-force
2	243.728 s	199.636 s
6	1448.431 s	4779.976 s

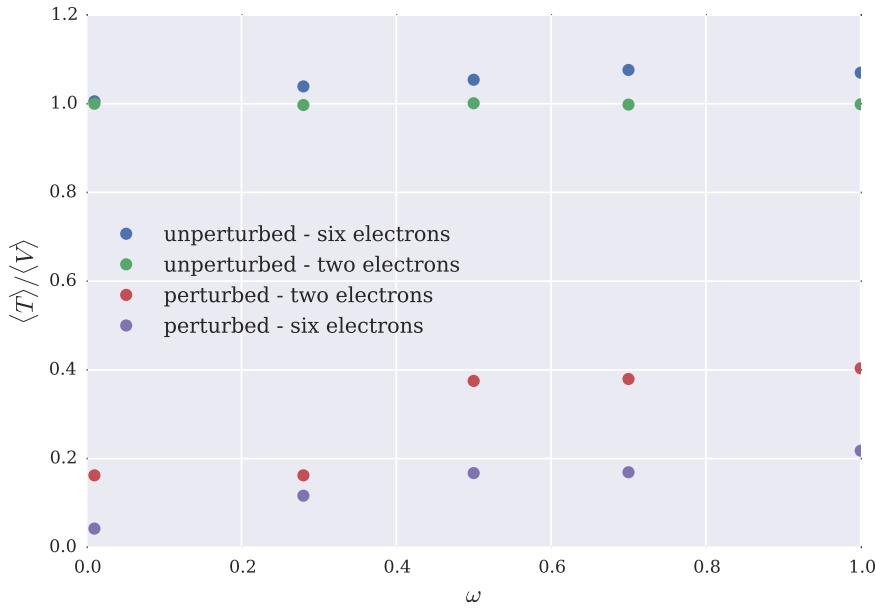


Figure 9: Shows the fraction of the mean kin. energy $\langle T \rangle$ to the mean pot. energy $\langle V \rangle$ for different values of ω . The calculations are done with either two or six electrons. The unperturbed functions are closed to unity the perturbed ones are much smaller. Additionally perturbed wavefunctions get a higher fraction for larger omega.

For two electrons it is apparent that the closed-form solution is not faster than the brute-force one. This is probably the case because the evaluation of the wavefunction for only two electrons takes not much time, whereas the calculation of the closed derived formulas inhibits many floating point operations. That the closed-form solution makes sense shows up clearly for six electrons. There the calculation is by a factor of approximately 3.3 faster, although elaborative calculations like the one of the inverse Slater matrix in the equations of section 3.6 are not stores and evaluated unnecessary often. Additionally further possible optimizations for the closed-form solution which are not possible in case of the brute force algorithm are not realized.

5 Conclusion

In this project, we have performed a Variational Monte Carlo simulation computing the energies of various electron systems.

In good accordance to Høgberget (2013) we have calculated the ground state energy of two electrons in a (harmonic oscillator) trap at $E = 3.0003$ as well as for diverse oscillator frequencies. Introducing importance sampling we have analysed the importance of the time step δt in the sampling noticing, that the simulation is stable for a range of $\delta t < 3$.

Moving on to six electrons it turned out, that the time step is responsible for the simulation stability. For inappropriate δt we experienced outliers in the energy calculation, that can be seen in figure 15 and 16. Overall the calculated energies correspond pretty well to those found by Høgberget (2013) and Lohne et al. (2011), which indicates that although those problems continue existing, we were able to extract suitable output from the simulation.

Another evidence, that the calculations are correct is given by the fact, that the virial-theorem is confirmed by our computations apart from small errors.

Furthermore, we were able to propose a relation of the variational parameters and the oscillator frequency in section 4.2.1.

In order to show the advantages of closed-form solutions towards brute-force derivations we compared the time profile. Here it showed off that especially for larger electron systems the closed-form can increase the velocity of the calculations considerably.

A 3D Plots

We will now show the energy's dependencies on the variational parameters α and β first for the case of two interacting electrons and then for the case of six interacting electrons in a harmonic oscillator potential.

