Fys4110: Project 2

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Abstract

I continue the study of many interacting particles in an isotropic two dimensional harmonic oscillator from [1], where I studied the problem with Hartree-Fock methods. Here I study a parametrized class of wavefunctions based on a slater determinant and a jastrow factor of the form in equation 7. I use the Metropolis algorithm with importance sampling to estimate the energy, and the blocking method to estimate the errors. I attempted to minimize the energy with respect to the parameters, but ran into problems and ended up using the best of a small set. The resulting estimates for ground state energies for 2,6 and 12 particles with oscillator strengths $\omega = 1$,0.5, 0.1, 0.05 and 0.01 in atomic units are found in tables 5,6 and 7. For $\omega = 1$ and 0.5 [5] inludes benchmark values found by diffusion Monte Carlo methods that fit well with these results.

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1   Introduction

In this project I continue the study of many interacting particles in an isotropic two dimensional harmonic oscillator. In project 1 [1] I used Hartree-Fock methods to construct the Slater determinant of linear combinations of single particle non-interacting states that minimized the energy. In this project I would like to improve this estimate of the ground state by adding a Jastrow factor. Then the energy cannot be found with Hartree-Fock methods, but rather from direct integration of the Hamiltonean. Rather than using the slater determinant from the HF calculations I will use a new set of trial wavefunctions consisting of a singly parametrized slater determinant and a singly parametrized jastrow factor. I will then try to minimize the energy with respect to these parameters. I will do this using the Metropolis algorithm to perform the integrals.

2   Physical Problem

We will study several Coulomb-interacting electrons in an isotropic two dimensional harmonic oscillator. The full Hamiltonean of the problem with N particles and using atomic units is

$$H = \sum_i^N -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 + \sum_{i<j}^N \frac{1}{r_{ij}},$$

(1)

where $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$. The non-interacting hamiltonean

$$H_0 = \sum_i^N -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2,$$

(2)

has as an analytical ground state solution (up to normalisation) the slater determinant

$$\mathcal{A}\left(\psi_1 \ldots \psi_N; \boldsymbol{r}_1 \ldots \boldsymbol{r}_N\right) = \begin{vmatrix} \psi_1(\boldsymbol{r}_1) & \cdots & \psi_N(\boldsymbol{r}_1) \\ \vdots & \ddots & \vdots \\ \psi_1(\boldsymbol{r}_N) & \cdots & \psi_N(\boldsymbol{r}_N) \end{vmatrix},$$

(3)

where

$$\psi_i(\boldsymbol{r}) = \chi_i \psi_{n_x, n_y}(\boldsymbol{r}) = \chi_i H_{n_x}(\sqrt{\omega}x) H_{n_y}(\sqrt{\omega}y) \exp(-\frac{r^2}{2}),$$

(4)

are the N lowest energy single particle wave eigenstates, H_n is the nth Hermite polynomial and ξ is a spin state spinor. The general ground state for the interacting case is not known.

3 Trial wave functions

3.1 2 Particle Case

For the two particle case I will aproximate the ground state with the parametrized trial wavefunction

$$\psi_T = \exp\left(-\alpha\omega(r_1^2 + r_2^2) - \frac{r_{12}}{1 + \beta r_{12}}\right),$$

(5)

with α and β as free parameters.

3.2 Slater case

For the many particle case we will use the non-interacting ground state Slater determinant for a modified potential of strength $\alpha\omega$ multiplied with a Jastrow factor with one free parameter. We could used Slater determinants from linear combinations of different non-interacting single particle states as found in [1] by Hartree-Fock methods, however this turned out to be too complicated too do in our timeframe. Instead we will compare the Hartree-Fock approach to adding a Jastrow factor to this modified ground state.

$$\psi_T = \mathcal{A}\left(\psi_1(\alpha) \ldots \psi_N(\alpha); \boldsymbol{r}_1 \ldots \boldsymbol{r}_N\right) \prod_{i<j}^N \exp\left(-\frac{a_{ij}r_{ij}}{1 + \beta r_{ij}}\right),$$

(6)

where ψ_i is the non-interacting single particle state with the ith lowest energy, and a_{ij} is 1 when the particles have anti-paralell spins and $1/3$ when paralell. Since we are talking about spin $1/2$ electrons there are two spin configurations for each spatial configuration for the single particle states that go into the Slater determinant. However the hamiltonean 1 is independent of spin. Wen can exploit this to simplify the wavefunction we use. If we let the $N/2$ first particles be in one spin state and the next $N/2$ in the other we may use a product of Slater determinants with only the particles in the same spin state in each:

$$\psi_T = \mathcal{A}\left(\psi_{1,\downarrow}(\alpha) \ldots \psi_{N/2,\downarrow}(\alpha); \boldsymbol{r}_1 \ldots \boldsymbol{r}_{N/2}\right) \mathcal{A}\left(\psi_{1\uparrow}(\alpha) \ldots \psi_{N/2\uparrow}(\alpha); \boldsymbol{r}_{N/2+1} \ldots \boldsymbol{r}_N\right) \prod_{i<j}^N \exp\left(-\frac{a_{ij}r_{ij}}{1 + \beta r_{ij}}\right).$$

(7)

In the 2 particle case this reduces to equation 5.

3.3 Steepest Descent

To find the optimal values for α and β start with an initial guess and traverse the parameter space by going down the steepest descent.

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}_{n+1} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}_n - \gamma \nabla_{\alpha,\beta} \langle E \rangle, \tag{8}$$

where γ is a parameter of the search and $\nabla_{\alpha,\beta}$ is the gradient operator in parameter space. From [6] the derivatives are

$$\frac{\partial \langle E \rangle}{\partial \alpha} = 2 \left(\left\langle \frac{1}{\psi_T} \frac{\partial \psi_T}{\partial \alpha} E \right\rangle - \left\langle \frac{1}{\psi_T} \frac{\partial \psi_T}{\partial \alpha} \right\rangle \langle E \rangle \right) \tag{9}$$

and

$$\frac{\partial \langle E \rangle}{\partial \beta} = 2 \left(\left\langle \frac{1}{\psi_T} \frac{\partial \psi_T}{\partial \beta} E \right\rangle - \left\langle \frac{1}{\psi_T} \frac{\partial \psi_T}{\partial \beta} \right\rangle \langle E \rangle \right) \tag{10}$$

The expressions in each case are found in appedices B.3 and C.3.

4 Monte-Carlo Integration

In this project I will estimate the energy of the trial wavefunctions with Monte-Carlo (MC) integration. MC integration is a method of estimating the value of integrals on the form

$$\langle F \rangle = \int F(x_1, \ldots, x_N) p(x_1, \ldots, x_N) \prod_{k=1}^{N} \mathrm{d}x_k, \tag{11}$$

where $p(x_1, \ldots, x_N)$ is a probability density function. MC integration is then based on drawing points $\boldsymbol{r}_i$ according to p and evaluating F in these points

$$F_i \equiv F(\boldsymbol{r}_i). \tag{12}$$

Then defining

$$\overline{F} \equiv \frac{1}{N} \sum_{i=1}^{N} F_i \tag{13}$$

we have that

$$\langle F \rangle = \lim_{N \to \infty} \overline{F}. \tag{14}$$

Since we cannot draw infinite points we use $\overline{F}$ as an estimate of $\langle F \rangle$.

In order to estimate an integral in this way we thus need a method to draw positions according to p, a way to compute F_i and a way to estimate the error in the integration.

4.1 The Metropolis Algorithm

The Metropolis algorithm is a way to draw points according to a probability density function p. It is based on semi randomly-walking through the space. One advantage of the method is that the pdf does not need to be normalised, which is convenient. We can thus rewrite equation 11 to

$$\langle F \rangle = \frac{\int F(x_1, \ldots, x_N) p(x_1, \ldots, x_N) \prod_{k=1}^{N} \mathrm{d}x_k}{\int p(x_1, \ldots, x_N) \prod_{k=1}^{N} \mathrm{d}x_k}. \tag{15}$$

One disadvantage is that as the each point is only a relatively small step from the last the correlations between points are high enough that we have to take them into account.

