

## Project 2

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June 3, 2021

### Abstract

Rust is used to develop a ground state solver for fermionic systems in an harmonic oscillator potential, utilizing the variational principle, Monte Carlo integration and two different implementations of the Metropolis-Hastings algorithm. The results are compared with analytical solutions to the corresponding systems.

The effect of the so-called Jastrow factor shows a **increase/decrease** on energies, onebody densities and ... at **these conditions - eg system  $N = 2$  and this result** on the higher number of particles.

# Chapter 1

## Introduction

Quantum dots are considered as point particles with confined electrons, usually existing in semiconductor materials, with different electrical and optical properties compared to its host. The difference in properties are due to quantum mechanical effects, yielding quantification of the energy of the system. The technology is utilized in photovoltaic devices to enhance performance, in LED's, photodetectors and more.

This paper presents a numerical study of such quantum dots confined in a Harmonic Oscillator potential. The system in question consists of closed shell configurations, from two to 20 electrons. The energy of the ground state is calculated using variational Monte Carlo, where a set of parameters are optimized in order to obtain accurate calculations as possible. For the simplest system (??) the numerical results are compared to analytical calculations.

The report first gives an overview of the theoretical background for the system and the methods. Derivation of the analytical expressions for the simplest system are presented, in order to give a benchmark to which we can compare the performance and accuracy of our numerical solver. Thereafter we present the methodology behind our numerical solver. Then the results from the calculations are presented, before a discussion and **suggestions for future work** are given. Hidden calculations and notation are presented in Appendix.

# Chapter 2

## Theory

We consider a system of electrons situated in an isotropic harmonic oscillator potential. We will use Hartree's atomic units<sup>1</sup> in order to get the idealized Hamiltonian presented below:

$$H = \sum_{i=1}^N \left( -\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 |\mathbf{r}_i|^2 \right) + \sum_{i < j} \frac{1}{r_{ij}}. \quad (2.1)$$

Here  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$  is the distance between two electrons. The first sum is the single particle harmonic oscillator potential. Because electrons repel each other, we also get the latter repulsive sum as part of the Hamiltonian - the perturbation of the system.

### 2.1 The unperturbed wave function

Disregarding interactions, there is a closed-form solution for the Hamiltonian shown in equation (2.1) for a single particle. The solutions follows [2]:

$$\phi_{n_x, n_y}(x, y, \alpha) = A H_{n_x}(\sqrt{\alpha\omega}x) H_{n_y}(\sqrt{\alpha\omega}y) \exp \left[ -\frac{\alpha\omega}{2}(x^2 + y^2) \right]. \quad (2.2)$$

Here,  $H_{n_i}$  are Hermite polynomials (see A.1), and  $A$  is the normalization constant. For the lowest lying state, we have  $n_x = n_y = 0$  and hence the energy of a non-interacting fermion  $\epsilon$  is:

$$\epsilon_{n_x, n_y} = \omega(n_x + n_y + 1) = \omega. \quad (2.3)$$

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<sup>1</sup> $\hbar = c = e = m_e = 1$ , see [1].

The Pauli exclusion principle states that two fermions can not occupy the same quantum state simultaneously. For each state  $(n_x, n_y)$  a fermion may have spin up or down, which means it can be occupied by at most two fermions. Using this principle, the ground state energies of the closed-shell configurations  $N = 2, 6, 12$  and 20 can easily be calculated using equation (2.3). The energies are given in table ??.

Table: The ground state energy of  $N$  non-interacting particles in an isotropic harmonic potential well.  $\omega$  is the oscillator frequency. Energies are given in Hartree's atomic units. | **Number of particles**  $N$  |  $E$  (a.u) | | —: | — | 2 |  $2\omega$  | | 6 |  $10\omega$  | | 12 |  $28\omega$  | | 20 |  $60\omega$  | {#tbl:energies}

These energies serve as great values to benchmark our program against.