A.1 Two electron perturbed case

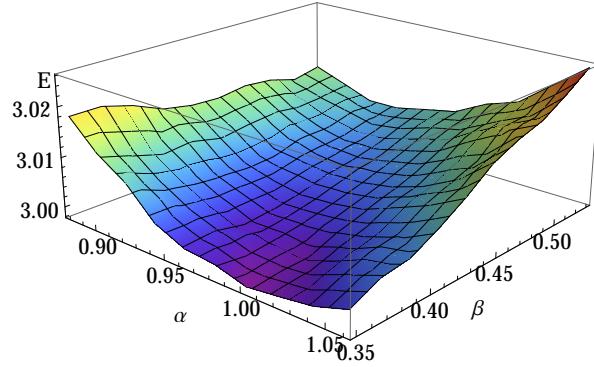


Figure 10: Plot of α - and β -dependencies of the ground state energy for two interacting electrons at the harmonic oscillator frequency $\omega = 1$

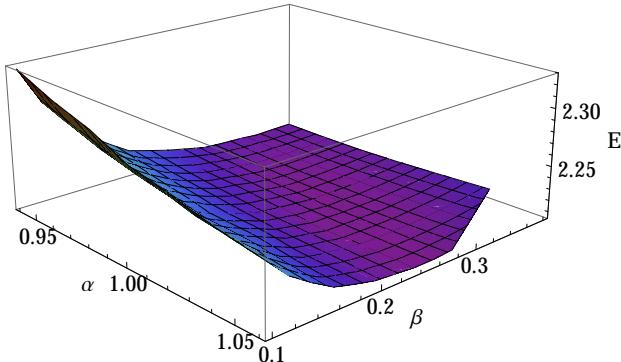


Figure 11: Plot of α - and β -dependencies of the ground state energy for two interacting electrons at the harmonic oscillator frequency $\omega = 0.7$

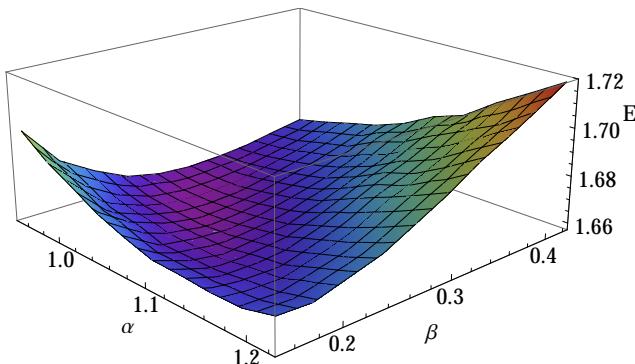


Figure 12: Plot of α - and β -dependencies of the ground state energy for two interacting electrons at the harmonic oscillator frequency $\omega = 0.5$

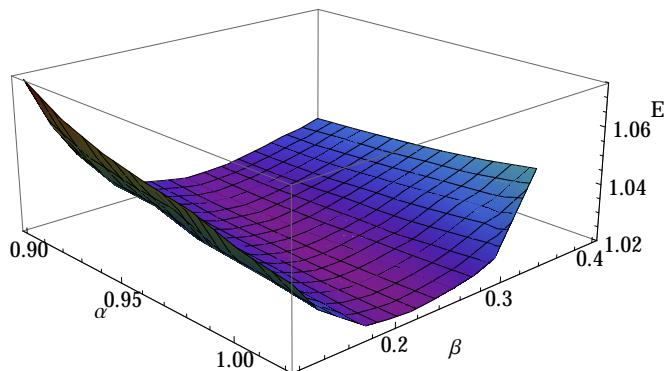


Figure 13: Plot of α - and β -dependencies of the ground state energy for two interacting electrons at the harmonic oscillator frequency $\omega = 0.28$

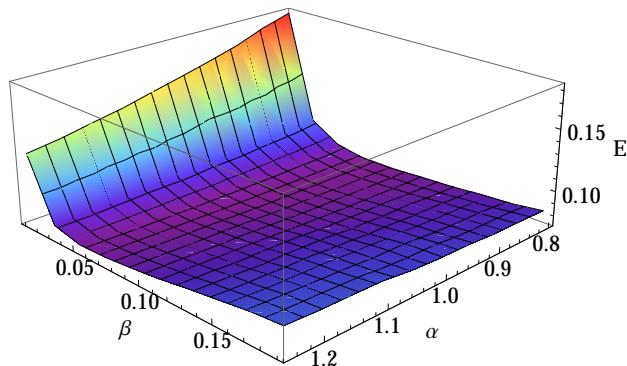


Figure 14: Plot of α - and β -dependencies of the ground state energy for two interacting electrons at the harmonic oscillator frequency $\omega = 0.01$

