Project 2

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Abstract

Many theoretical physics systems involve the many-body Schrödinger equation (SE) and modelling a quantum dot is one of them. The problem with the many-body SE is that it is very hard or impossible to solve it analytically. Therefore, numerical solution are necessary to gain insight into the behaviour of many-body systems of particles. In this particular project I am working with quantum Variational Monte Carlo (VMC) methods to solve the many-body SE for fermions in an harmonic oscillator trap, which here represents the quantum dot. I am looking at full-shell systems of two, six and twelve fermions in harmonic oscillator traps of different strengths, i.e. trap frequencies, and investigating the different systems by comparing expectation energies and one-body densities. Additionally, I look at how these properties change by introducing interaction between the particles with a Jastrow factor.

Contents

1 Introduction

The main objective of this project is to investigate the many-body problem of simulating a quantum dot. A quantum dot is basically electrons that are trapped in an electrical potential. In this project, the potential is modelled as a harmonic oscillator potential. This assumption is ... (maybe not accurate because ...), but it is an easy potential to start with and the potential can later be expanded and most of the code can be reused as it is. Furthermore, we use a trial wavefunction with one (two) fitting parameters for the case without (with) a Jastrow factor to represent the interaction between the particles. This trial wave function is not the exact wave function, hence the simulation can only approximate the exact values for the ground state energy.

The report starts out by introducing the system with the representative equations and analysis tools. Most of the numerical tools used in the programming in this project has already been described in detail in project 1 [1], but some additional things are explained or more thoroughly elaborated on in the theory and method part of this report.

Furthermore, the results and discussion part first analyses how different important parameters have been chosen, i.e. choise of evaluation of the double derivative, step size of sampling techniques and method and parameters of the optimization. In addition the expectation energies and the one-body densities of the systems involves are compared and evaluated. At last, an evaluation of code's efficiently

is made and some concluding remarks are stated.

2 Theory and method

In this project we investigate a fermionic system of $N = 2$, 6 and 12 electrons, where N is the number of particles. It is a so-called closed shell-system. The Hamiltonian used to model this system is

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

where

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

is the single particle part and

$$\hat{H}_1 = \sum_{i<j} \frac{1}{r_{ij}}, \tag{2}$$

represent the interaction potential between particles. The Hamiltonian is written in atomic units, which implies that $\hbar = 1, m = 1$, the unit of length is $a_0 = {}^{4\pi\epsilon_0\hbar^2}/_{m_e e^2}$ and the unit of energy is $E_h = {}^{\hbar^2}/_{m_e a_0^2}$. We also have $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$ and ω is the oscillator frequency. Later we will study the dependence of the system on the oscillator frequency.

2.1 Two particle system

The single particle wave function in two dimensions is

$$\phi_{n_x,n_y}(x, y) = AH_{n_x}(\sqrt{\omega}x)H_{n_y}(\sqrt{\omega}y) \exp\left(-\omega(x^2 + y^2)/2.\right. \tag{3}$$

where the functions $H_{n_x}(\sqrt{\omega}x)$ are Hermite polynomials, while A is a normalization constant. The relevant Hermite polynomials in this project are listed in Appendix D. ω is the trap frequency.

For the lowest-lying state, E_{00} (see Fig. 1), we have $n_x = n_y = 0$ and an energy $\epsilon_{n_x,n_y} = \omega(n_x + n_y + 1) = \omega$, the total energy of the lowest-lying state is hence 2ω because there is room for two electrons with opposite spins.

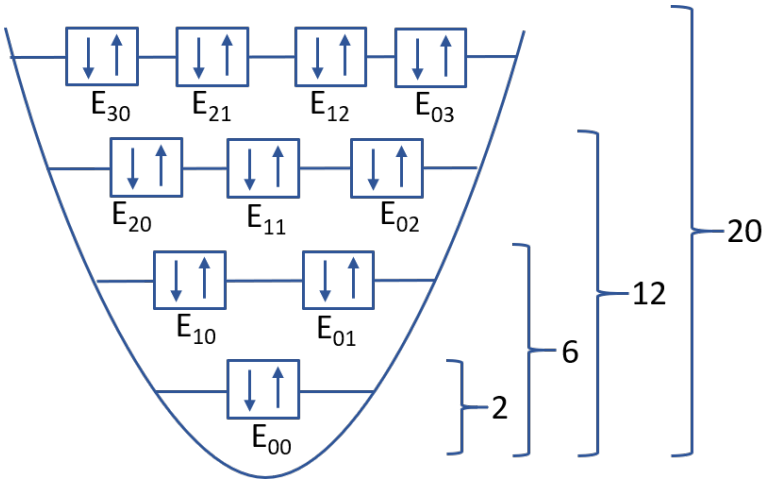

Figure 1: •

The expectation value can be found by solving the equation

$$\langle E \rangle = \frac{\int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \psi_T^*(\boldsymbol{r}_1, \boldsymbol{r}_2) \hat{H}(\boldsymbol{r}_1, \boldsymbol{r}_2) \psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2)}{\int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \psi_T^*(\boldsymbol{r}_1, \boldsymbol{r}_2) \psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2)}. \tag{4}$$

We will use Variational Monte Carlo (VMC) methods to evaluate the Eq. 4 [1]. The exact wave function for two not interacting electrons in the ground state is given by

$$\Phi(\boldsymbol{r}_1, \boldsymbol{r}_2) = C \exp\left(-\omega(r_1^2 + r_2^2)/2\right),$$

where $r_i = \sqrt{x_i^2 + y_i^2}$ and C is a normalization constant. The trial wavefunction we use for the not interacting case is

$$\Phi(\boldsymbol{r}_1, \boldsymbol{r}_2) = C \exp\left(-\alpha\omega(r_1^2 + r_2^2)/2\right). \tag{5}$$

with the parameter α. From the exact wave function we know that $\alpha = 1$ for the situation without interaction. On the other hand, for the interacting case, the trial wave function for the two-electron system is

$$\psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2) = C \exp\left(-\alpha\omega(r_1^2 + r_2^2)/2\right) \exp\left(\frac{a r_{12}}{(1 + \beta r_{12})}\right), \tag{6}$$

where we introduce another parameter, β, and a spin factor, a. a is 1 when the two electrons have anti-parallel spins and $1/3$ when they have the parallel spins (this is not relevant before we introduce more particles to the system, as can be seen from Fig. 1).

2.2 More particles

Since we are looking at closed shell systems, the next amount of particles are six. We can see this from Fig. 1, there are room for two electrons with opposite spin in two different states, in addition to the two in the lowest lying state. The trial wave function is now given by

$$\psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_6) = Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \ldots, \phi_6(\boldsymbol{r}_6)\right) \prod_{i<j}^{6} \exp\left(\frac{ar_{ij}}{(1+\beta r_{ij})}\right), \tag{7}$$

where

$$Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \ldots, \phi_6(\boldsymbol{r}_6)\right) = \begin{vmatrix} \phi_1(\boldsymbol{r}_1) & \phi_2(\boldsymbol{r}_1) & \cdots & \phi_6(\boldsymbol{r}_1) \\ \phi_1(\boldsymbol{r}_2) & \phi_2(\boldsymbol{r}_2) & \cdots & \phi_6(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{r}_6) & \phi_2(\boldsymbol{r}_6) & \cdots & \phi_6(\boldsymbol{r}_6) \end{vmatrix}$$

is the Slater determinant. This determinant occurs because electron are indistinguishable particles and they are antisymmetric ... . The functions, $\phi_i(\boldsymbol{r}_j)$, are given by Eq. 3 and the notation is explained in Tab. 1.

Table 1: The relation between the notation used in the determinant (left) compared to Eq. 3 (right).