4.1.1 Detailed Balance

The Metropolis algorithm may be derived by demanding that the Markov chain of the random walk exhibits detailed balance. The criterion for detailed balance is

$$P(a)P(b|a) = P(b)P(a|b), \tag{16}$$

or rewritten

$$\frac{P(a)}{P(b)} = \frac{P(a|b)}{P(b|a)}. \tag{17}$$

We may split $P(a|b) = G(a|b)A(a|b)$, where $G(a|b)$ is the probability of proposing a move from b to a, while $A(a|b)$ is the probability of accepting a proposed move from b to a. The the detailed balance requirement may be rewritten as

$$\frac{A(a|b)}{A(b|a)} = \frac{P(a)G(b|a)}{P(b)G(a|b)}. \tag{18}$$

Now we choose an acceptance ratio that satisfies this requirement. The Metropolis choice is to use

$$A(a|b) = \min\left(1, \frac{P(a)G(b|a)}{P(b)G(a|b)}\right). \tag{19}$$

So the Metropolis algorithm for drawing points from a probability distrobution is

1. Draw a proposed move from the proposal distribution.

2. Evaluate the acceptance ratio a from equation 19.

3. Draw a random number $0 \leq r < 1$ from a uniform distribution.

4. If $a > r$ accept the move. Else reject the move.

5. Save position

6. return to point 1.

4.1.2 Symmetric Proposal Density

If the proposal probality $G(a|b) = G(b|a)$ the proposal distribution is called symmetric and drops out of the acceptance ratio. Thus there is less to calculate for each loop in the algortihm. However symmetric proposal densities lead to many proposed steps being rejected, and thus to higher corelations between the points.

4.1.3 Importance Sampling

If we instead choose a non-symmetric proposal distribution we may choose one to maximise the acceptance rate. If we choose a proposal distribution so that the probability of proposing a move into an area with a higher probability is higher than the probability of proposing a move into an area with a lower probability, in other words if $P(a) > P(b)$ then $G(a|b) > G(b|a)$, we will increase the acceptance rate. We need to make sure that the proposal distribution preserves ergodicity, which means that the whole space may be reached from any point with enough steps. So the probability of proposing a move into an area with lower probability must be non-zero. The obvious way to ensure proposals into higher probability is to use the gradient of p:

$$\frac{1}{p}\nabla p = \frac{1}{|\psi_T|^2}\nabla|\psi|^2 = \frac{2}{\psi_T}\nabla\psi \equiv 2F, \tag{20}$$

where I have used that the wavefunction is real. If we only move one particle at a time in one direction at a time we only need the derivative with respect to that particle in that dimension. One choice that uses this and preserves ergodicity is

$$x_{i,n+1} = x_{i,n} + \sigma\chi + \sigma^2 F(x_{i,n}), \tag{21}$$

where χ is a random variable from a gaussian distribution about 0 with standard deviation 1. From [6] the proposal distribution from this rule is

$$G(x_{i,n+1}|x_{i,n}) = \exp\left(-\frac{(x_{i,n+1} - x_{i,n} - \sigma^2 F(x_{i,n}))^2}{2\sigma^2}\right). \tag{22}$$

4.1.4 Equilibrriation

The metropolis algorithm requires a starting point for the walker, but this cosen starting point may bias the distribution toward points close to it. To account for this one should let the algorithm run until the probability distribution is in equilibrium, i.e. is independent of time before saving the points. This process is called equilibriation or burn-in.

4.2 Local Energy

In quantum mechanics the probability distribution is given by $|\psi|^2$ and the expectation value for an operator O is given by

$$\langle O \rangle = \frac{\int \psi^* O \psi \prod_i dx_i}{\int |\psi|^2 \prod_i dx_i}, \tag{23}$$

This is not exactly on the form of equation 15, but it can be rewritten in terms of local variables given by

$$O_L = \frac{1}{\psi} O \psi, \tag{24}$$

so that the expectation value is

$$\langle O \rangle = \frac{\int |\psi|^2 O_L \prod_i dx_i}{\int |\psi|^2 \prod_i dx_i}. \tag{25}$$

So the expectation value of the energy is given by

$$\langle E \rangle = \frac{\int |\psi|^2 E_L \prod_i dx_i}{\int |\psi|^2 \prod_i dx_i}, \tag{26}$$

with

$$E_L = \frac{1}{\psi} H \psi,. \tag{27}$$

4.2.1 2 Particle Case

We might compute the local energy by numerical differentiation, however we will see that that is inefficient compared to calculating the derivative analytically. In the two particle case with hamiltonean given by equation 1 and trial wavefunction by equation 5 the anaytical expression for the local energy is

$$E_L(r_1, r_2) = \left[\frac{1}{2}(1 - \alpha)\omega(r_1^2 + r_2^2) + 2\alpha\omega\right] - \frac{a}{(1 + \beta r_{12})^2}\left[\frac{a}{(1 + \beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{(1 + \beta r_{12})} - \alpha\omega r_{12}\right] + \frac{1}{r_{12}}, \tag{28}$$

as shown in appendix B.2.

4.2.2 Slater Case

In the N particle case with hamiltonean given by equation 1 and trial wavefunction by equation 7 the local energy is given by

$$E_L = -\frac{1}{2}\left(\frac{\nabla^2|S_\downarrow|}{|S_\downarrow|} + \frac{\nabla^2|S_\uparrow|}{|S_\uparrow|} + \frac{\nabla^2 J}{J} + \left(\frac{\nabla|S_\downarrow|}{|S_\downarrow|} + \frac{\nabla|S_\uparrow|}{|S_\uparrow|}\right) \cdot \frac{\nabla J}{J}\right) + \frac{1}{2}\omega^2 \sum_i r_i^2 + \sum_{i<j} \frac{1}{r_{ij}}, \tag{29}$$

where the expressions for the laplacians are derived in appendix C.2 and are too big to include here.

4.3 Error Estimation and Blocking

Let $\{ F_i \}$ be a finite set of consecutive measurements of the quantity F on a system in equilibrium, in other words the probability distribution for the measurements is independent of time. For a true average of $\langle F \rangle$ the error of each measurement is given by

$$e_i = F_i - \langle F \rangle, \tag{30}$$

while the error in the mean of the measurements $\overline{F}$ is given by

$$E = \overline{F} - \langle F \rangle. \tag{31}$$

The variance of F is given by

$$\sigma_F^2 = \left\langle (F - \langle F \rangle)^2 \right\rangle = \left\langle e^2 \right\rangle, \tag{32}$$

while the variance of $\overline{F}$ is given by

$$\sigma_{\overline{F}}^2 = \left\langle (\overline{F} - \langle F \rangle)^2 \right\rangle = \left\langle E^2 \right\rangle, \tag{33}$$

noting that $E = (\sum_i e_i)/n$ we see that

$$\sigma_{\overline{F}}^2 = \left\langle \left(\frac{1}{n} \sum_i e_i \right)^2 \right\rangle = \frac{1}{n^2} \sum_{i,j} \langle e_i e_j \rangle. \tag{34}$$

4.3.1 Uncorrelated Data [1]

For uncorrelated data

$$\langle e_i e_j \rangle = 0, \tag{35}$$

when $i \neq j$ and so equation 34 says

$$\sigma_{\overline{F}}^2 = \frac{1}{n} \left\langle e^2 \right\rangle = \frac{1}{n} \sigma_F^2. \tag{36}$$

These quantities depend on the true average $\langle F \rangle$ and are thus unknown, so we instead look at the following known quantity

$$d_i = F_i - \overline{F} = e_i - E, \tag{37}$$

with mean square

$$\overline{d^2} = \frac{1}{n} \sum_n (e_i - E)^2 = \frac{1}{n} \sum_i e_i^2 - E^2. \tag{38}$$

We note that the true average of this is

$$\left\langle \overline{d^2} \right\rangle = \sigma_F^2 - \sigma_{\overline{F}}^2 = (n-1)\sigma_{\overline{F}}^2, \tag{39}$$

or

$$\sigma_{\overline{F}}^2 = \frac{\left\langle \overline{d^2} \right\rangle}{n-1}. \tag{40}$$

We still don't know $\left\langle \overline{d^2} \right\rangle$, but we can estimate it with $\overline{d^2}$. And so our estimate of $\sqrt{\langle E^2 \rangle}$ is

$$\sqrt{\langle E^2 \rangle} = \sigma_{\overline{F}} \approx \sqrt{\frac{\overline{d^2}}{n-1}}. \tag{41}$$

If the measurements come with errors the errors propagate as

$$\sigma_{\overline{F}}^2 = \frac{1}{n^2} \sum_i \sigma_{F_i}^2. \tag{42}$$

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[1] This section is based on the treatment in [2]

4.3.2 Correlations and Blocking [2]

When the data is correlated $\langle e_i e_j \rangle$ is not generally 0 and so equation 34 reads

$$\sigma_{\bar{F}}^2 = \frac{1}{n} \left\langle e^2 \right\rangle + \frac{2}{n^2} \sum_{i<j} \langle e_i e_j \rangle \tag{43}$$

The time independence of the pdf means that $\langle e_i e_j \rangle$ should only depend on the relative distance between i and j: $t \equiv |i - j|$ [3]. So we can define $C(t) = \langle e_i e_j \rangle$ and write

$$\sigma_{\bar{F}}^2 = \frac{1}{n} \left[C(0) + 2 \sum_{t=0}^{n-1} \left(1 - \frac{t}{n} \right) C(t) \right]. \tag{44}$$

For finite correlation time there exists some $t = t_{max}$ for which $C(t > t_{max}) = 0$. If

$$\sigma_{\bar{F}}^2 = \frac{1}{n} \left[C(0) + 2 \sum_{t=0}^{t_{max}} \left(1 - \frac{t}{n} \right) C(t) \right]. \tag{45}$$

We know how to estimate $C(0)$ from above, but $C(t > 0)$ is more complicated. The blocking method allows us to build $C(t > 0)$ into a new $C(0)$ which we can estimate in the regular way.