## 2.2 The complete wave function

Single harmonic oscillators are solvable analytically, but introducing the repulsive perturbation forces us to tackle the problem differently. We choose a variational Monte Carlo approach, and use the Slater-Jastrow type of trial wave function, namely

$$\Psi_T(\mathbf{R}, \alpha, \beta) = \Psi_D \Psi_J = \det(D(\mathbf{R}, \alpha)) \exp(J(\mathbf{R}, \beta)),$$

where  $D(\mathbf{R})$  is a Slater matrix and  $J(\mathbf{R})$  is a Padé-Jastrow correlation function.  $\mathbf{R}$  here represents the set of all the individual particle's positions, and  $\alpha$  and  $\beta$  are the variational parameters. Following [2], our ansatz for the factors of this trial wave function is:

$$\begin{aligned} \Psi_D &= \det(D(\mathbf{R}, \alpha)), & D_{ij} &= \phi_j(\mathbf{r}_i, \alpha), \\ \Psi_J &= \prod_{i < j}^N \exp\left(\frac{ar_{ij}}{1 + \beta r_{ij}}\right). \end{aligned} \tag{2.4}$$

$\phi_j(\mathbf{r}_i)$  is the single particle wave function for the  $i$ -th fermion, as shown in (2.2), with  $j$  being an index describing each unique quantum state<sup>2</sup>. The coefficient  $a = 1$  when the electrons  $i$  and  $j$  have anti-parallel spins, and  $a = \frac{1}{3}$  when their spins are parallel. The index notation on the product is as explained in A.2.

### 2.2.1 A system of $N = 2$ fermions

Expanding the ansatz (2.4) for a system of two fermions, the trial wave function is reduced to:

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<sup>2</sup>E.g.  $(0, 0, \uparrow)$ ,  $(2, 1, \downarrow)$ , etc.

$$\Psi_T(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left( -\frac{\alpha\omega (|\mathbf{r}_1|^2 + |\mathbf{r}_2|^2)}{2} \right) \exp \left( \frac{ar_{12}}{1 + \beta r_{12}} \right).$$

The total spin in the ground state of this system is simply zero as the two fermions are paired with opposite spins.

## 2.3 Local energy

We define the *local energy* of a wave function as:

$$E_L \equiv \frac{1}{\Psi} H \Psi.$$

As shown in B.1, the local energy for a two-fermion system is:

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

The numerical local (kinetic) energy is calculated using the derivative of the velocity utilizing the two point approximation of the first derivative

$$\frac{dg(x)}{dx} \approx \frac{g(x + \Delta x) - g(x - \Delta x)}{2\Delta x}$$

Second derivative by three point approximation

$$\frac{d^2g(x)}{dx^2} \approx \frac{g(x + \Delta x) - 2g(x) + g(x - \Delta x)}{\Delta x^2}$$

$\Delta x$  is the stepsize which we let run towards zero. The error is proportional to  $(\Delta x^2)$ .

## 2.4 Quantum Force

Importance sampling requires the quantum force, which for the two-fermion case is given by

$$F = -2\alpha\omega \mathbf{r}_1 + \frac{2a}{r_{12}(1 + \beta r_{12})^2} \mathbf{r}_{12} - 2\alpha\omega \mathbf{r}_2 + \frac{2a}{r_{12}(1 + \beta r_{12})^2} \mathbf{r}_{21},$$

or generally as

$$F = 2 \frac{\nabla \Psi_T}{\Psi_T}$$

as shown in Appendix B.1.

## 2.5 Slater determinant

The Slater determinant is a crucial, time consuming part of the trial wavefunction and hence the Metropolis algorithm, in evaluating the quantum force, and when computing the local energy and other observables. Standard Gaussian elimination determinant calculation for a  $N \times N$  matrix is in the order of  $N^3$ . Our gradient and Laplacian requires  $N \cdot \dim$  determinant calculations. Hence, it is important to optimize.

Calculating the transition probability of the trial wavefunction  $\Psi_{old}(\mathbf{R})/\Psi_{new}(\mathbf{R})$  requires a computation of the ratio of the determinants  $\det(D_{old}(\mathbf{R}))/\det(D_{new}(\mathbf{R}))$ . Instead of recalculating the whole determinant for each step, the algorithm can be optimized using Sherman-Morrison formula, reducing the computational cost of evaluating the ratio of the determinants with a factor of  $N$  of the move is accepted.

## 2.6 Onebody density

The one body density is a useful entity in quantum mechanics, helping visualizing and optimizing the wavefunction as well as calculating excitation energies. It describes the probability of finding any of the  $N$  electrons in the volume  $d\mathbf{r}_1$ . The density is defined as [ref:Hogberger2013?](#)

$$\rho(\mathbf{r}_1) = \int_{\mathbf{r}_2} \int_{\mathbf{r}_3} \cdots \int_{\mathbf{r}_N} |\psi(\mathbf{r}_1, \dots, \mathbf{r}_N)|^2 d\mathbf{r}_2 \dots d\mathbf{r}_N \quad (2.5)$$

Notice the integration of the wavefunction,  $\psi$ , squared is over all but the first coordinate. It is normalized with the number of particles, not unity.