ϕ_1	$\phi_{n_x=0,n_y=0}$	ϕ_7	$\phi_{n_x=2,n_y=0}$
ϕ_2	$\phi_{n_x=0,n_y=0}$	ϕ_8	$\phi_{n_x=2,n_y=0}$
ϕ_3	$\phi_{n_x=1,n_y=0}$	ϕ_9	$\phi_{n_x=1,n_y=1}$
ϕ_4	$\phi_{n_x=1,n_y=0}$	ϕ_{10}	$\phi_{n_x=1,n_y=1}$
ϕ_5	$\phi_{n_x=0,n_y=1}$	ϕ_{11}	$\phi_{n_x=0,n_y=2}$
ϕ_6	$\phi_{n_x=0,n_y=1}$	ϕ_{12}	$\phi_{n_x=0,n_y=2}$

Similarly if we include another "shell" in our system we get 12 particles and the trial wavefunction is

$$\psi_T(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_{12}) = Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \ldots, \phi_{12}(\boldsymbol{r}_{12})\right) \prod_{i<j}^{12} \exp\left(\frac{ar_{ij}}{(1+\beta r_{ij})}\right). \tag{8}$$

The determinant have the same structure as for six particles and the relation to the single-particle wave functions are shown in Tab. 1.

2.3 One-body density

The radial one-body density is a measure of the spacial distribution of the electrons with respect to the distance from the middle of the harmonic oscillator trap. To calculate the radial one-body density, we want to sample the position of the electrons. The distance from the origin to a set cut-off is separated into bins with a length Δr. For every Monte Carlo step, the distance between the electron's position and the origin is calculated, and the bin that corresponds to the current distance get a count. In the end, you have an array corresponding to the different bins with counts corresponding to how many times an electron was found to have that particular distance to the origin. This array is normalized by dividing by the number of Monte Carlo steps. However, to get the density, we have to divide the number in the bins with the area or volume the bin represents. Because we have two-dimensional

problem in this project and we calculate the radial one-body density, we divide bin i with the area $A = \pi(r_i + \Delta r)^2 - \pi r_i^2$ where r_i is distance from the origin to bin i. *normalized to the number of particles. Mention. Should happen automatically... Does not happen automatically for me, but I have notice that Even has the same scale on the y-axis.*[2]

2.4 Virial theorem

The virial theorem gives a relation between the time-average total kinetic energy, $\langle T \rangle$, and the time-average external potential energy, $\langle V_{ext} \rangle$, that is

$$2 \langle T \rangle = n \langle V_{ext} \rangle \tag{9}$$

where $V(r) = Br^n$. In our case when we do not include interaction $n = 2$ from the external potential term in Eq. 1, and therefore the average kinetic energy should be equal to the average potential energy. This can be used as a test to see if the simulations executed are correct.

2.5 Trap frequency

The trap frequency changes the external potential felt by the electrons. Figure 2 shows how a larger trap frequency, ω, results in a narrower external potential. In this narrow harmonic oscillator trap, the electrons are forced to be closer to each other. Later, we will investigate how ω affects the energy when the electrons are interacting with each other through the potential given in Eq. 2

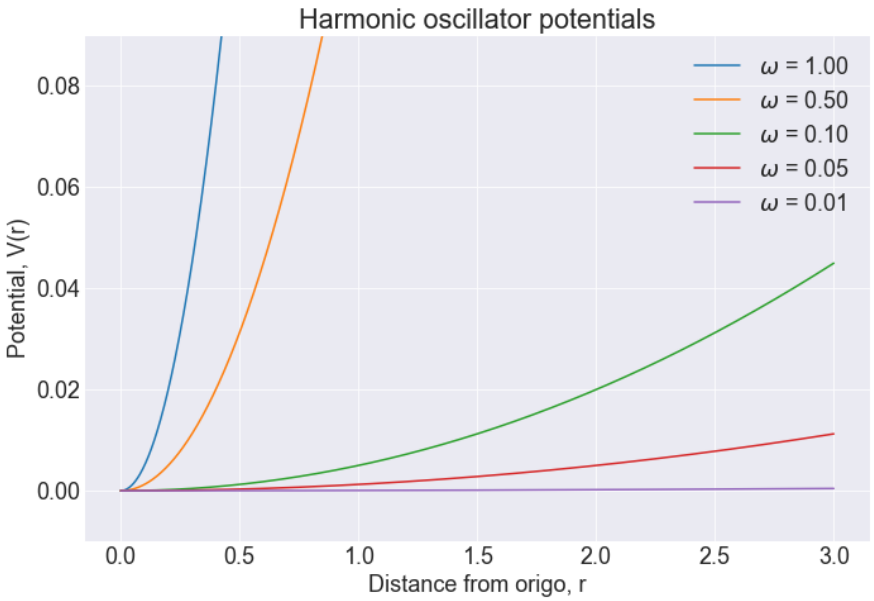

Figure 2: Illustration of how the potential changes when the trap frequency changes.

2.6 Evaluating the error

Standard error of the mean (SEM):

$$\text{SEM} = \frac{\sigma}{\sqrt{N}} \tag{10}$$

where N is the number of observations, in our case the number of Monte Carlo cycles.

2.7 The program

2.7.1 Initialization

2.7.2 Metropolis steps

2.7.3 Sampling

2.8 Improving performance and effiency

2.8.1 Vectorization

Solving as vectors instead of scalars - using more of memory - is sort of parallel.

2.8.2 Parallelizing

Doing operations in parallell instead of secquentially. In this case, we want more MC cycles in less time. I chose to parallellize with cmake. I am generating files that contain E_L. I get the same data if I run the same code (with different seeds for the random number generator) in 4 proseccors for MC cycles/4 or the same code for MC cycles in one proscessor. Embarrasing parallellization - very simple. Need different file name.

2.8.3 Reducing computational cost

Decrease floating point operations (flops) by smarter code and use of ratios.

3 Results and discussion

3.1 Two electrons in two dimensions

We start with the simple case of two electrons in a harmonic oscillator trap. These electrons do not interact with each other and the trial wavefunction is given by Eq. 5.

3.1.1 Brute force sampling

First, brute force sampling was used to calculate the new position and evaluate the metropolis ratio. The double derivative of the wavefunction, used to calculate the kinetic energy part of the expectation energy, was evaluated both analytically and numerically. Table 2 shows the energy for different values for the parameter α. The numbers show that the standard error of the mean (SEM) is underestimating the deviations. From Tab. 2 one can observe that including the correlations, i.e. mainly correlations between one state and the next where only one particle is moved, increases the deviation, giving us σ_b. This value is also an estimate of the error, but probably a more true estimate of the error.

From Tab. 2 one can also observe that $\alpha = 1.0$ gives zero standard deviation and is therefore the optimal parameter. By comparing the results for the analytical and the numerical cases one can observe that the SEM and σ_b is similar for both cases, especially around the ground state ($\alpha = 1.0$). If he expectation energies from the analytical case and the numerical cases are compared, they differ with values at the scale of 10^{-3}, which is reasonable with a σ_b around 10^{-3} to 10^{-2}. At last one can observe, both from the individual CPU time measurements and the mean CPU time of these 10

measurements (though with different αs), that the analytical solution of the double derivative is much faster and more efficient than the numerical case.

Table 2: Comparing the results for analytical/numerical evaluation of the double derivative. Here $\langle E_L \rangle$ is the expectation value for the energy given in atomic units (a.u.) and CPU time is in units of seconds. σ_B is the standard deviation after resampling with the blocking method and SEM is the standard deviation of the mean. Number of MC cycles are 2^{21}.

Analytical:					Numerical:				
α:	$\langle E_L \rangle$:	SEM:	σ_B:	CPU time:	α:	$\langle E_L \rangle$:	SEM:	σ_B:	CPU time:
0.50	2.49402	0.00073	0.01022	5.57812	0.50	2.49991	0.00073	0.01093	18.20310
0.60	2.26441	0.00052	0.00690	5.76562	0.60	2.26412	0.00053	0.00727	18.21880
0.70	2.13118	0.00035	0.00448	5.92188	0.70	2.13039	0.00036	0.00436	18.62500
0.80	2.05016	0.00022	0.00263	5.67188	0.80	2.04993	0.00022	0.00269	18.46880
0.90	2.01015	0.00010	0.00116	5.96875	0.90	2.01160	0.00010	0.00118	18.46880
1.00	2.00000	0.00000	0.00000	5.62500	1.00	2.00000	0.00000	0.00000	18.31250
1.10	2.00871	0.00009	0.00102	6.20312	1.10	2.00825	0.00009	0.00097	18.35940
1.20	2.03402	0.00018	0.00175	6.34375	1.20	2.03308	0.00018	0.00170	18.31250
1.30	2.07259	0.00026	0.00244	5.95312	1.30	2.06460	0.00026	0.00243	20.23440
1.40	2.11041	0.00034	0.00311	6.15625	1.40	2.11803	0.00033	0.00308	19.00000
Mean CPU time: 5.91875					Mean CPU time: 18.62033				

3.1.2 Including importance sampling

Figure 3 compare the expectation value of the energy and the acceptance rate of brute force sampling and importance sampling. It can be observed from the right part of the figure that the acceptance rate of both methods increase with decreasing step size, but one can also observe that the acceptance is lower for importance sampling than brute force sampling at large step sizes. These observations could indicate that a small step size would be ideal for both methods.