If we transform the data set $\{ F_i \}$ into another set $\{ \tilde{F}_i \}$, where

$$\tilde{F}_i = \frac{1}{B} \sum_{j=1}^{B} F_{(i-1)B+j}, \tag{46}$$

where B is a whole number called the block size. Call $\tilde{F}_i$ a block. Expanding $\tilde{C}(0)$ we see that

$$\begin{aligned}
\tilde{C}(0) &= \left\langle \tilde{F}_i^2 \right\rangle - \left\langle \tilde{F}_i \right\rangle^2 \\
&= \frac{1}{B^2} \sum_{a,b}^{B} \langle F_{i+a} F_{i+b} \rangle - \langle F_{i+a} \rangle \langle F_{i+b} \rangle \\
&= \frac{1}{B^2} \sum_{a,b}^{B} C(|a-b|) \\
&= \frac{1}{B} C(0) + \frac{2}{B} \sum_{t=1}^{B-1} \left(1 - \frac{t}{B} \right) C(t),
\end{aligned}$$

and so

$$\frac{\tilde{C}(0)}{N/B} = \frac{1}{N} \left[C(0) + 2 \sum_{t=1}^{B-1} \left(1 - \frac{t}{B} \right) C(t) \right], \tag{47}$$

comparing with equation 45 we see that blocking has incorporated part of the error from correlations into $\tilde{C}(0)$! So, for an appropriate block size an improved estimate of the error is

$$\sigma_{\bar{F}}^2 \approx \frac{\sigma_{\tilde{F}}^2}{N/B - 1}. \tag{48}$$

To find the approriate block size we may plot this estimate as a function of block size, and choose a value where this seems to flatten.

5 Implementation

The code is found at `https://github.com/khhelland/Fys4411/tree/master/2/src`.

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[2]This section is based on [3]

Table 1: Table of blocksizes.

N	importance samling?	blocksize from plot	chosen blocksize
2	no	250 000	250 000
	yes	200 000	250 000
6	no	400 000	500 000
	yes	156 250	250 000
12	no	500 000	500 000
	yes	100 000	250 000

5.1 Structure

The code is set up as two classes one for the two particle case and a generalisation for 2,6 or 12 particles. The 2 particle class i called vmc and the many particles class is called slatervmc. Both classes are initialized with a steplenght, frequency, variational parameters and a seed for the random number generator. To run the integration both classes have a member function called run, which takes the number of MC cycles and a blocksize. The classes have public booleans that can be set to determine whether or not to switch on the interaction, jastrow factor, importance sampling and, in the 2 particle case, numerical differentiation. Both classes have member functions that write the energies to file, and functions that perform a steepest descent parameter optimization. Due to problems with the automatic steepest descent getting stuck in local minima or becomming unstable there is a manual steepest descent which uses a static steplength and simply prints updated parameters untill stopped. The idea is to use it by starting it with a relatively large stepsize, see how it behaves, and then try again with a better initial guess and smaller stepsize.

Due to time constraints the code is somewhat messy, but hopefully it is readable anyway. Due to the time constraints not alot of time has been put into optimization, and there are several obvious inefficiencies.

5.2 Paralellization

To run several integrations in paralell I used OpenMPI. The file paramain.cpp includes the MPI commands necesary to set up paralell processes and collect the results.

6 Results

6.1 Cost of numerical differentiation

I timed the program with 10^7 MC cycles without the jastrow factor or interaction with both analytical and numerical differentiation in local energy. The analytical aproach took on average 3.32 s while the numerical approach took on average 11.78 s. I conclude that the analytical approach is more efficient and move forward using only the analytical expressions.

6.2 Blocking

Plots of the estimated error as a function of blocksize are found in figures 1 through 6. In table 1 I have collected the blocksizes where the plots seem to flatten, and the blocksize I chose to work with. I chose slightly bigger blocksizes than seem necessary from the plots.

6.3 Steepest Descent Optimization

For the two particle case the automatic steepet descent algorithm seemed to work fine. It consistently found the same point for a lot of different starting points, which seems to me to indicate that it really

Figure 1: Error as a function of block size for 2 particles with 1×10^7 MC cycles without importance sampling. The error seems to flatten after a blocksize of 250 000.

Figure 2: Error as a function of block size for 2 particles with 1×10^7 MC cycles with importance sampling. The error seems to flatten after a blocksize of 200 000.
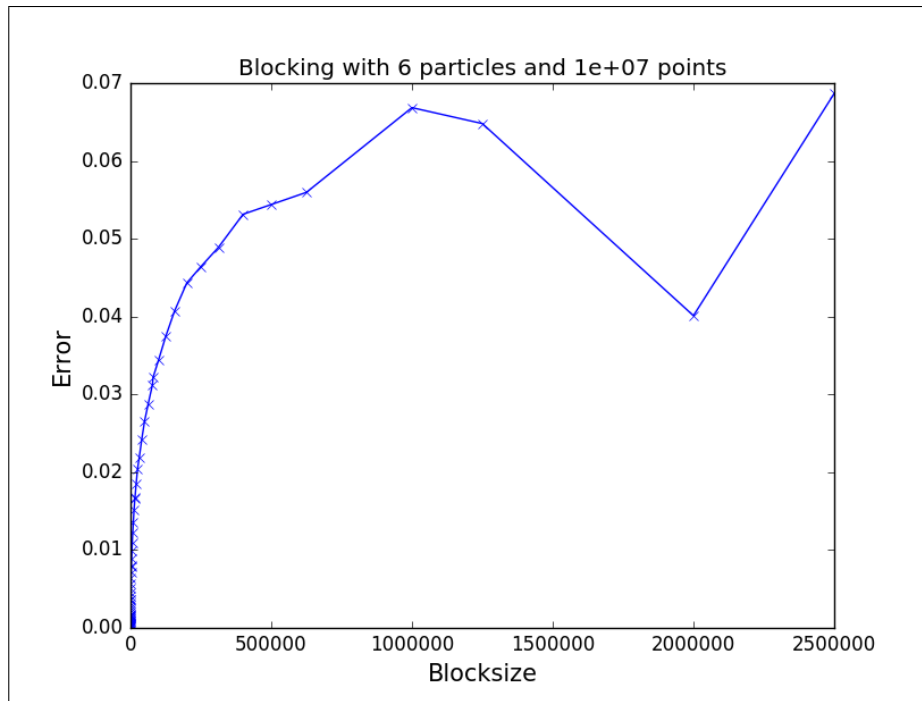
Figure 3: Error as a function of block size for 6 particles with 1×10^7 MC cycles without importance sampling. The error seems to flatten after a blocksize of 400 000.
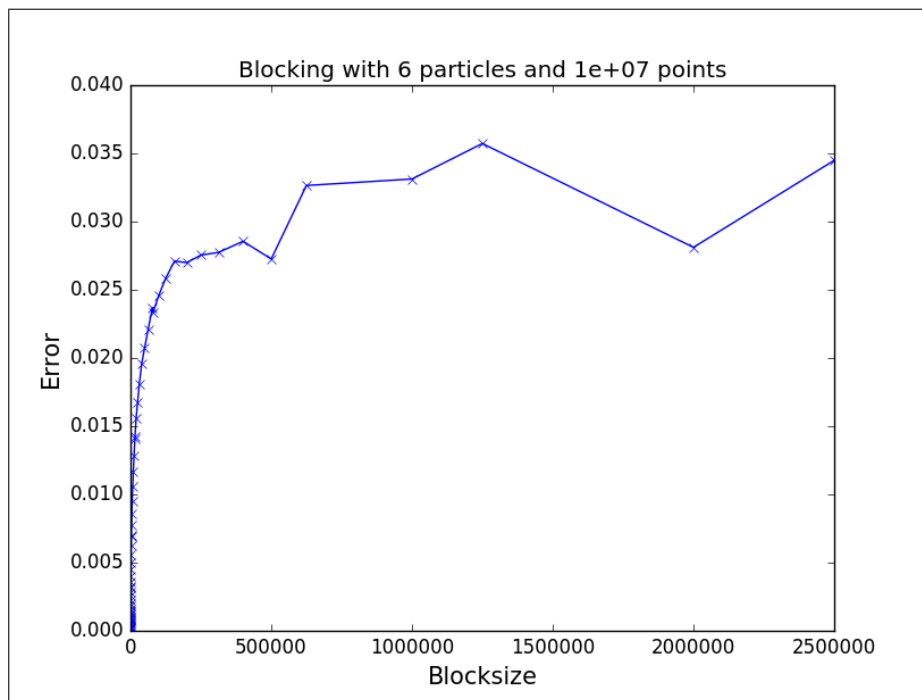
Figure 4: Error as a function of block size for 6 particles with 1×10^7 MC cycles with importance sampling. The error seems to flatten after a blocksize of 156 250.