By the Pauli principle, no electrons can occupy the same state, making the integral a bit simpler. This is accounted for by the repulsion/perturbation term in the Hamiltonian.

## 2.7 The Virial Theorem

The Virial theorem relates the average time  $\langle T \rangle$  for the total kinetic and potential energy in a system of  $N$  particles by the following equation

$$\langle T \rangle = -\frac{1}{2} \sum_{k=1}^N \langle \mathbf{F}_{\mathbf{k}} \cdot \mathbf{r}_{\mathbf{k}} \rangle$$

,

where  $\mathbf{F}_{\mathbf{k}}$  and  $\mathbf{r}_{\mathbf{k}}$  is the force on and position of particle  $k$  respectively. The theorem allows for calculations of the average total kinetic energy of complex systems, independent of temperature.

The more relevant quantum mechanical version of the theorem, the potential around the confined particles are considered instead of the force, hence,

$$2\langle T \rangle = -\frac{1}{2} \sum_n \langle X_n \frac{dV}{dX_n} \rangle$$

where  $V$  is the potential. For a Harmonic oscillator  $V = \frac{1}{2}kx^2$ .



# Chapter 3

## Method

### 3.1 Variational Monte Carlo

Our variational Monte Carlo approach is as explained in our previous work [3]. Roughly, it proceeds by proposing a change to the system  $\mathbf{R} \mapsto \mathbf{R}'$  by changing the position of a single particle  $\mathbf{r}_i$ . The choice of this particle and how it moves is done both randomly and by way of the *quantum force*, both explained by [3]. From the states  $\mathbf{R}$  and  $\mathbf{R}'$ , and the trial wave function  $\Psi_T$ , we evaluate an acceptance factor, that determines whether or not we accept the proposed changed system. The flowchart shown in figure 3.1 briefly describes this process.

Regardless of whether the new step is accepted or not, the desired quantities - in our case the energy, its gradient and their composites - are sampled in Monte Carlo integration. The integrated values are then used in steepest gradient descent [3] to find the optimal variational parameters.

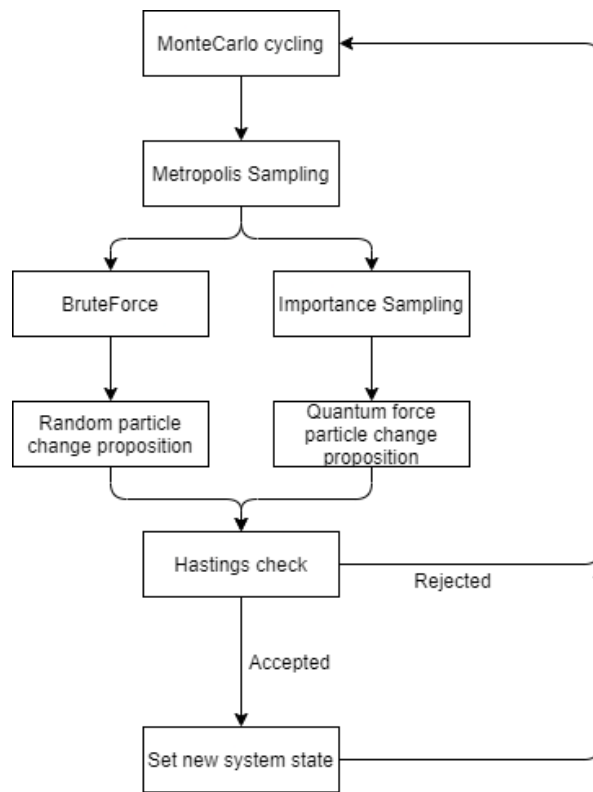


Figure 3.1: Flowchart showcasing our Monte Carlo sampling

## 3.2 Optimization of the wave function ratio

In our approach, the most time-consuming calculation is the evaluation of the wave function. For each proposed step in the Metropolis algorithm, we need to evaluate it to determine the acceptance factor, and if the step is accepted, yet another evaluation is needed (although this might be stored for reuse). This is expensive, so we need to optimize this process to scale well with the size of the system.