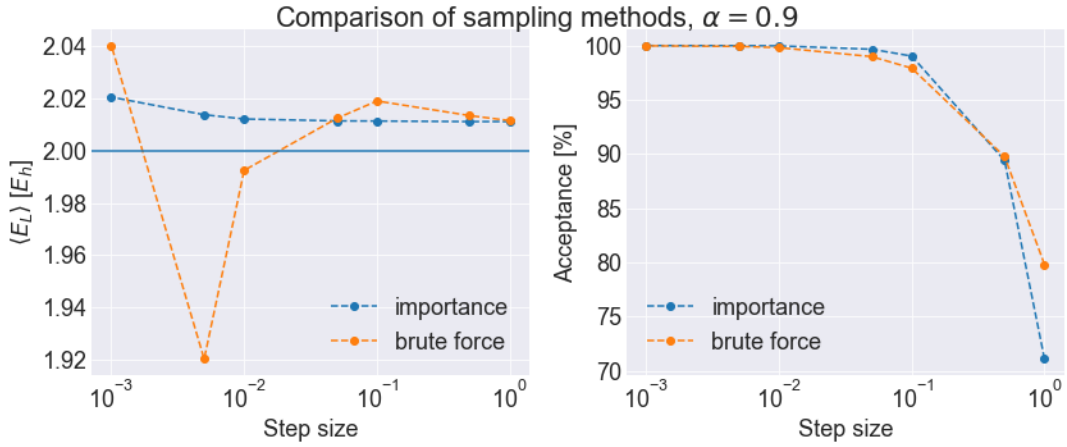

Figure 3: Left: Expectation energies after 2^{21} MC cycles for different step sizes. Right: Percentage of accepted steps for different step sizes. Here importance sampling and brute force sampling is compared.

From the left part of the figure it can be observed that one of the expectation values for the energies

are lower than the ground state energy ($dl = 0.005$ with brute force sampling) when these calculations where done with $\alpha = 0.9$. However, in Tab. 3 which compare the result of brute force sampling and importance sampling for different step sizes one can observe that the standard deviation from the blocking method is larger for the case of brute force sampling with a step size of 0.005. However, the SEM does not indicate anything to be special about this result.

Table 3: Comparing the results for importance/brute force sampling. Here the parameter α is set to 0.9 and number of MC cycles are 2^{21}. Acc. is short for acceptance and is here given in % and t_{CPU} is the CPU time used by the program in units of seconds. The rest of the values are as described in Tab. 2.

	Brute force:					Importance:				
dl:	$\langle E_L \rangle$:	SEM:	σ_B:	Acc.:	t_{CPU}:	$\langle E_L \rangle$:	SEM:	σ_B:	Acc.:	t_{CPU}:
1.000	2.010	0.00010	0.00066	79.832	6.625	2.011	0.00010	0.00022	71.078	8.531
0.500	2.011	0.00010	0.00112	89.794	7.266	2.011	0.00010	0.00023	89.343	8.672
0.100	2.015	0.00011	0.00549	97.919	7.078	2.011	0.00010	0.00047	99.049	8.859
0.050	2.007	0.00011	0.00946	99.001	7.016	2.011	0.00010	0.00068	99.662	8.188
0.010	2.002	0.00007	0.01510	99.788	6.953	2.007	0.00010	0.00136	99.968	8.281
0.005	1.942	0.00006	0.02140	99.916	6.578	2.010	0.00010	0.00199	99.989	8.547
0.001	2.118	0.00002	0.00371	99.974	6.531	2.007	0.00010	0.00410	99.999	8.016
	Mean CPU time: 6.86384					Mean CPU time: 8.44197				

I took a closer look at the actual local energies for the brute force sampling method. Figure 4 shows how the energy is not stable for steps sizes smaller than 0.01, so even though the step sizes 0.001 and 0.01 seems to give reasonable expectation values for the energy (see Tab. 3 and Fig. 3), Fig. 4 seems to show that that is sort of a lucky shot. I also saw this by running the calculation with brute force sampling and the step size, 0.005, with different seeds for the random number generator. The expectation energy for five different runs where $\langle E_L \rangle$ = 1.91487, 2.03452, 1.90805, 1.88356 and 1.9284. From Fig. 4 one can observe that even $dl = 0.1$ seems to be too small since it also results in the local energy varying slowly and taking longer "trips" to higher energies and using many steps to get back down again, but for this step size the "trips" to higher energies are more frequent than for the smaller step sizes. I concluded that a step size of 0.5 is the best choice for the brute force sampling because it gives reasonable changes of the local energy and an acceptance rate of $\sim$ 90 % (see Fig. 3).

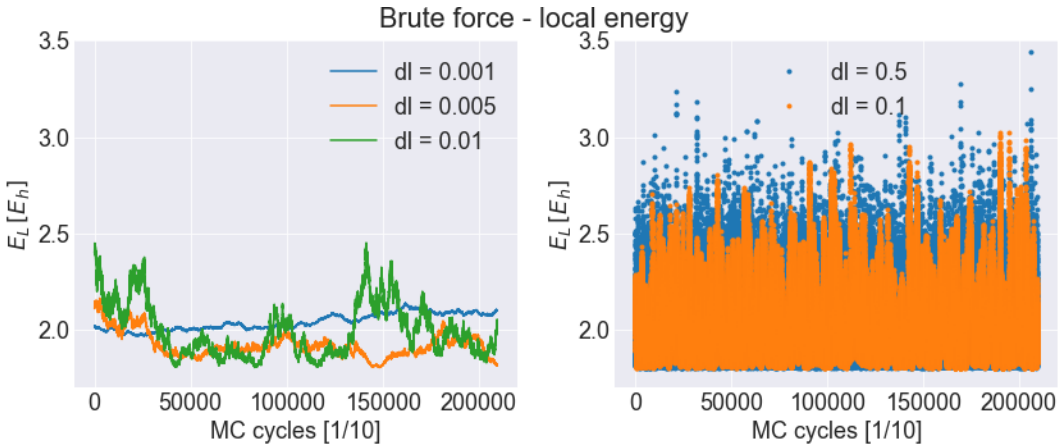

Figure 4: The local energy for every tenth MC cycle for brute force sampling at different step sizes, dl. a) shows the smaller step sizes and b) some that are a bit larger.

Proceeding to evaluate the energy, Table 4 shows how the energy changes with different trap frequencies, ω. From Tab. 4 one can observe that the mean distance is increasing with decreasing trap frequency. This is as expected from Fig. 2, where the potential is broadened with decreasing trap frequency ang hence is not forcing the particels closer together. The mean distance is a bit different for brute force sampling compared to importance sampling, but the similarity might imporve if more MC cycles are used. The other value show, however, no large difference between the results from brute force sampling and importance sampling. But to be able to compare the sampling methods more thoroughly it is better to look at the case where the system is not in the ground state.

Table 4: Ground state energy of two electrons in harmonic oscillator trap. Here $\overline{r}_{12}$ is the mean distance between the two electrons at positions $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ and $\langle E_L \rangle$, $\langle T \rangle$, $\langle V_{ext} \rangle$ and $\langle V_{int} \rangle$ are the expectation value of the local energy, kinetic energy, potential energy and interaction energy, respectively. The rest of the values are as explained in Tab. 2. Number of MC cycles are 2^{23}.