Figure 5: Error as a function of block size for 12 particles with 1×10^7 MC cycles without importance sampling. The error seems to flatten after a blocksize of 500 000.

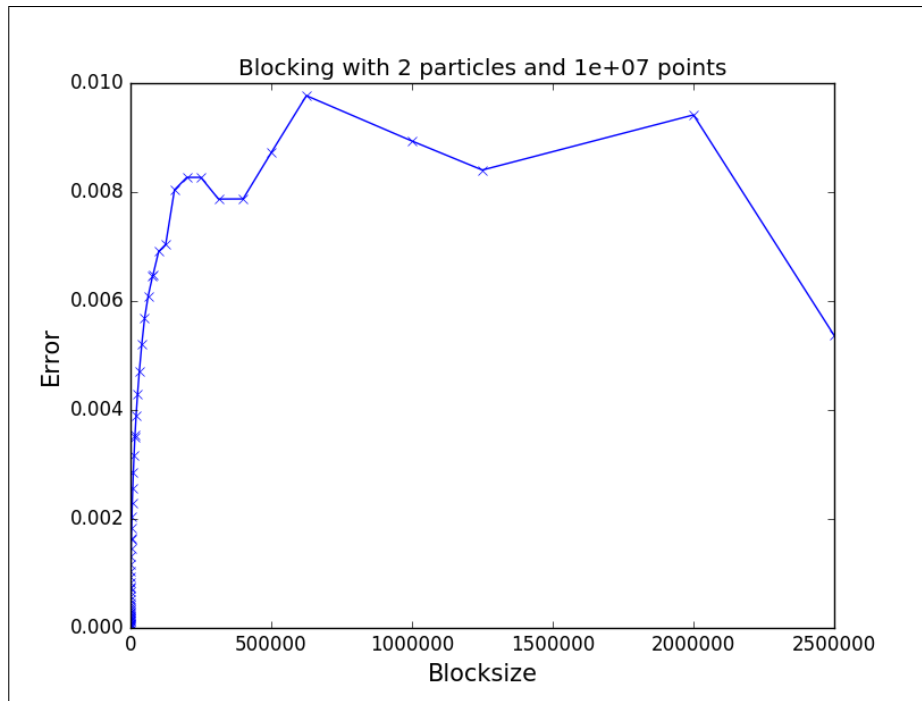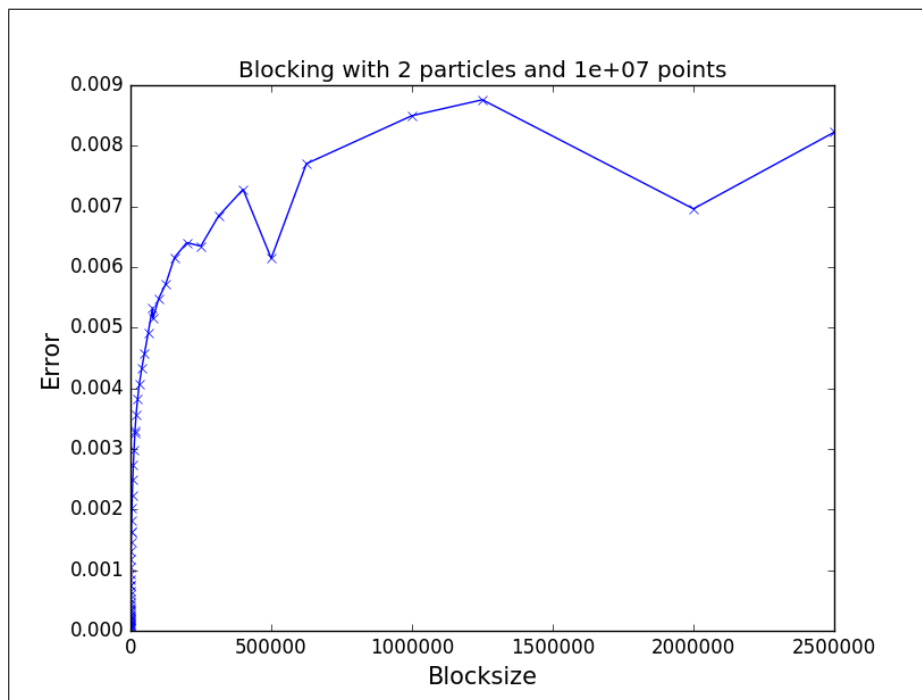Figure 6: Error as a function of block size for 12 particles with 1×10^7 MC cycles with importance sampling. The error seems to flatten after a blocksize of 100 000.
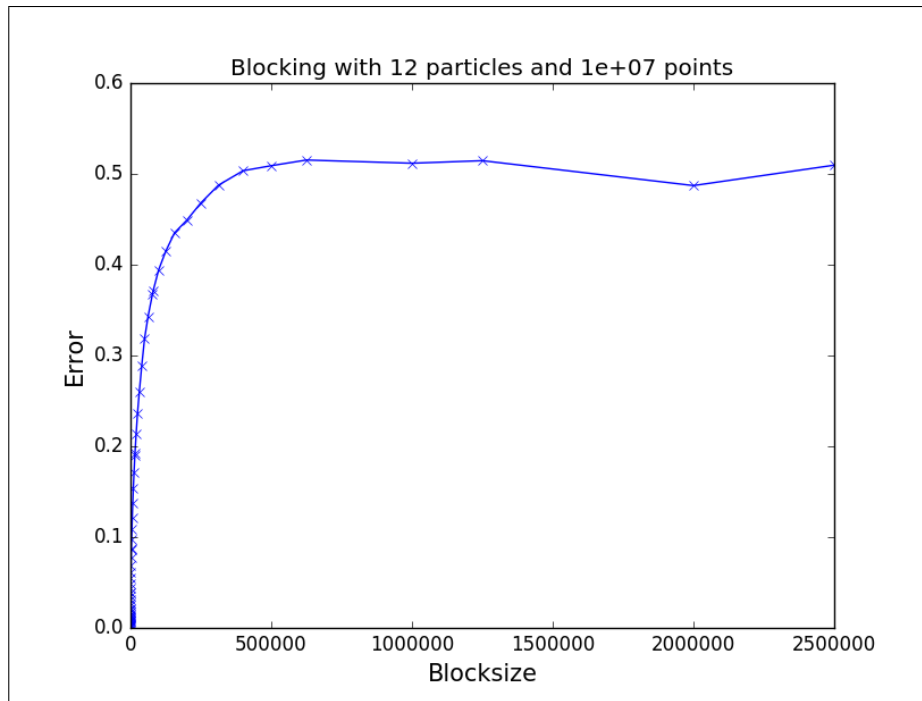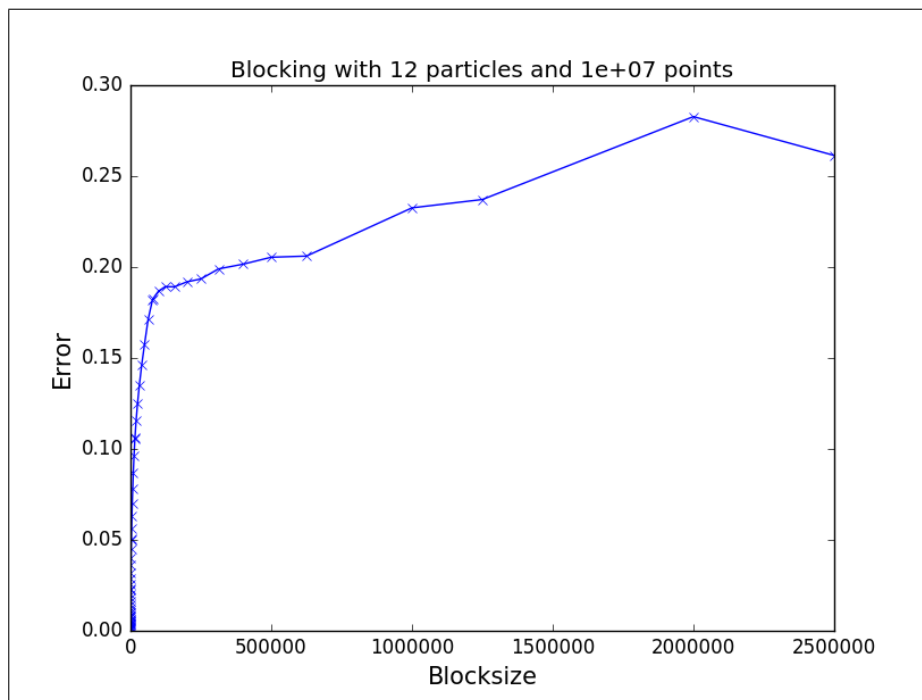
Table 2: Table of "optimal" parameters found by steepest descent.