As previously stated, we find the acceptance factor in our Metropolis algorithm by introducing the proposed system change  $\mathbf{R} \mapsto \mathbf{R}'$  in our Metropolis algorithm, with a single particle change  $\mathbf{r}_p \mapsto \mathbf{r}'_p$ . The acceptance factor depends on the wave function ratio  $\mathcal{R}$ , which we can split up like this:

$$\mathcal{R} = \frac{\Psi_T(\mathbf{R}')}{\Psi_T(\mathbf{R})} = \frac{\Psi_D(\mathbf{R}')}{\Psi_D(\mathbf{R})} \cdot \frac{\Psi_J(\mathbf{R}')}{\Psi_J(\mathbf{R})} = \mathcal{R}_D \mathcal{R}_J.$$

We will optimize each of these ratios separately.

### 3.2.1 Optimizing $\mathcal{R}_D$

Each new ratio  $\mathcal{R}_D = \frac{\det(D(\mathbf{R}'))}{\det(D(\mathbf{R}))}$  would require  $\mathcal{O}(N^3)$  operations if done with Gaussian elimination. However, as found by [4], this is decreased to  $\mathcal{O}(N)$  by utilizing the inverse matrix  $D^{-1}$  as such:

$$\mathcal{R}_D = 1 + \mathbf{v}_p^T D^{-1} \mathbf{e}_p, \quad \text{where } \mathbf{v}_p = \begin{bmatrix} \phi_1(\mathbf{r}'_p) - \phi_1(\mathbf{r}_p) \\ \vdots \\ \phi_N(\mathbf{r}'_p) - \phi_N(\mathbf{r}_p) \end{bmatrix}.$$

$\mathbf{e}_p$  is simply the unit vector with 1 on the  $p$ -th entry and zero everywhere else. It serves the purpose of extracting the  $p$ -th column from  $D^{-1}$ .

Now, how do we calculate  $D^{-1}$  effectively? Once again, Gaussian elimination gives us an  $\mathcal{O}(N^3)$  cost, which is no-go. However, if we do the matrix inversion with Gaussian elimination initially, to acquire  $D_0^{-1}$ , we can iteratively find the succeeding inversions by using a special case of the *Sherman-Morrison-Woodbury formula*<sup>1</sup> [5], which states:

$$(D + D^{-1} \mathbf{e}_p \mathbf{v}_p^T)^{-1} = D^{-1} - \frac{D^{-1} \mathbf{e}_p \mathbf{v}_p^T D^{-1}}{1 + \mathbf{v}_p^T D^{-1} \mathbf{e}_p}.$$

We introduce the index  $k$ , referring to an arbitrary Monte Carlo step. Recognizing  $D_k + D_k^{-1} \mathbf{e}_p \mathbf{v}_p^T$  as  $D_{k+1}$  [4], we can simplify this to the iterative statement

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<sup>1</sup>Which, confusingly, is just called the *Sherman-Morrison formula*.

$$D_{k+1}^{-1} = \left( \mathbf{I} - \frac{D_k^{-1} \mathbf{e}_p \mathbf{v}_p^T}{\mathcal{R}_{D,k}} \right) D_k^{-1}.$$

This has an operation complexity of  $\mathcal{O}(N)$ .

### 3.2.2 Optimizing $\mathcal{R}_J$

We consider the ratio

$$\mathcal{R}_J = \frac{\Psi'_J}{\Psi_J} = \prod_{i < j}^N \frac{\exp(J(r'_{ij}, \beta))}{\exp(J(r_{ij}, \beta))}.$$

This naive operation scales in the order of  $\mathcal{O}\left(\frac{N^2(N-1)}{2}\right)$ . It is however easily optimized, by employing the fact that we only move one particle's position  $\mathbf{r}_p$ , which means only distances  $r_{pj}$  are changed. We thus get

$$\mathcal{R}_J = \prod_{i \neq p}^N \frac{\exp(J(r'_{pi}, \beta))}{\exp(J(r_{pi}, \beta))} = \exp\left(\sum_{i \neq p}^N J(r'_{pi}, \beta) - J(r_{pi}, \beta)\right),$$

which scales in the order of  $\mathcal{O}(N-1)$  operations.

## 3.3 Testing

Testing in Rust is normally divided in two categories: *unit tests* and *integration tests*. Unit tests are small codes to test specific functions inside the code. These tests are normally written in the same file as the functions themselves, but inside a module annotated with `#[cfg(test)]`.