	Brute force:					Importance:				
ω	α	$\langle E_L \rangle$	$\overline{r}_{12}$	$\langle T \rangle$	$\langle V_{ext} \rangle$	α	$\langle E_L \rangle$	$\overline{r}_{12}$	$\langle T \rangle$	$\langle V_{ext} \rangle$
1.00	1	2.00	1.250	1.0008	0.9992	1	2.00	1.254	0.9982	1.0018
0.50	1	1.00	1.775	0.4971	0.5029	1	1.00	1.781	0.4973	0.5027
0.10	1	0.20	3.967	0.0996	0.1004	1	0.20	4.046	0.0987	0.1013
0.05	1	0.10	5.638	0.0497	0.0503	1	0.10	5.534	0.0512	0.0488
0.01	1	0.02	12.631	0.0099	0.0101	1	0.02	12.488	0.0101	0.0099

Table 5 shows the expectation value for the energy for various parameters, $alpha$. The calculated expectation values for the energy for the two different sampling methods are similar, especially close to the correct parameter α, varying only by $\pm 10^{-2}$. The SEM is here underestimating the error compared to σ_b from the blocking resampling technique for both sampling methods. However, what is different is that σ_b is larger for importance sampling than for brute force sampling. *Why is that? Is it just estimating the error more correctly (but the blocking code is the same), or is there a larger error resulting from importance sampling?*. At last, one can observe that the CPU time of the the importance sampling method is larger than brute force sampling which is expected because of the

calculation of the gradient and the quantum force. But we know from Fig. 3 that the acceptance rate of brute force sampling is around 90 % compared to importance sampling which should be close to 100 % and this makes the importance sampling technique more effective in terms of MC cycles.

Table 5: Comparing the results for brute force sampling/importance sampling. Values are as explained in Tab. 2. Number of MC cycles are 2^{21}.

	Brute force:				Importance:			
α:	$\langle E_L \rangle$:	SEM:	σ_B:	CPU time:	$\langle E_L \rangle$:	SEM:	σ_B:	CPU time:
0.50	2.49074	0.00072	0.01030	6.26562	2.52950	0.00075	0.01952	8.53125
0.60	2.27645	0.00053	0.00721	6.53125	2.26531	0.00052	0.01281	8.62500
0.70	2.12481	0.00036	0.00451	6.59375	2.12449	0.00036	0.00813	8.76562
0.80	2.04873	0.00022	0.00265	6.68750	2.04797	0.00022	0.00454	9.37500
0.90	2.01135	0.00010	0.00115	6.82812	2.01171	0.00010	0.00203	8.81250
1.00	2.00000	0.00000	0.00000	6.75000	2.00000	0.00000	0.00000	8.76562
1.10	2.00863	0.00009	0.00097	6.59375	2.00954	0.00009	0.00171	8.40625
1.20	2.03343	0.00018	0.00174	7.29688	2.03276	0.00018	0.00305	8.50000
1.30	2.07103	0.00026	0.00246	6.75000	2.07363	0.00026	0.00440	8.67188
1.40	2.11725	0.00033	0.00317	6.70312	2.10697	0.00034	0.00536	8.67188
	Mean CPU time: 6.7000				Mean CPU time: 8.7125			

3.1.3 Including optimization

Because there are two parameters to optimize, I chose this time to experiment with the minimization rate during the actual optimization. I started out using a minimization rate, $\gamma = 0.5$. It resulted in the fewest steps until the parameter value stabilized both for guesses close to the optimal value and for guesses far away from the optimal value, but for the smallest trap frequencies I had to use $\gamma = 0.1$ or 0.2. For the case of two interacting fermions, the parameters were optimized by trying out different first guesses for α and β and tuning γ so that the parameters stabilized during the first 200 iterations. The optimal parameters were extracted from the mean of the last 50 iterations. An example run is shown in Fig. 5 for $\omega = 0.5$.

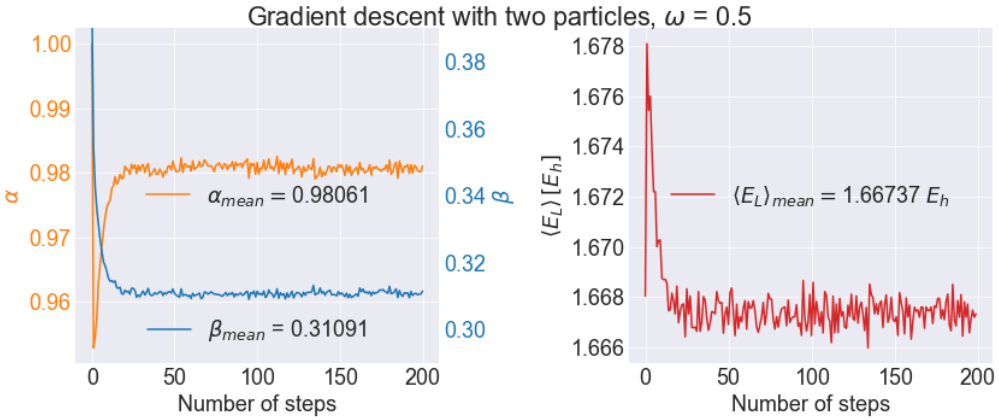

Figure 5: Left: The developement of the parameters during the steps of gradient descent. The values α_{mean} and β_{mean} printed on the figure is the mean of the last 50 values. Right: The expectation value after 2^{19} number of MC cycles. Here also, the value printed on the figure is the mean of the last 50 iterations.

For the system with six interacting fermions, the method described above was used for the largest ωs (i.e. $\omega = 1.0, 0.5, 0.1$), but for the smaller ones I had to use a smaller minimization rate (i.e. 0.01-0.05) and I also had to move step by step from $\omega = 0.1$ to $\omega = 0.01$ with the step size of $\Delta\omega = 0.01$. I found the parameters for the current ω and used that as a guess for the next ω. I tried to do it in a more efficent way and let the simple gradient descent method find the minimum on its own, but with this unguided method, the optimization ended up in local minima at higher energies or going to infinite energies. To improve the code, I attempted to use the extended gradient descent method, described in project 1, which utilize the previous gradient to find the new parameter [1]. But the attempt did not improve the behavoir described earlier. Compared to project 1, this systems local energy dependence on the parameters ($\langle E_L \rangle (\alpha, \beta)$), is more complicated, and also involve two paramters instead of one, which makes it harder to optimize the parameters with this simple gradient descent method.

Is the value calculated from the mean of 50 2^{19} with slightly different αs and βs, which values are oscillating around the optimal value, better than one calculation with the mean values of α and β for 2^{21} number of MC cycles? Maybe if I also could calculate the standard deviation and also save the local energies so that I get σ_b?

3.1.4 Including interaction

Here is the results of the expectation values approximating the ground state energy for two interacitng electrons in a harmonic oscillator trap. The equations used to model the system is as described in the theory part of this report. That includes the trial wavefunction (see Eq. 6) with the Jastrow factor that is used to model the many-body wavefunction. Table 6 and 7 show the results of the calculations with the optimal parameters found with the gradient descent method for brute force and importance sampling, respectively.

Table 6: Ground state energy of two interacting electrons in harmonic oscillator trap found with brute force sampling. Here $\overline{r}_{12}$, $\langle T \rangle$, $\langle V_{ext} \rangle$ and $\langle V_{int} \rangle$ are as explain in Tab. 4. The rest of the values are as explained in Tab. 2 . Number of MC cycles are 2^{23}.