N	ω	α (no Jastrow)	α	β
2	1	0.767	0.985	0.402
	0.5	0.691	0.976	0.328
	0.1	0.511	0.948	0.170
	0.05	0.438	0.916	0.155
	0.01	0.278	0.940	0.097
6	1	0.599	0.998	0.491
	0.5	0.532	0.956	0.475
	0.1	0.378	0.80	0.21
	0.05	0.314	0.5	0.15
	0.01	0.314	0.5	0.1
12	1	0.556	1	0.4
	0.5	0.478	1	0.3
	0.1	0.313	0.8	0.2
	0.05	0.260	0.6	0.1
	0.01	0.150	0.1	0.1

found a global minimum. However for the 6 and 12 particle cases the automatic algorithm produced very eratic results, and I decided to do the search manually. This seemed to work for the case with no jastrow factor, but failed with the jastrow factor. I discovered that the energy was very unstable as a function of the number of MC cycles, and that I probably needed to use 10^7 cycles to get reasonable results. One integral with 10^7 cycles took about 1 minute for 6 particles and about 3 or 4 minutes for 12 particles. Using this many points in a manual steepest descent search would be a grueling task, while an automatic search would have taken too much time. Therefore I decided to just calculate the energy of a few parameter combinations chosen based on the optimal parameters for the two particle case and chose the set that gave the lowest energy. Thus it may be a bit of a stretch to call these the optimal parameters. The parameters I ended up with are found in table 2.

6.4 Benchmarks

When the interaction is turned off, setting $\alpha = 1$ and turning off the jastrow factor make the trial wavefunctions 5 and 7 the known ground states with energies $2\omega, 10\omega$ and 28ω for the 2,6 and 12 particle case, respsectively. Since the ground state is an eigenstate the local energy for these states should be equal to the total energy at every point. Thus the MC integration should find the exact energies with zero variance, yielding an error estimate of zero. For these ground states it is also known that the expectation value for the kinetic and potential energies should be exactly half the total energy. However, the states are not eigenstates for kinetic and potential energy, so we can not expect to find this exactly. We may use this to see how well the error estimation based on blocking works, simply by comparing the deviation of the calculated values for $\overline{K}$ and $\overline{V}$ with the true means $\langle K \rangle = \langle V \rangle = \langle E \rangle /2$ and the expected error. I have calculations with blocking and 10^7 MC cycles for wavefunctions without jastrow factors, $\alpha = 1$ and no interaction in table 3. We see that in all cases $\overline{E} = \langle E \rangle$ exactly, with expected error equal to zero up to numerical precision. $\overline{K}$ and $\overline{V}$ are not exact, which is as expected, but they deviate from their exact values by much more than the expected error, especially for low ω.

When we turn on the interaction Taut has shown in [4] that the ground state energy for 2 particles and $\omega = 1$ is exactly 3 a.u.. Also [5] includes ground state energies for certain frequencies found by diffusion monte carlo methods. In [1] I used Hartree-Fock methods to build a slater determinant out of linear combinations of single particle wavefunctions and minimized the energy, which is another way to aproximate the ground state. I have collected these results in 4.

Table 3: Results from calculations with blocking and 10^7 MC cycles for wavefunctions without jastrow factors, $\alpha = 1$ and no interaction.

N	ω	$\overline{K}$	$\sigma_{\overline{K}}$	$\overline{V}$	$\sigma_{\overline{V}}$	$\overline{E}$	$\sigma_{\overline{E}}$	$\langle E \rangle$
2	1	1.05317	0.00131343	0.946828	0.00131343	2	-1.13869e-16	2
	0.5	0.535774	0.000661513	0.464226	0.000661513	1	0	1
	0.1	0.106852	9.89911e-05	0.093148	9.89911e-05	0.2	8.89602e-19	0.2
	0.05	0.054874	2.20498e-05	0.045126	2.20498e-05	0.1	8.89602e-20	0.1
	0.01	0.0151137	3.01902e-07	0.00488625	3.01902e-07	0.02	2.78001e-21	0.02
6	1	5.06396	0.0234623	4.93604	0.0234623	10	3.64381e-16	10
	0.5	2.52148	0.0100633	2.47852	0.0100633	5	-2.73286e-16	5
	0.1	0.570124	0.000367148	0.429876	0.000367148	1	5.69345e-18	1
	0.05	0.333559	6.76897e-05	0.166441	6.76897e-05	0.5	0	0.5
	0.01	0.0870228	6.50881e-07	0.0129772	6.50881e-07	0.1	1.3344e-19	0.1
12	1	13.8033	0.121219	14.1967	0.121219	28	0	28
	0.5	7.01541	0.0417814	6.98459	0.0417814	14	0	14
	0.1	1.51871	0.00237558	1.28129	0.00237558	2.8	6.83214e-17	2.8
	0.05	0.835721	0.000725358	0.564279	0.000725358	1.4	-3.98542e-17	1.4
	0.01	0.230431	1.24871e-05	0.0495693	1.24871e-05	0.28	-3.55841e-19	0.28

Table 4: Reference values for ground state energies found by, diffusion monte carlo collected from [5] (a), Hartree-Fock methods from [1] (b) and the exact value for 2 particles and $\omega = 1$ from [4] (c).

N	ω	$\overline{E}_a$	$\overline{E}_b$	E_c
2	1	3.00000	3.16191	3
	0.5	1.65975	2.8386	
6	1	20.1597	20.7192	
	0.5	11.7888	17.8352	
12	1	65.700	66.912	
	0.5	39.159	56.6229	

Table 5: Results of 4 paralell integrations with 10^7 MC cycles each for 2 particles. The variation parameters chosen are those from table 2 and the expected errors have been calculated with the blocking method with blocksizes according to table 1.The "J?" collumn indicates whether the jastrow factor was included or not.

ω	J?	$\overline{K}$	$\sigma_{\overline{K}}$	$\overline{V}$	$\sigma_{\overline{V}}$	$\overline{E}$	$\sigma_{\overline{E}}$	$\overline{r_{12}}$	time
1	yes	0.896043	0.0185009	2.10496	0.0183245	3.001	0.000765124	1.64293	5.58495
	no	0.762656	0.0164748	2.37302	0.0257503	3.13568	0.0210561	1.44959	3.64587
0.5	yes	0.442345	0.0140292	1.21753	0.0136653	1.65988	0.00105956	2.49304	5.59341
	no	0.339068	0.0106497	1.44792	0.0220222	1.78699	0.0200221	2.17777	3.76321
0.1	yes	0.0854813	0.00428608	0.356026	0.00398314	0.441507	0.000934913	6.88561	5.64161
	no	0.0449886	0.00241899	0.465024	0.011365	0.510013	0.0110211	5.90909	3.67108
0.05	yes	0.0373425	0.00353373	0.216955	0.00317596	0.254297	0.000806016	10.1328	5.61539
	no	0.0192918	0.00111495	0.313173	0.0112679	0.332465	0.0114061	8.95725	3.63865
0.01	yes	0.00715056	0.000859333	0.0695279	0.000865545	0.0766784	0.000473462	23.3606	5.547
	no	0.00399493	0.000103827	0.125667	0.00787434	0.129662	0.00790149	15.8172	3.63274

Table 6: Results of 4 paralell integrations with 10^7 MC cycles each for 6 particles. The variation parameters chosen are those from table 2 and the expected errors have been calculated with the blocking method with blocksizes according to table 1.The "J?" collumn indicates whether the jastrow factor was included or not.