On the other hand, integration tests are written externally to the library, and is made to test the integration of the functions in the program. These tests are often much larger than unit tests, and are made to make sure that the internal functions work well with each other, from the standpoint of an external user. Therefore, integration tests are normally written in a separate `tests` directory at the same level as the `src` directory.

We will write mainly unit tests in our program, to ensure that our functions return the expected values, and to reduce the mental overhead of debugging when making larger changes to the codebase.

More on testing can be found in the official documentation of the Rust programming language [6].

## 3.4 Evaluation and performance of the VMC solver

The first performance evaluations are done for a case with two electrons in a quantum dot with frequency of  $\hbar\omega = 1$ .

### 3.4.1 Performance evaluation of different energy calculation methods

The performance of the analytical expression for the local energy is compared to the performance of the numerical derivation of the kinetic energy in results section ???. This test is performed without importance sampling and the Jastrow factor. Following this, importance sampling is added and tested only with the analytical expression for the local energy. Lastly, a blocking analysis is performed in order to obtain the optimal standard deviation.

The energy should equal 2.0 atomic units with a variance exactly equal to zero.

### 3.4.2 Evaluating the variational parameters

By using the steepest descent method, the best variational parameters,  $\alpha$  and  $\beta$  are found. The results for this is found in section 4.2.

### 3.4.3 Computation of the two electron system

The minimum energy of the system is computed and compared to Taut's work . In addition, the mean distance between the two electrons and the onebody density is calculated for the best variational parameters. These results are also compared with the results from the same computations, where only the pure harmonic oscillator wavefunctions are used, and where pure HO wavefunctions are used but without the Jastrow factor.

Lastly the expectation value for the kinetic energy is calculated with  $\omega \in 0.01, 0.05, 0.1, 0.5, 1.0$ .

## 3.5 Increasing computational performance

Being able to simulate many-body system at large scale without running out of time is crucial. Hence taking advantage of available tools such as compilation flags (e.g. for vectorization) and parallelization is important. The Rust language provides a great set of such tools - similar to the ones used in C++, but safer.

Since we run many different simulations with unique parameters, we parallelize over these simulations, to keep the logic of our program simple. This allows us to utilize all our cores' computation power, while still not needing to program concurrently. For future work, parallelization should be done further into the

“core” of the program, in order to increase performance in single runs. For details on how we do vectorization in Rust, see [3].

# Chapter 4

## Results

### 4.1 Two fermions

To validate our algorithm a simulation of the simplest case with two electrons without the Jastrow factor and perturbation was done, expecting an energy-output of exactly 2 a.u and a variance of 0. The results, together with a performance analysis(see below), is listed in Table 4.1.

A performance analysis, taking the average time over 10 runs, of the analytical expression for the local energy, numerical derivation of the kinetic energy and the analytical local energy with importance sampling is shown in table 4.1 below.

Table 4.1: Results from computations of the expectation value of the energy using both Importance Sampling and the Metropolis algorithm for both the analytical expression for the local energy(see equation ??) and numerical derivation of the kinetic energy. To compare the performance of the different configurations, the algorithms are timed over 10 runs and averaged.

Sampling method	Average time [s]	$\langle E \rangle$	$\langle E_{kinetic} \rangle$	$\sigma^2$	$\sigma_{blocking}$
Analytical w/ Metropolis	<i>time</i>				
Analytical w/ Importance Sampling	<i>time</i>				
Numerical w/ Metropolis	<i>time</i>				

Sampling method	Avarage time [s]	$\langle E \rangle$	$\langle E_{kinetic} \rangle$	$\sigma^2$	$\sigma_{\text{blocking}}$
Numerical w/ Importance Sampling	<i>time</i>				

The **blocking analysis** shows that the optimal standard deviation is *FILL*.

## 4.2 Evaluating the variational parameters

To obtain the optimal variational parameters for the ground state energy, the steepest decent method is implemented in the Variatonal Monte Carlo calculations. The result, with and without the Jastrow factor are shown in Table ??  
The table also

Table 4.2: Optimal variatonal parameters for the different systems without the Jastrow factor, for comparison.  
{#tbl:results-variational-parameters}

N	$\omega$	$\alpha$	$\alpha_{\text{wo J}}$	$\beta$	$\langle E \rangle$	$\sigma_{\text{blocking}}$	$\langle E_k \rangle$	$\langle E_p \rangle$	$\langle r_{12} \rangle$
2	1								
	0.5								
	0.1								
	0.05								
	0.01								
-----:									
6	1								
	0.5								
	0.1								
	0.05								
	0.01								
-----									
12	1								
	0.5								
	0.1								
	0.05								
	0.01								
-----									
20	1								
	0.5								
	0.1								
	0.05								
	0.01								



### 4.3 Computations for the two electron system

By using the variational parameters  $\alpha = FILLME$  and  $\beta = FILLME$ , the calculation of minimum energy for the system has been compared to Taut's analytical values in table ???. This table also contains the mean distance between the two electrons and the onebody density. Calculations are done with interaction, purely Harmonic Oscillator wavefunctions and pure HO wavefunctions without the Jastrow factor.