ω	α	β	$\langle E_L \rangle$	SEM	σ_B	$\overline{r}_{12}$	$\langle T \rangle$	$\langle V_{ext} \rangle$	$\langle V_{int} \rangle$
1.00	0.98847	0.39965	3.0068	0.00001	0.00009	1.636	0.8944	1.2990	0.8135
0.50	0.98061	0.31091	1.6674	0.00001	0.00010	2.481	0.4488	0.7051	0.5135
0.10	0.94693	0.17764	0.4486	0.00001	0.00011	6.695	0.1003	0.1767	0.1716
0.05	0.92747	0.13815	0.2609	0.00000	0.00011	10.389	0.0533	0.0997	0.1076
0.01	0.88398	0.07287	0.0777	0.00000	0.00006	29.177	0.0129	0.0284	0.0364

Table 7: Ground state energy of two interacting electrons in harmonic oscillator trap found with importance sampling. Here $\overline{r}_{12}$, $\langle T \rangle$, $\langle V_{ext} \rangle$ and $\langle V_{int} \rangle$as explain in Tab. 4. The rest of the values are as explained in Tab. 2. Number of MC cycles are 2^{23}

ω	α	β	$\langle E_L \rangle$	SEM	σ_B	$\overline{r}_{12}$	$\langle T \rangle$	$\langle V_{ext} \rangle$	$\langle V_{int} \rangle$
1.00	0.98846	0.39954	3.0069	0.00001	0.00018	1.643	0.8931	1.3052	0.8086
0.50	0.98082	0.31068	1.6674	0.00001	0.00019	2.481	0.4547	0.6997	0.5130
0.10	0.94734	0.17810	0.4486	0.00001	0.00023	6.724	0.0989	0.1787	0.1710
0.05	0.92262	0.14090	0.2610	0.00000	0.00021	10.333	0.0495	0.1024	0.1091
0.01	0.88305	0.07366	0.0776	0.00000	0.00010	29.293	0.0131	0.0283	0.0362

From Tab. 6 and 7 one can observe that the two sampling methods give approximately the same results. The different expectation values for the different energies are very similar and the mean distance is also very similar. However, the standard deviation from the blocking resampling method are different. Importance sampling seems to result in larger σ_B here as well as for the case without interaction (see Tab. 5).

The results above show that the energy of the system is decreasing with decreasing trap frequency, ω. One can slo observe that the potential energy dominates for large trap frequencies ($\omega = 1.0$ and $\omega = 0.5$), but for the smaller ωs the interaction energy and the potential energy is approximately equal. For all ω, the kinetic energy is the smallest one. *Does this make sense? What is the potential energy? The energy stored in the force from the trap - keeping the electorns together - stronger trapping force - stronger potential energy. What is kinetic energy? Momentum? Why does it decrease with trap frequency? Because potential energy is less? Without interaction - energy oscillates between potential energy and kinetic energy - energy is conserved.*

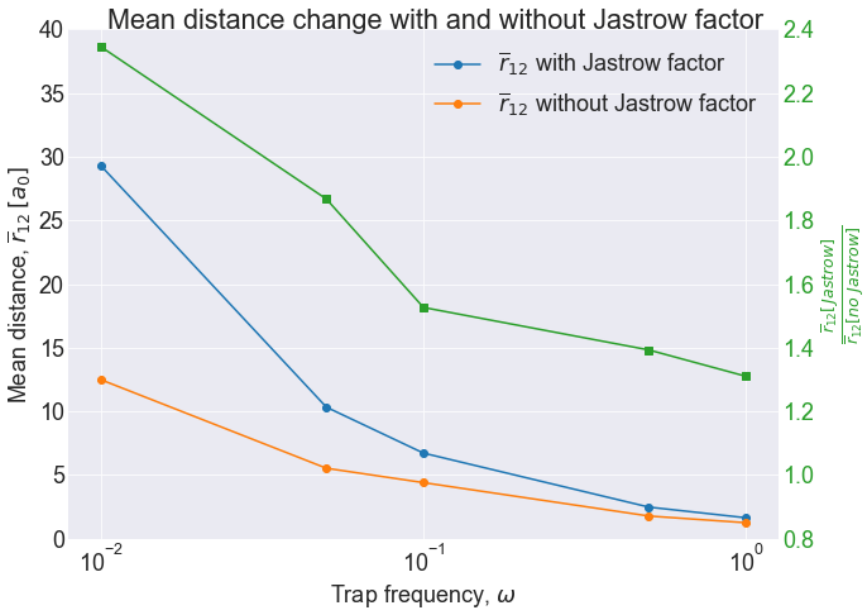

Figure 6: The mean distance between the two particles, calculated with importance sampling, compared for the situation with and without the Jastrow factor and at different trap frequencies.

Figure 6 shows the combined results from Tab. 4 and 7. One can observe that the mean distance is larger for the case with interaction. This is expected since the interaciton potential (see Eq. 2) is a repulsive potential, and will hence force the electrons further apart. One can also observe that the ratio of the two different cases increase with decreasing trap frequency, i.e. the mean distance increases more for smaller trap frequencies. *is that as expected? Why? Does that mean that the trap frequency is more important than the interaction?*

3.1.5 One-body density

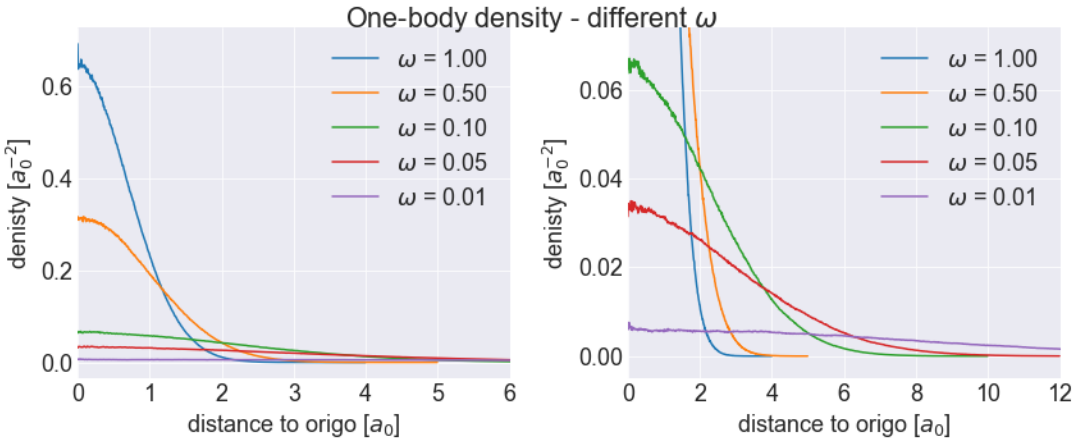

Figure 7: •

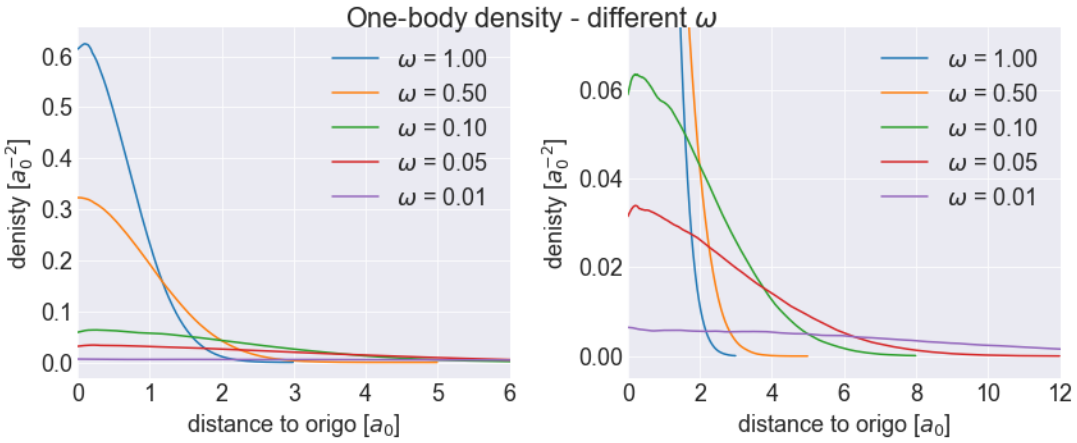

Figure 8: •

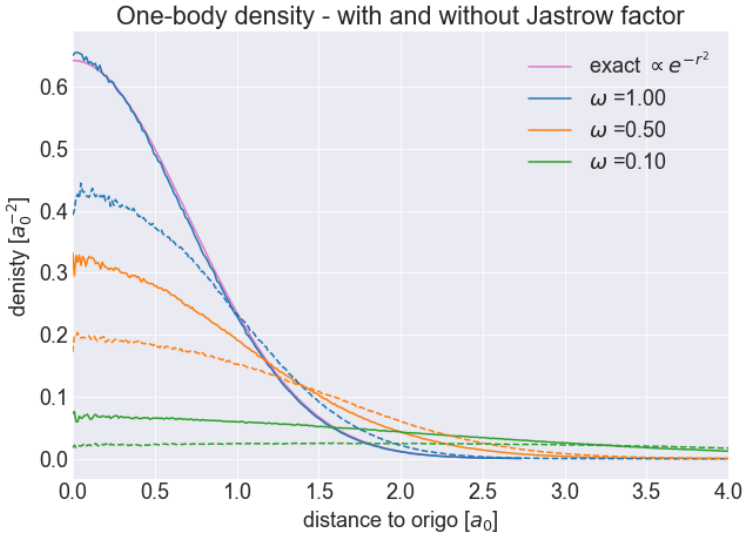

Figure 9: Dashed lines are with the Jastrow factor. Normal lines is without Jastrow factor.