ω	J?	$\overline{K}$	$\sigma_{\overline{K}}$	$\overline{V}$	$\sigma_{\overline{V}}$	$\overline{E}$	$\sigma_{\overline{E}}$	time
1	yes	3.68271	0.06032	16.5068	0.0529771	20.1895	0.0145315	57.8832
	no	2.99233	0.0545036	17.7254	0.0956411	20.7177	0.0708336	16.7907
0.5	yes	1.85946	0.0391915	9.998	0.0339211	11.8575	0.0168981	60.13
	no	1.32267	0.0255294	10.9755	0.0623592	12.2981	0.0541781	16.6152
0.1	yes	0.296443	0.0125718	3.2867	0.011232	3.58314	0.00453845	57.2104
	no	0.206651	0.00398447	3.62807	0.0352785	3.83472	0.0372295	16.665
0.05	yes	0.0682081	0.0117284	2.15215	0.00884077	2.22035	0.0134219	62.8669
	no	0.101616	0.00179862	2.48552	0.0430841	2.58714	0.0442215	17.0087
0.01	yes	-0.138742	0.0221044	0.825324	0.0161958	0.686582	0.00717069	65.096
	no	0.027521	0.000172539	1.68502	0.0554644	1.71254	0.0555953	16.6392

6.5 MC Integration

I ran the integration with 10^7 MC cycles in 4 paralell processes. I assumed that the 4 results were uncorrelated when calculating the expected error, meaning I used equation 42. I collected the results in tables 5,6 and 7.

6.6 Onebody Densities

The onebody density for a multiparticle wavefunction $\psi(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N)$ is

$$\int |\psi|^2 \prod_{i=2}^{N} d\boldsymbol{r}_i. \tag{49}$$

Figure 7 shows the onebody density of the 2 particle trial wavefunction for $\omega = 1$ and optimal parameters both with and without the jastrow factor.

6.7 Cost and paralellization

Let T be the time it takes to run a program and T_N be the time it takes to run a paralellized version of the program in N processes. The paralellization is done in such a way that the paralellized program

Table 7: Results of 4 paralell integrations with 10^7 MC cycles each for 12 particles. The variation parameters chosen are those from table 2 and the expected errors have been calculated with the blocking method with blocksizes according to table 1.The "J?" collumn indicates whether the jastrow factor was included or not.

ω	J?	$\overline{K}$	$\sigma_{\overline{K}}$	$\overline{V}$	$\sigma_{\overline{V}}$	$\overline{E}$	$\sigma_{\overline{E}}$	time
1	yes	8.54277	0.13305	57.6363	0.124573	66.179	0.0544664	362.953
	no	7.75721	0.138949	59.6794	0.201069	67.4366	0.152718	98.2915
0.5	yes	4.2585	0.0757153	35.2696	0.0653093	39.5281	0.0356756	357.436
	no	3.21622	0.0626376	37.1745	0.149676	40.3907	0.124732	86.3928
0.1	yes	0.600904	0.0505859	11.6492	0.031241	12.2501	0.0245983	360.226
	no	0.541136	0.010503	13.0991	0.14344	13.6402	0.1504	86.9919
0.05	yes	-0.627686	0.167751	7.73977	0.0363206	7.11209	0.159102	407.275
	no	0.276648	0.00368362	9.61352	0.214207	9.89016	0.217163	80.9301
0.01	yes	-1.89996	0.20771	3.49049	0.0992233	1.59053	0.111508	389.397
	no	0.0403921	8.45161e-05	7.47626	0.28336	7.51665	0.283431	84.4429
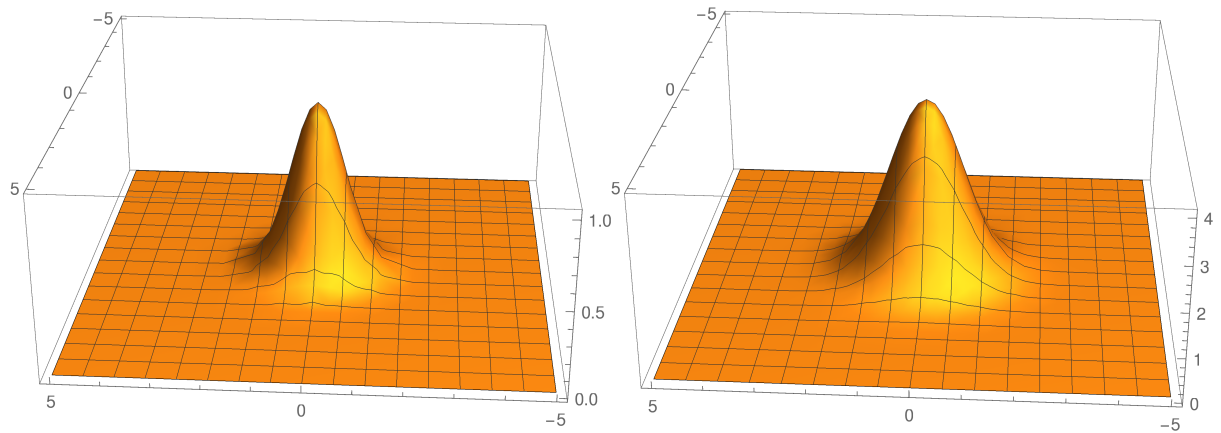
(a) With Jastrow

(b) Without Jastrow

Figure 7: Onebody density for 2 particles, $\omega = 1$ with optimal parameters.

performs the task to be performed N times. So in our case if it takes T to perform an integral with 10^7 MC cycles then T_N is the time it takes to perform N integrals with 10^7 MC cycles each. Let f be the fraction of T that is parallizable so that

$$T_N = fT + (1-f)NT, \tag{50}$$

then

$$f = \frac{NT - T_N}{NT - T}. \tag{51}$$

N is chosen while T and T_N are measurable so f is now a measurable quantity. I ran the program for 2 particles with 10^7 MC cycles 10 times both paralellized on 4 cores and non-parallelizes. The average time used was $T = 11.84$ s and $T_4 = 13.51$ s. Then $f = 0.95$. Theoretically f is 1 as each process is completely independent so 0.95 is quite low. This is partially due to the overhead of distributing and governing the jobs, but i think most of the difference is due to synchronization holdup. The time use for each process has some variability, but re-gathering results from the distributed processes requires all jobs to be finished. Thus every process must wait on the slowest process, which means that T_N goes as the average of the slowest of N processes, while T is just the average time use for a process.

7 Discussion

7.1 Errors

As mentioned the kinetic and potential energy expectation values of harmonic oscillator eigenstates are exactly equal to half the energy. Thus we know the absolute error of the estimates for kinetic and potential energy in table 3. Comparing with the error estimates from the blocking analysis, we see that the error estimates badly underestimate the true error. In fact they seem to miss by about an order of magnitude. The blocksize was chosen based on analysing calculations of the total energy and so perhaps this only shows that I should have used a different blocksize based on what quantity I am looking at, but most of the correlations should come from the points chosen from the probability distribution, and the function we apply to these should not matter. Thus I think this may be an indication that I have underestimated the errors even after blocking.

Also note that the error estimates for $\overline{K}$ and $\overline{V}$ are bigger than those for $\overline{E}$, which seems weird at first glance, after all $E = K + V$. The reason for this is that the local energy is calculated from the local kinetic and potential energy at each integration point, and the quadratic terms in K_L and V_L partially cancel. Thus E_L varies less with position that both K_L and V_L making the uncertainty smaller.

In tables 6 and 7 we see that for small ω and the Jastrow factor switched on $\overline{K}$ can be negative and the estimated error is too small to make up. This is obviously wrong, and could indicate that there is a bug in the code and throw into question the rest of the results. However, I have already noted that the estimated error for K and V is too small by at least an order of magnitude. Taking this into account makes $\overline{K} > 0$ be within the error.

7.2 Average distance between particles

In the 2 particle case I included a calculation of the average relative distance of the particles, found in table 5. We see that the distance increases dramatically when ω decreases, and that the distance is greater in cases where the jastrow factor is included. In figure 7 we saw that the onebody density was more condensed about the origin with the jastrow factor than without. These results seem contradictory at first glance, but I suppose there are details in the wavefunction that are missed by simply looking at a plot of the onebody density.

7.3 Comparison of results with and without Jastrow factor

Looking at tables 5, 6 and 7 we see that the energy estimates $\overline{E}$ are consistently lower when the jastrow factor is used. The jastrow factor seems to be more important for higher numebers of particles and lower ω. This makes sense as the factor is supposed to account for the interactions of the particles,

which naturally are more important the more particles there are and the stronger the interaction is compared to the confining potential.

7.4 Comparison of results with benchmark values

Comparing the results to table 4 we see that in the 2 particle case the energies with the jastrow factor are equal to the diffusion MC results within the errors. For 6 and 12 particles the diffusion MC energies are mostly outside of the error ranges of my results. This is probably due to the parameter optimization not working as well as I had hoped, but could also be a reflection of an overoptimistic estimation of the error. If we compare instead with the Hartree-Fock results we find that my results give lower energies both with and without the jastrow factor, especially for $\omega = 0.5$.