Calculation type	Minimum energy	Taut's analytical energies	Mean particle distance	Onebody Density
All included	<i>FILL</i>	$2\omega$	1	1
Purely HO	<i>FILL</i>	$2\omega$	1	1
Purely HO, no Jastrow	<i>FILL</i>	$2\omega$	1	1

Lastly the expectation value for the kinetic energy and the potential energy is computed using  $\omega \in 0.01, 0.05, 0.1, 0.5, 1.0$ . With interaction and the Jastrow factor.

$\omega$	$\langle E_k \rangle$	$\langle E_p \rangle$
0.01	1	1
0.05	1	1
0.1	1	1
0.5	1	1
1.0	1	1

### 4.4 Ground state energies

### 4.5 One body densities

The one body density is computed for 2 and 6 particles with the optimal parameters obtained during the previous calculations and  $\omega = 1$ . The calculations are executed with and without the Jastrow factor (**and perturbation**)??? for comparison and analysis of their influence.

The one-body densities are calculated with and without the Jastrow factor for two (2) and (6) fermions. The results is shown in figure ?? below

One Body densities for 2 and 6 fermions with and without the Jastrow factor. The computations are done with  $\alpha = FILL$ ,  $\beta = FILL$  and  $\omega = 1$

## 4.6 Performance analysis

Lastly a analysis of the algorithms are given for  $N = 6$  electrons, *FILLIN* Monte Carlo cycles, optimal variational parameters  $\omega = 1$  and without the Jastrow factor. The analysis is done by comparing the avarage time used for a calculation with and without vecotrization. The procedure is repeated with paralellization, expecting approximatly a 100% speedup. The quantities which are calculated are **FILL INN**. The most time consuming part is the **FILL INN** , and hence the clock is started here. The results are presented in table ??.  
**ADD SOME MORE DESCRIPTION OF HOW HERE**

Table 4.5: Results from performance analysis with and without vectorization and compile flags. The time is avaraged over 10 runs with **FILL INN** MC cycles. The sampling method is the **Brute Force Metropolis OR Importance sampling**

Optimization/compile flags	$\bar{t}$ [s]
<b>With vectorization</b>	
Flag 1	
Flag 2	
Flag 2	
<b>Without Vectorization</b>	
Flag 1	
Flag 2	
Flag 3	
<b>Parallelization</b>	

## Chapter 5

# Discussion

### 5.1 Verification/ Two electrons

As a validation test for our algorithm we calculated the energy without the Jastrow factor for  $N = 2$  electrons, expecting a energy of  $-2.0$  a.u and a variance of zero. Running this system with the Metropolis (and Importance sampling) method returned a energy of  $FILL$  ( $FILL$ ) and a variance of  $FILL$  ( $FILL$ ). Together with the energy and statistical calculations, a performance analysis showed a **FILL- large, intermediate..** difference in time consumption. The analytical algorithm used  $FILL$  seconds, while the numerical approach used  $FILL$  seconds. Comparing the two sampling methods in question, the **Metropolis/Importance** sampling was **faster/slower** than the **Metropolis/Importance**.

### 5.2 Variational parameters

The variational parameters were obtained using the Steepest Gradient Decent method both with and without the Jastrow factor. The results are to be found in Table ???. Without the factor our calculations returned  $\alpha = FILL$ , with the expectation of  $\alpha = 1$ . With the Jastrow factor, there is an additional variational parameter,  $\beta$ .

### 5.3 Energy minima

The results from the energy minima calculations are also listed in Table ??.

The obtained mean distance between two fermions shows to be strongly (inverse) **dependent/independent** on the frequency,  $\omega$ , which is **expected/unexpected**. Decreasing the frequency with a factor of  $FILL$

increases the distance with a factor of  $FILL$ . Looking at the energy, there is a **decrease/increase** in energy when **decreasing** the frequency.