3.2 Extending to more particles

3.3 Six particles

Table 8: Ground state energy of six electrons in harmonic oscillator trap. Here $\langle E_L \rangle$, $\langle T \rangle$ and $\langle V_{ext} \rangle$ are as explain in Tab. 4. Number of MC cycles are 2^{23}.

ω	$\langle E_L \rangle$	$\langle T \rangle$	$\langle V_{ext} \rangle$
1.00	10.00	4.9865	5.0135
0.50	5.00	2.4973	2.5027
0.10	1.00	0.4861	0.5139
0.05	0.50	0.2483	0.2517
0.01	0.10	0.0454	0.0546

Table 9: Ground state energy of six interacting electrons in harmonic oscillator trap found with importance sampling. Number of MC cycles are 2^{23}.

ω	α	β	$\langle E_L \rangle$	SEM	σ_B	$\langle T \rangle$	$\langle V_{ext} \rangle$	$\langle V_{int} \rangle$
1.00	0.71567	0.49372	20.4492	0.00022	0.00813	2.3429	10.7076	7.3988
0.50	0.75823	0.34260	11.9868	0.00011	0.00522	1.3226	5.8094	4.8548
0.10	0.78852	0.15041	3.6542	0.00003	0.00416	0.2951	1.7035	1.6556
0.05	0.76518	0.10733	2.2223	0.00003	0.00436	0.1178	1.0882	1.0162
0.01	0.64907	0.05085	0.7191	0.00001	0.00586	0.0021	0.3803	0.3367

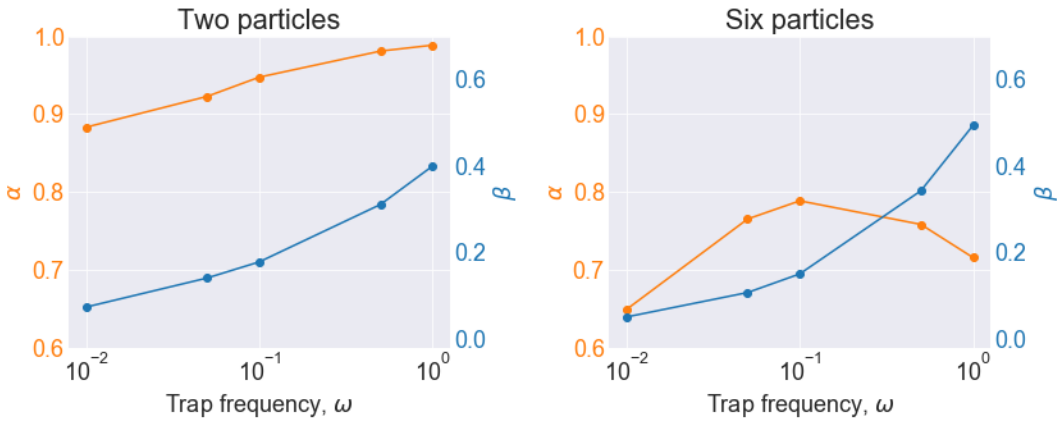

Figure 10: •

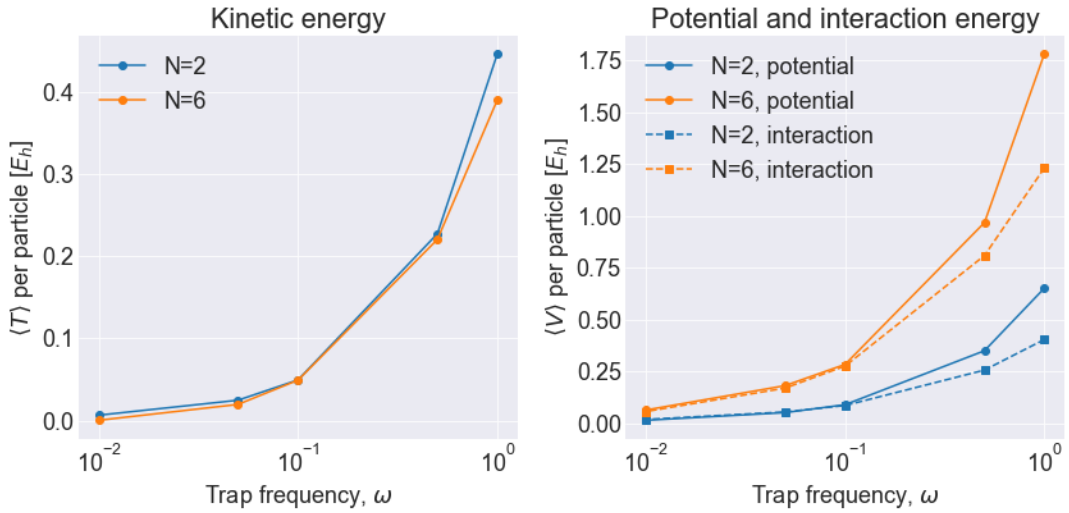

Figure 11: •

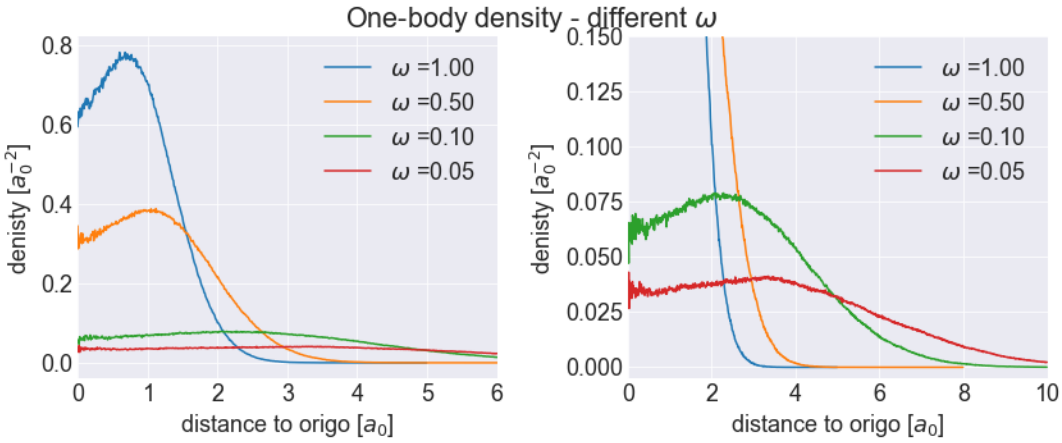

Figure 12: •

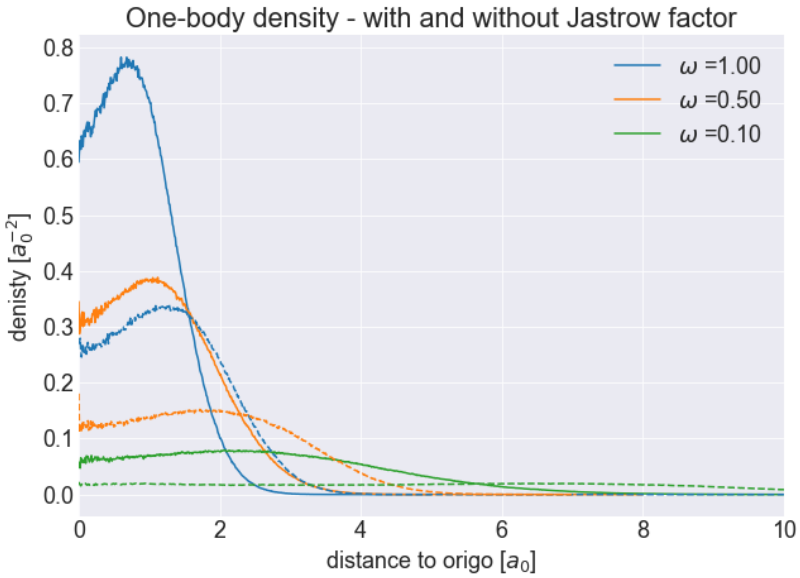

Figure 13: Dashed lines are with the Jastrow factor. Normal lines is without Jastrow factor.