7.5 The virial theorem

The virial theorem states that

$$\langle T \rangle = \frac{1}{2} \sum_{k}^{N} \langle \nabla_k V \cdot \boldsymbol{r}_k \rangle, \tag{52}$$

in our case this yields

$$\langle T \rangle = \langle V_{HO} \rangle - \frac{1}{2} \langle V_I \rangle. \tag{53}$$

As I have not calculated $\overline{V}_{HO}$ or $\overline{V}_I$ there is no straightforward way to check if this is obeyed. But rewriting

$$\langle V \rangle = \langle T \rangle + \frac{3}{2} \langle V_I \rangle, \tag{54}$$

we at least see that we should expect the potential energy to be higher than the kinetic, especially when interactions grow more important, i.e. when the frequency is low and number of particles high. This relationship seems to be borne out by the data.

8 Conclusion

Even with the strange results of negative kinetic energy, I think the results are mostly trustworthy and probably quite close to the true ground energies. There are two main problems. We have seen that the estimated errors for kinetic and potential energy are too small by an order of magnitude, which leads me to question the error estimates for the total energy as well.

The other main problem is the parameter optimisation. As mentioned I needed to use 10^7 MC cycles for the integrals for many particles to be fairly accurate, which took too much time to perform a proper steepest descent search. Thus the wavefunctions I ended up integrating are probably not really the optimal wavefunctions from our class. For better results, this is what I would first and foremost try to improve. As noted the code has not been properly optimized and doing so may decrease the cost enough too make the steepest descent take considerably less time. Else one might put more effort into making a robust automatic steepest descent function that can run unsupervised for as long as it takes. One could also try another optimization method like for example the conjugate gradient method.

A A Note About Cofactors and Determinants

Determinants can be somewhat hard to work with, following [6] we may use cofactors to do some trickery. For a matrix A with elements A_{ij} the cofactors C_{ij} are given by $(-1)^{i+j}M_{ij}$, with M_{ij} being the determinant of the matrix formed by deliting the ith row and jth collumn from A. There two properties of cofactors that will be important here are

$$|A|\mathbf{1} = AC^T \Leftrightarrow |A| = \sum_j A_{ij}C_{ij}, \tag{55}$$

and thus

$$A^{-1} = \frac{1}{|A|} C^T \Leftrightarrow A_{ij}^{-1} = \frac{1}{|A|} C_{ji}, \tag{56}$$

and the fact that C_{ij} is independent of row i and collumn j of A.

B Derivatives of the 2 particle trial wavefunction

In the course of the project we needed analytical expressions for different derivatives of the 2 particle trial wavefunction 5. I have collected the differentiations here.

B.1 Gradient

In order to compute the driftforce for importance sampling we needed

$$\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial z},$$

where $z_i = x_1, x_2, y_1, y_2$. As ψ_T is an exponential

$$
\begin{aligned}
\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial z_i} &= \frac{\partial}{\partial z_i} \left(-\frac{1}{2}\alpha\omega(r_1^2 + r_2^2) + \frac{ar_{12}}{1 + \beta r_{12}} \right) \\
&= -\alpha\omega z_i + a \left(\frac{1}{1 + \beta r_{12}} - \frac{r_{12}\beta}{(1 + \beta r_{12})^2} \right) \frac{\partial r_{12}}{\partial z_i} \\
&= -\alpha\omega z_i + \frac{a}{(1 + \beta r_{12})^2} \frac{\partial r_{12}}{\partial z_i} \\
&= -\alpha\omega z_i + \frac{a}{(1 + \beta r_{12})^2} \frac{(z_i - z_j)}{r_{12}},
\end{aligned}
$$

where z_j is the coordinate of the other particle along the same dimension as z_i, so for example when $z_i = x_2, z_j = x_1$.

B.2 Laplacian

The local energy is defined as

$$E_L(\boldsymbol{r_1}, \boldsymbol{r_2}) = \frac{1}{\psi_T} H \psi_T.$$

In our case the Hamiltonean is

$$H = \sum_{i=1}^{2} -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 + \frac{1}{r_{12}}.$$

The laplacian is

$$\sum_i \nabla^2 = \sum_i \frac{\partial^2}{\partial z_i^2},$$

where z_i is the same as above.

Again since ψ_T is an exponential we have

$$
\begin{aligned}
\frac{1}{\psi_T} \frac{\partial^2 \psi_T}{\partial z_i^2} &= \frac{\partial^2}{\partial z_i^2} \left(-\alpha\omega(r_1^2 + r_2^2)/2 + \frac{ar_{12}}{1 + \beta r_{12}} \right) + \left(\frac{\partial}{\partial z_i} \left(-\alpha\omega(r_1^2 + r_2^2)/2 + \frac{ar_{12}}{1 + \beta r_{12}} \right) \right)^2 \\
&= \frac{\partial}{\partial z_i} \left(-\alpha\omega z_i + \frac{a}{(1 + \beta r_{12})^2} \frac{(z_i - z_j)}{r_{12}} \right) + \left(-\alpha\omega z_i + \frac{a}{(1 + \beta r_{12})^2} \frac{(z_i - z_j)}{r_{12}} \right)^2 \\
&= -\alpha\omega + \frac{a}{(1 + \beta r_{12})^2 r_{12}} - \frac{2a\beta(z_i - z_j)^2}{(1 + \beta r_{12})^3 r_{12}^2} - \frac{a(z_i - z_j)^2}{(1 + \beta r_{12})^2 r_{12}^3} + \alpha^2\omega^2 z_i^2 - \frac{2\alpha\omega a z_i(z_i - z_j)}{(1 + \beta r_{12})^2 r_{12}} + \frac{a^2(z_i - z_j)^2}{(1 + \beta r_{12})^4 r_{12}^2}.
\end{aligned}
$$

So, because the ψ_T is symmetric under $1 \leftrightarrow 2$ and $x \leftrightarrow y$:

$$\frac{1}{\psi_T} \sum_i \nabla_i^2 \psi_T = \alpha\omega(r_1^2 + r_2^2) - 4\alpha\omega + \frac{2a^2}{(1+\beta r_{12})^4} + \frac{4a}{(1+\beta r_{12})^2 r_{12}} - \frac{4a\beta}{(1+\beta r_{12})^3} - \frac{2a}{(1+\beta r_{12})^2 r_{12}} - \frac{2\alpha\omega a r_{12}}{(1+\beta r_{12})^2}$$

and finally:

$$\frac{1}{\psi_T} \sum_i \nabla_i^2 \psi_T = \alpha\omega(r_1^2 + r_2^2) - 4\alpha\omega + \frac{2a}{(1+\beta r_{12})^2} \left[\frac{a}{(1+\beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{(1+\beta r_{12})} - \alpha\omega r_{12} \right]$$

Using this expression we have the local energy as

$$E_L(\mathbf{r_1}, \mathbf{r_2}) = \left[\frac{1}{2}(1-\alpha)\omega(r_1^2 + r_2^2) + 2\alpha\omega \right] - \frac{a}{(1+\beta r_{12})^2} \left[\frac{a}{(1+\beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{(1+\beta r_{12})} - \alpha\omega r_{12} \right] + \frac{1}{r_{12}},$$

where the second term contains the terms from the Jastrow-factor and the cross term and the third is the interaction term.

B.3 Derivatives w.r.t α and β

In order to find the optimal parameters α and β we needed the derivatives of ψ_T with respect to these.

$$\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial \alpha} = -\frac{1}{2}\omega(r_1^2 + r_2^2).$$

$$\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial \beta} = -\frac{a r_{12}^2}{(1+\beta r_{12})^2}.$$

C Derivatives of the N particle trial wavefunction

In the course of the project we needed analytical expressions for different derivatives of the N particle trial wavefunction 7. I have collected the differentiations here.