## 5.4 One Body density

The results from the one body density calculations utilizing optimal parameters are shown in Figure ?? . With perturbation (interaction term), there is a (small?) **increas/decrease**

## 5.5 Performance analysis

Table ?? gives an overview of the performance analysis of running our algorithm with and without vectorization and parallelization for  $N = 6$  electrons.

## Chapter 6

## Conclusion

# Appendix A

## Definitions and notation

### A.1 Hermite polynomials

The Hermite polynomials are the solutions to the following contour integral [7]:

$$H_n(z) = \frac{n!}{2\pi i} \oint e^{-t^2 - tz} t^{-n-1} dt.$$

In this report, we will consider the real Hermite polynomials, and only up to order of four. A computationally efficient way of finding these is given by the following sequence:

$$H_n(x) = c_{n+m}x^n + c_{n-1+m}x^{n-1} \dots + c_mx^0, \quad m = \sum_{i=1}^n i$$

where the coefficients  $c_n$  are given by the triangle sequence shown in (A.1).

$$c_i = 1, 0, 2, -2, 0, 4, 0, -12, 0, 8, 12, 0, -48, \dots \quad (\text{A.1})$$

This is just a selection of the sequence, more can be found from the work by [8].

### A.2 Index notation for sums and products

For products and sums, the following convention is used:

$$\sum_{i < j}^N = \sum_{i=1}^N \sum_{j=i+1}^N, \quad \text{or} \quad \prod_{i < j}^N = \prod_{i=1}^N \prod_{j=i+1}^N$$

# Appendix B

## Derivations

### B.1 Analytical derivation of the Quantum Force, Laplacian and Local energy of two-fermion systems

The trial wavefunction of a two-particle system is

$$\Psi_T(\mathbf{r}_1, \mathbf{r}_2) = \Psi_1 * \Psi_2 = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \exp\left(\frac{ar_{12}}{1 + \beta r_{12}}\right)$$

The Laplacian is the double derivative in all dimensions, defined as:

$$\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

The calculations: First we change the laplacian to work with a cartesian twodi-  
mensional system:

$$\Delta f = \frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2} + \frac{\partial^2 f}{\partial y_1^2} + \frac{\partial^2 f}{\partial y_2^2}$$

Then the wavefunction is inserted.

$$\Delta \Psi_T = \frac{\partial^2 \Psi_T}{\partial x_1^2} + \frac{\partial^2 \Psi_T}{\partial x_2^2} + \frac{\partial^2 \Psi_T}{\partial y_1^2} + \frac{\partial^2 \Psi_T}{\partial y_2^2}$$

We see that the trial wavefunction is composed of two exponential terms, and to do the derivative, we can use the derivative product rule twice.

$$(fg)'' = (f'g + fg')' = f''g + 2f'g' + fg'' \quad (\text{B.1})$$

where

$$f = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2)$$

$$g = \exp\left(\frac{ar_{12}}{1 + \beta r_{12}}\right)$$

The two following equalities are then used to find the first derivative of  $f$  and  $g$

$$\frac{\partial r_1}{\partial x_1} = x_1/r_1, \quad \frac{\partial r_{12}}{\partial x_1} = (x_1 - x_2)/r_1$$

$$\frac{\partial f}{\partial x_1} = -\alpha\omega x_1 f, \quad \nabla_i f = -\alpha\omega f \mathbf{r}_i \quad (\text{B.2})$$

Where  $i$  denotes the specific particle, and the particle position  $r_i$  equals  $(x_i, y_i)$ . For the second term  $g$  we have

$$\frac{\partial g}{\partial x_1} = g \frac{a(x_1 - x_2)}{r_{12}(1 + \beta r_{12})^2}, \quad \nabla_i g = g \frac{a}{r_{12}(1 + \beta r_{12})^2} \mathbf{r}_{ij} \quad (\text{B.3})$$

Where  $j$  is the opposite particle of  $i$  and the distance from  $j$  to  $i$ ,  $\mathbf{r}_{ij} = (x_i - x_j, y_i - y_j)$ .