A.2 Six electron perturbed case

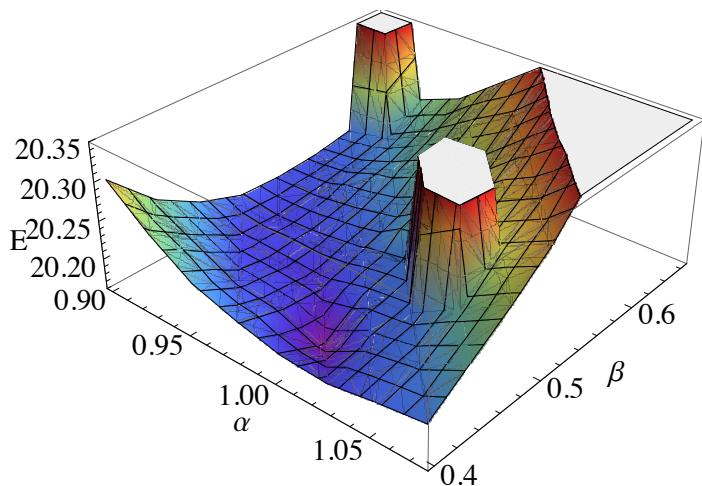


Figure 15: Plot of α - and β -dependencies of the ground state energy for six interacting electrons at the harmonic oscillator frequency $\omega = 1$

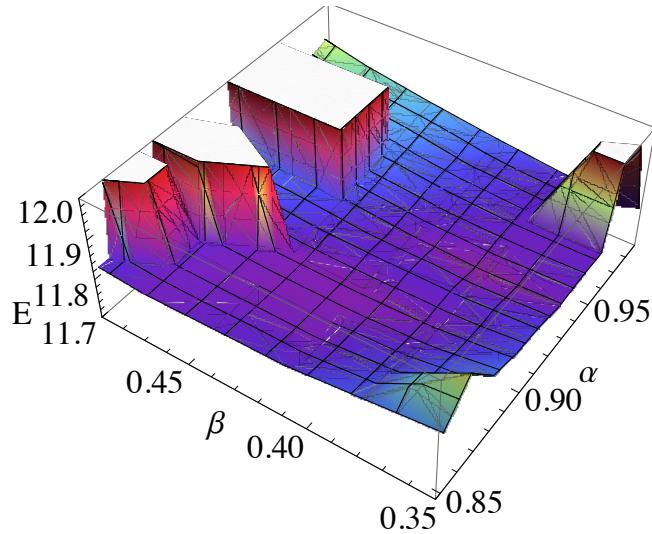


Figure 16: Plot of α - and β -dependencies of the ground state energy for six interacting electrons at the harmonic oscillator frequency $\omega = 0.5$

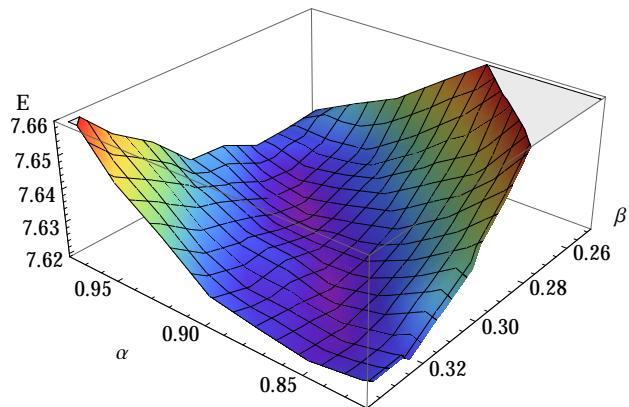


Figure 17: Plot of α - and β -dependencies of the ground state energy for six interacting electrons at the harmonic oscillator frequency $\omega = 0.28$

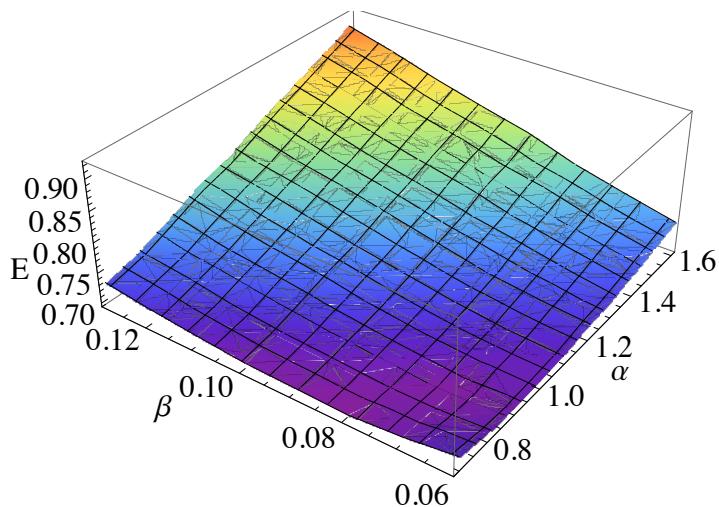


Figure 18: Plot of α - and β -dependencies of the ground state energy for six interacting electrons at the harmonic oscillator frequency $\omega = 0.01$

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