C.1 Gradient

We note that for any coordinate z_i only one of the determinants depends on it. So

$$\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial z_i} = \frac{1}{|s|} \frac{\partial |s|}{\partial z_i} + \frac{1}{J} \frac{\partial J}{\partial z_i}.$$

For the derivative of the determinant we exploit the properties noted in section A to see that

$$\frac{1}{|s|} \frac{\partial |s|}{\partial z_i} = \frac{1}{|s|} \sum_j \frac{\partial s_{ij}}{\partial z_i} C_{ij},$$

since C_{ij} is independent of z_i. Rewriting $C_{ij} = |s| s_{ji}^{-1}$ we find

$$\frac{1}{|s|} \frac{\partial |s|}{\partial z_i} = \sum_j \frac{\partial s_{ij}}{\partial z_i} s_{ji}^{-1}.$$

From section B.1 it is clear that

$$\frac{1}{J} \frac{\partial J}{\partial z_i} = \sum_{j \neq i} \frac{a_{ij}}{(1+\beta r_{ij})^2} \frac{(z_i - z_j)}{r_{ij}},$$

so

$$\frac{1}{\psi_T} \frac{\partial \psi_T}{\partial z_i} = \sum_j \frac{\partial s_{ij}}{\partial z_i} s_{ji}^{-1} + \sum_{j \neq i} \frac{a_{ij}}{(1+\beta r_{ij})^2} \frac{(z_i - z_j)}{r_{ij}}.$$

C.2 Laplacian

Writing $\psi_T = \psi_S J$ we can write the Laplacian as

$$\frac{\nabla^2 \psi_T}{\psi_T} = \frac{\nabla^2 \psi_S}{\psi_S} + \frac{\nabla^2 J}{J} + 2\frac{\nabla \psi_S}{\psi_S} \cdot \frac{\nabla J}{J},$$

expanding the Slater part $\psi_S = |S|_\downarrow |S|_\uparrow$ we find

$$\frac{\nabla^2 \psi_T}{\psi_T} = \frac{\nabla^2 |S|_\downarrow}{|S|_\downarrow} + \frac{\nabla^2 |S|_\uparrow}{|S|_\uparrow} + \frac{\nabla^2 J}{J} + 2\left(\frac{\nabla |S|_\downarrow}{|S|_\downarrow} + \frac{\nabla |S|_\uparrow}{|S|_\uparrow}\right) \cdot \frac{\nabla J}{J},$$

noting that there is no cross-term between the determinants as they depend on different coordinates. By the same arguments as above we find

$$\frac{1}{|S|}\frac{\partial^2 |S|}{\partial z_i^2} = \sum_j \frac{\partial^2 s_{ij}}{\partial z_i^2} s_{ji}^{-1},$$

which means that

$$\begin{aligned}
\frac{\nabla^2 \psi_s}{\psi_s} &= \sum_{ij} (\nabla^2 s_{ij}^\downarrow) s_{ji}^{\downarrow,-1} + (\nabla^2 s_{ij}^\uparrow) s_{ji}^{\uparrow,-1} \\
&= \sum_{ij}^{N/2} (\nabla^2 \psi_{\downarrow,j}(\boldsymbol{r}_i)) s_{ji}^{\downarrow,-1} + (\nabla^2 \psi_{\uparrow,j}(\boldsymbol{r}_i)) s_{ji}^{\uparrow,-1} \\
&= \sum_{ij}^{N/2} (\alpha^2 \omega^2 r_i^2 - 2\alpha\omega(n_{x,j} + n_{y,j} + 1))\psi_j(\boldsymbol{r}_i) s_{ji}^{\downarrow,-1} + (\alpha^2 \omega^2 r_{i+N/2}^2 - 2\alpha\omega(n_{x,j} + n_{y,j} + 1))\psi_j(\boldsymbol{r}_{i+N/2}) s_{ji}^{\uparrow,-1} \\
&= \sum_{ij}^{N/2} (\alpha^2 \omega^2 r_i^2 - 2\alpha\omega(n_{x,j} + n_{y,j} + 1)) s_{ij}^\downarrow s_{ji}^{\downarrow,-1} + (\alpha^2 \omega^2 r_{i+N/2}^2 - 2\alpha\omega(n_{x,j} + n_{y,j} + 1)) s_{ij}^\uparrow s_{ji}^{\uparrow,-1} \\
&= \sum_{i=1}^{N} \alpha^2 \omega^2 r_i^2 - 4\alpha\omega \sum_j^{N/2} (n_{x,j} + n_{y,j} + 1),
\end{aligned}$$

where I have used that $\sum_j s_{ij} s_{ji}^{-1} = \sum_i s_{ji}^{-1} s_{ij} = 1$. For the jastrow part

$$\frac{1}{J}\frac{\partial^2 J}{\partial z_i^2} = \sum_{j\neq i} \frac{\partial^2 f_{ij}}{\partial z_i^2} + \left(\sum_{j\neq i} \frac{\partial f_{ij}}{\partial z_i}\right)^2,$$

with $f_{ij} = a_{ij} r_{ij}/(1 + \beta r_{ij})$, so

$$\frac{1}{J}\frac{\partial^2 J}{\partial z_i^2} = \sum_{j\neq i} \frac{a_{ij}}{(1+\beta r_{ij})^2}\left[\frac{1}{r_{ij}}\left(1 - \left(\frac{(z_i - z_j)}{r_{ij}}\right)^2\right) - \frac{2\beta}{(1+\beta r_{ij})}\left(\frac{(z_i - z_j)}{r_{ij}}\right)^2\right] + \left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial z_i}\right)^2,$$

and

$$\frac{\nabla_i^2 J}{J} = \sum_{j\neq i}\frac{a_{ij}}{(1+\beta r_{ij})^2}\left[\frac{1}{r_{ij}} - \frac{2\beta}{(1+\beta r_{ij})}\right] + \left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial x_i}\right)^2 + \left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial y_i}\right)^2,$$

and finally

$$\frac{\nabla^2 J}{J} = 2\sum_{j<i}\frac{a_{ij}}{(1+\beta r_{ij})^2}\left[\frac{1}{r_{ij}} - \frac{2\beta}{(1+\beta r_{ij})}\right] + \sum_i\left[\left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial x_i}\right)^2 + \left(\sum_{j\neq i}\frac{\partial f_{ij}}{\partial y_i}\right)^2\right],$$

The cross terms become

$$2\left(\frac{\nabla |S|_\downarrow}{|S|_\downarrow} + \frac{\nabla |S|_\uparrow}{|S|_\uparrow}\right) \cdot \frac{\nabla J}{J} = 2\sum_i\left(\frac{1}{|s|}\frac{\partial |s|}{\partial x_i}\frac{1}{J}\frac{\partial J}{\partial x_i} + \frac{1}{|s|}\frac{\partial |s|}{\partial y_i}\frac{1}{J}\frac{\partial J}{\partial y_i}\right).$$

C.3 Derivative w.r.t α and β

The many particle generalizations of the formulas from section B.3. For α we again need the derivative of a determinant, but the arguments for the adjugate C^T being independent of the diffentiation variable used above is no longer valid. Luckily Jacobis formula says that we may still use a similar expression:

$$\frac{1}{|A|}\frac{\mathrm{d}|A|}{\mathrm{d}\alpha} = \sum_{i,j}\frac{\mathrm{d}A_{ij}}{\mathrm{d}\alpha}A_{ji}^{-1}.$$

In our case we then have

$$\frac{1}{\psi_T}\frac{\partial\psi_T}{\partial\alpha} = \sum_{i,j}\frac{\partial\psi_i(\boldsymbol{r}_j)}{\partial\alpha}s_{ji}^{\downarrow,-1} + \frac{\partial\psi_i(\boldsymbol{r}_{j+N/2})}{\partial\alpha}s_{ji}^{\uparrow,-1}.$$

$$\begin{aligned}
\frac{\partial\psi_i(\boldsymbol{r})}{\partial\alpha} &= \omega\frac{\partial\psi_i(\boldsymbol{r})}{\partial\alpha\omega}\\
&= \omega\left(\frac{\partial\sqrt{\alpha\omega}x}{\partial\alpha}H'_{n_x}(\sqrt{\alpha\omega}x)H_{n_y}(\sqrt{\alpha\omega}y) + \frac{\partial\sqrt{\alpha\omega}y}{\partial\alpha}H_{n_x}(\sqrt{\alpha\omega}x)H'_{n_y}(\sqrt{\alpha\omega}y)\right.\\
&\quad\left. -\frac{1}{2}(x^2+y^2)H_{n_x}(\sqrt{\alpha\omega}x)H_{n_y}(\sqrt{\alpha\omega}y)\right)e^{-\alpha\omega(x^2+y^2)/2}\\
&= \omega\left(\frac{xn_x}{\sqrt{\alpha\omega}}H_{n_x-1}(\sqrt{\alpha\omega}x)H_{n_y}(\sqrt{\alpha\omega}y) + \frac{yn_y}{\sqrt{\alpha\omega}}H_{n_x}(\sqrt{\alpha\omega}x)H_{n_y-1}(\sqrt{\alpha\omega}y)\right.\\
&\quad\left. -\frac{1}{2}(x^2+y^2)H_{n_x}(\sqrt{\alpha\omega}x)H_{n_y}(\sqrt{\alpha\omega}y)\right)e^{-\alpha\omega(x^2+y^2)/2}.
\end{aligned}$$

The β derivative is a lot simpler:

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

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