From this we can actually find an analytical solution to the *quantum force* used in importance sampling, defined as

$$F = 2 \frac{\nabla \Psi_T}{\Psi_T} = 2 \frac{f'g + fg'}{fg}$$

$$F = -2\alpha\omega \mathbf{r}_1 + \frac{2a}{r_{12}(1 + \beta r_{12})^2} \mathbf{r}_{12} - 2\alpha\omega \mathbf{r}_2 + \frac{2a}{r_{12}(1 + \beta r_{12})^2} \mathbf{r}_{21}$$

Next, we calculate the Laplacian, or double derivative, of the first term,  $f$ .

$$\frac{\partial^2 f}{\partial x_1^2} = f(\alpha^2 \omega^2 x_1^2 - \alpha\omega), \quad \nabla^2 f = f(\alpha^2 \omega^2 (r_1^2 + r_2^2) - 4\alpha\omega) \quad (\text{B.4})$$

And the second term,  $g$ .



$$\frac{\partial^2 g}{\partial x_1^2} = g \left[ \frac{a^2 (x_1 - x_2)^2}{r_{12}^2 (1 + \beta r_{12})^4} + \frac{a r_{12} (1 + \beta r_{12})^2}{r_{12}^2 (1 + \beta r_{12})^4} - \frac{a (x_1 - x_2) \left[ (x_1 - x_2) / r_{12} (1 + \beta r_{12})^2 + 2 r_{12} (1 + \beta r_{12}) \beta (x_1 - x_2) / r_{12} \right]}{r_{12}^2 (1 + \beta r_{12})^4} \right]$$

$$\frac{\partial^2 g}{\partial x_1^2} = g \left[ \frac{a^2 (x_1 - x_2)^2}{r_{12}^2 (1 + \beta r_{12})^4} + \frac{a}{r_{12} (1 + \beta r_{12})^2} - \frac{a (x_1 - x_2)^2}{r_{12}^3 (1 + \beta r_{12})^2} - \frac{2 a \beta (x_1 - x_2)^2}{r_{12}^2 (1 + \beta r_{12})^3} \right]$$

With this, we get

$$\nabla^2 g = g \left[ \frac{2a^2}{(1 + \beta r_{12})^4} + \frac{4a}{r_{12} (1 + \beta r_{12})^2} - \frac{2a}{r_{12} (1 + \beta r_{12})^2} - \frac{2a\beta}{(1 + \beta r_{12})^3} \right]$$

Which can be further shortened by pulling  $\frac{2a}{(1 + \beta r_{12})^2}$  outside the brackets to:

$$\nabla^2 g = g \frac{2a}{(1 + \beta r_{12})^2} \left[ \frac{a}{(1 + \beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{1 + \beta r_{12}} \right] \quad (\text{B.5})$$

Now, by inserting  $f''$ ,  $g''$ ,  $f'$  and  $g'$  from equations B.4, B.5, B.2 and B.3 into equation B.1, we actually obtain the *Laplacian* of the trial wavefunction  $\nabla^2 \Psi_T$ . First we simplify the middle term:

$$\begin{aligned} \nabla f \nabla g &= -fg \frac{a\alpha\omega}{r_{12} (1 + \beta r_{12})^2} [x_1 (x_1 - x_2) + y_1 (y_1 - y_2) - x_2 (x_1 - x_2) - y_2 (y_1 - y_2)] \\ &= -fg \frac{a\alpha\omega}{r_{12} (1 + \beta r_{12})^2} [(x_1 - x_2) (x_1 - x_2) + (y_1 - y_2) (y_1 - y_2)] \\ &= -fg \frac{a\alpha\omega r_{12}}{(1 + \beta r_{12})^2} \end{aligned}$$

And then, we insert the double derivatives.

$$\begin{aligned} \frac{\nabla^2 \Psi_T}{\Psi_T} &= 2\alpha^2 \omega^2 (r_1^2 + r_2^2) - 4\alpha\omega - \frac{2a\alpha\omega r_{12}}{(1 + \beta r_{12})^2} + \\ &\quad \frac{2a}{(1 + \beta r_{12})^2} \left[ \frac{a}{(1 + \beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{1 + \beta r_{12}} \right] \end{aligned}$$

Now, by the relation  $E_L = \frac{1}{\Psi_T} H \Psi_T$  we can get the analytical expression for the *local energy*:

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

$$\frac{2a}{(1 + \beta r_{12})^2} \left[ \frac{a}{(1 + \beta r_{12})^2} + \frac{1}{r_{12}} - \frac{2\beta}{1 + \beta r_{12}} \right] +$$

$$\frac{1}{2} \omega^2 (r_1^2 + r_2^2) + \frac{1}{r_{12}}$$

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