3.4 Twelve particles

Table 10: Number of MC cycles are 2^{23}.

ω	$\langle E_L \rangle$	$\langle T \rangle$	$\langle V_{ext} \rangle$
1.00	28.00	14.0117	13.9883
0.50	14.00	7.0463	6.9537
0.10	2.80	1.4084	1.3916
0.05	1.40	0.6901	0.7099
0.01	0.28	0.1419	0.1381

Table 11: Ground state energy of twelve interacting electrons in harmonic oscillator trap found with importance sampling. Number of MC cycles are 2^{23}

ω	α	β	$\langle E_L \rangle$	SEM	σ_B	$\langle T \rangle$	$\langle V_{ext} \rangle$	$\langle V_{int} \rangle$

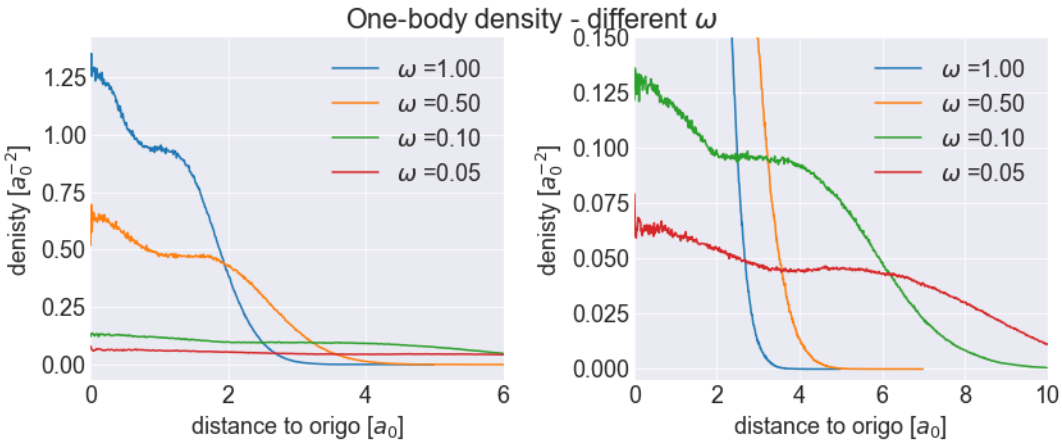

Figure 14: Had to use MC 2 24 to get smooth graphs.

3.5 Efficiency

Show results or errors of attempt to make parts of code more efficient.

3.6 Performance analysis

3.6.1 Vectorization

3.6.2 Parallellization

Chose to parallellize using cmake.

4 Conclusion

Appendices

A Iteration - derivatives with regards to parameters

$$\frac{\partial \psi_T}{\partial \alpha} = -\frac{\omega}{2} \sum_i^N r_i^2 \tag{11}$$

$$\frac{\partial \psi_T}{\partial \beta} = -\sum_{i<j}^N \frac{a_{ij} r_{ij}^2}{(1+\beta r_{ij})^2} \tag{12}$$

B Dealing with the Slater determinant efficiently

Determening a determinant numerically is a costly operation, so we want to do some alteration to increase the efficency of the code.

B.1 Slater determinant

The Slater determinant is contain the single-particle wave function of the number of particles included in the system evaluated at the posistion for all particles included because electrons are indistinguishable. The determinant is written as

$$D = Det\left(\phi_1(\boldsymbol{r}_1), \phi_2(\boldsymbol{r}_2), \ldots, \phi_N(\boldsymbol{r}_N)\right) = \begin{vmatrix} \phi_1(\boldsymbol{r}_1) & \phi_2(\boldsymbol{r}_1) & \cdots & \phi_N(\boldsymbol{r}_1) \\ \phi_1(\boldsymbol{r}_2) & \phi_2(\boldsymbol{r}_2) & \cdots & \phi_N(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{r}_N) & \phi_2(\boldsymbol{r}_N) & \cdots & \phi_N(\boldsymbol{r}_N). \end{vmatrix}$$

Hence the rows represent different positions, r_i, and the coloumns represent different states. To simplify the calcualtions we want to have all states with spin up in one determinant and all states with spin down in another determinant. For six particles we then get

$$D = D_\uparrow D_\downarrow = \begin{vmatrix} \phi_1(\boldsymbol{r}_1) & \phi_3(\boldsymbol{r}_1) & \phi_5(\boldsymbol{r}_1) \\ \phi_1(\boldsymbol{r}_2) & \phi_3(\boldsymbol{r}_2) & \phi_5(\boldsymbol{r}_2) \\ \phi_1(\boldsymbol{r}_3) & \phi_3(\boldsymbol{r}_3) & \phi_5(\boldsymbol{r}_3) \end{vmatrix} \begin{vmatrix} \phi_2(\boldsymbol{r}_4) & \phi_4(\boldsymbol{r}_4) & \phi_6(\boldsymbol{r}_4) \\ \phi_2(\boldsymbol{r}_5) & \phi_4(\boldsymbol{r}_5) & \phi_6(\boldsymbol{r}_5) \\ \phi_2(\boldsymbol{r}_6) & \phi_4(\boldsymbol{r}_6) & \phi_6(\boldsymbol{r}_6) \end{vmatrix}.$$

We see this from Tab. 1 and Eq. 3. *Mister anti-symmertrien, men expectation value er lik.*

The trial wavefunction can therefore be rewritten to

$$\psi_T = D_\uparrow D_\downarrow \psi_C$$

where ψ_C is the correlation part of the trial wavefunction. Now we only have to update one of these matrises when we move a particle, depending on which spin the particle has.

B.2 The Metropolis ratio

In the metropolis test we calculate the ratio bewteen the wavefunction before and after a proposed move, but now the wavefunction includes a determinant which is costly to calculate. We therefore want to utilize some relations from linear algebra to simplify the ratio and make the algorithm more efficent. The ratio between the Slater determinant part of the wavefunction, ψ_{SD}, is

$$R = \frac{\psi_{SD}(\boldsymbol{r}^{new})}{\psi_{SD}(\boldsymbol{r}^{old})} = \frac{\sum_i^N d_{ij}(\boldsymbol{r}^{new}) C_{ij}(\boldsymbol{r}^{new})}{\sum_i^N d_{ij}(\boldsymbol{r}^{old}) C_{ij}(\boldsymbol{r}^{old})}. \tag{13}$$

where $d_{ij} = \psi_i(j)$

Here we have used the fact that when you calculate a determinant, you break it down into a sum of

smaller determinants times a factor:

$$D = \begin{vmatrix} d_{11} & d_{12} & \cdots & d_{1N} \\ d_{21} & d_{22} & \cdots & d_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ d_{N1} & d_{N2} & \cdots & d_{NN} \end{vmatrix} = \sum_{i}^{N} d_{ij} C_{ij}.$$

So if $dij = d_{11}$ then

$$C_{11} = \begin{vmatrix} d_{22} & d_{23} & \cdots & d_{2N} \\ d_{32} & d_{33} & \cdots & d_{3N} \\ \vdots & \vdots & \ddots & \vdots \\ d_{N2} & d_{N3} & \cdots & d_{NN} \end{vmatrix}.$$

We observe in Eq. 13 that if we move particle j from r_j^{old} to r_j^{new} the matrix C_{ij} is unchanged, we have only changed the d_{ij} in the original determinant D that is not included in C_{ij}. Equation 13 is then

$$R = \frac{\sum_i^N d_{ij}(\boldsymbol{r}^{new})}{\sum_i^N d_{ij}(\boldsymbol{r}^{old})} \tag{14}$$

We can simplify this even further with the relation

$$\sum_{k=1}^{N} d_{ik} d_{kj}^{-1} = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \tag{15}$$

The ratio can be rewritten as

$$R = \frac{\sum_i^N d_{ij}(\boldsymbol{r}^{new}) d_{ij}(\boldsymbol{r}^{old})^{-1}}{\sum_i^N d_{ij}(\boldsymbol{r}^{old}) d_{ij}(\boldsymbol{r}^{old})^{-1}} = \sum_{i}^{N} d_{ij}(\boldsymbol{r}^{new}) d_{ij}(\boldsymbol{r}^{old})^{-1}. \tag{16}$$

The consequence of these calculations are that we now only have to calculate the invers values of the determinant once to know the values for $d_{ij}(\boldsymbol{r}^{old})^{-1}$ and then update only the row of the position that was changed in the Slater determinant and calculate the invers of the determinant again only if the move is accepted.

B.3 Updating the inverse of the Slater determinant

After a move is accepted in the Metropolis test, the row in the Slater determinant representing that particle is updated, but the inverse of the Slater determinant also needs to be updated because the Slater determinant has changed. This could be done by simply calculating the inverse of the determinant, but this is costly and there is a more efficient way. The elements of the determinant d_{kj}^{-1}

(*hva betyr den $^{-1}$? At den skal opphøyes i minus 1 eller er det notasjon på at det er et element i den inverse matrisen?*) can be found through

$$d_{kj}^{-1}(\boldsymbol{r}^{new}) = \begin{cases} d_{kj}^{-1}(\boldsymbol{r}^{old}) - \frac{d_{kj}^{-1}(\boldsymbol{r}^{old})}{R} \sum_{l=1}^{N} d_{il}^{-1}(\boldsymbol{r}^{new}) d_{lj}^{-1}(\boldsymbol{r}^{old}) & \text{if } i \neq j \\ \frac{d_{kj}^{-1}(\boldsymbol{r}^{old})}{R} \sum_{l=1}^{N} d_{il}^{-1}(\boldsymbol{r}^{old}) d_{lj}^{-1}(\boldsymbol{r}^{old}) & \text{if } i = j \end{cases},$$

where i is the number of the row representing the particle that was moved.

C Energies

$$E_{n_x n_y} = \hbar\omega(n_x + n_y + \frac{d}{2}) \tag{17}$$

where d is the number of dimensions. In this project $d = 2$.

Table 12: The exact energies for the non-interacting case with different number of particles in a closed shell system.

Energies	
E_{00}	$\hbar\omega$
$E_{10} = E_{01}$	$2\hbar\omega$
$E_{20} = E_{02} = E_{11}$	$3\hbar\omega$
$E_{30} = E_{03} = E_{21} = E_{12}$	$4\hbar\omega$
$E_{N=2} = 2E_{00}$	$2\hbar\omega$
$E_{N=6} = E_{N=2} + 2E_{10} + 2E_{01}$	$10\hbar\omega$
$E_{N=12} = E_{N=6} + 2E_{20} + 2E_{02} + 2E_{11}$	$28\hbar\omega$
$E_{N=20} = E_{N=12} + 2E_{30} + 2E_{03} + 2E_{21} + 2E_{12}$	$60\hbar\omega$

D Hermite polynomials and the wavefunction derivatives

The relevant Hermite polynomials	
$H_0(\sqrt{\omega}x)$	1
$H_1(\sqrt{\omega}x)$	$2\sqrt{\omega}x$
$H_2(\sqrt{\omega}x)$	$4\omega x^2 - 2$
$H_3(\sqrt{\omega}x)$	$8\omega\sqrt{\omega}x^3 - 12\sqrt{\omega}x$

$$\phi_{n_x,n_y}(x,y) = AH_{n_x}(\sqrt{\omega}x)H_{n_y}(\sqrt{\omega}y)\exp\left(-\omega(x^2+y^2)/2.\right.$$

Table 13: $\psi_{n_x n_y}$

Trial wavefunctions for the different states	
ψ_{00}	$A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{01}	$2\sqrt{\omega}xA\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{10}	$2\sqrt{\omega}yA\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{20}	$(4\omega x^2-2)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{02}	$(4\omega y^2-2)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{11}	$4\omega xyA\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{30}	$(8\omega\sqrt{\omega}x^3-12\sqrt{\omega}x)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{03}	$(8\omega\sqrt{\omega}y^3-12\sqrt{\omega}y)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{21}	$(8\omega\sqrt{\omega}x^2y-4\sqrt{\omega}y)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
ψ_{12}	$(8\omega\sqrt{\omega}xy^2-4\sqrt{\omega}x)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$

Table 14: $\psi_{n_x n_y}$

The derivative of the trial wavefunctions for the different states	
$\nabla\psi_{00}$	$(-\alpha\omega x,-\alpha\omega y)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla\psi_{01}$	$-(\sqrt{\omega}(a\omega x^2-1),\alpha\omega^{3/2}xy)2A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla\psi_{10}$	$-(\alpha\omega^{3/2}xy,\sqrt{\omega}(a\omega y^2-1))2A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla\psi_{20}$	$-(2\alpha\omega^2x^3-\alpha\omega x-4\omega x,2\alpha\omega^2x^2y-\alpha\omega y)2A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla\psi_{02}$	$-(2\alpha\omega^2xy^2-\alpha\omega x,2\alpha\omega^2y^3-\alpha\omega y-4\omega y)2A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla\psi_{11}$	$(-4\omega y(\alpha\omega x^2-1),-4\omega x(\alpha\omega y^2-1))A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla\psi_{30}$	$(-4\sqrt{\omega}(2\alpha\omega^2x^4-3(\alpha+2)\omega x^2+3),-4\alpha\omega^{3/2}xy(2\omega x^2-3))A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla\psi_{03}$	$(-4\sqrt{\omega}(-4\alpha\omega^{3/2}xy(2\omega y^2-3),2\alpha\omega^2y^4-3(\alpha+2)\omega y^2+3))A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla\psi_{21}$	$(-4\sqrt{\omega}(\alpha\omega x^2(2\omega xy-1)-4\omega xy+1),-4\omega^{3/2}x(2x(\alpha\omega y^2-1)-\alpha y))A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla\psi_{12}$	$(-4\omega^{3/2}y(2y(\alpha\omega x^2-1)-\alpha x),-4\sqrt{\omega}(\alpha\omega y^2(2\omega xy-1)-4\omega xy+1))A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$

Table 15: $\psi_{n_x n_y}$

The double derivative of the trial wavefunctions for the different states

$\nabla^2\psi_{00}$	$(\alpha^2\omega^2 r^2 - \alpha\omega)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{01}$	$2\alpha\omega^{3/2}x(\alpha\omega r^2 - 4)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{10}$	$2\alpha\omega^{3/2}y(\alpha\omega r^2 - 4)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{20}$	$2\omega(\alpha^2\omega(2\omega x^2 - 1)r^2 + \alpha(2 - 12\omega x^2) + 4))A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{02}$	$2\omega(\alpha^2\omega(2\omega y^2 - 1)r^2 + \alpha(2 - 12\omega y^2) + 4))A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{11}$	$4\alpha\omega^2 xy(\alpha\omega r^2 - 6)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{30}$	$4\omega^{3/2}x(\alpha^2\omega(2\omega x^2 - 3)r^2 - 4\alpha(4\omega x^2 - 3) + 12)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{03}$	$4\omega^{3/2}y(\alpha^2\omega(2\omega y^2 - 3)r^2 - 4\alpha(4\omega y^2 - 3) + 12)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{21}$	$4\omega^{3/2}(\alpha^2\omega x r^2(2\omega xy - 1) + 4\alpha x(1 - 4\omega xy) + 4y)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$
$\nabla^2\psi_{12}$	$4\omega^{3/2}(\alpha^2\omega y r^2(2\omega xy - 1) + 4\alpha y(1 - 4\omega xy) + 4x)A\exp\left(\frac{-\alpha\omega r^2}{2}\right)$

E Evaluating the minimization rate

References

[1] Vilde M Reinertsen. Project 1, 2020.

[2] Even Marius Nordhagen. Studies of quantum dots using machine learning. Master's thesis, University of Oslo, 2019.