Project 2

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Chapter 1

Introduction

Chapter 2

Theory

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

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

Here $r_{ij} = |r_i - r_j|$ 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 (Hjorth-Jensen, 2021):

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

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 ϵ is:

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

[1] $\hbar = c = e = m_e = 1$, see (Hartree, 1928).

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 2.1.

Table 2.1: The ground state energy of N non-interacting particles in an isotropic harmonic potential well. ω is the oscillator frequency. Energies are given in Hartree's atomic units.

Number of particles N	E **(a.u)**
2	2ω
6	10ω
12	28ω
20	60ω

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 α and β are the variational parameters. Following Hjorth-Jensen (2021), our ansatz for the factors of this trial wave function is:

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

$\phi_j(\mathbf{r}_i)$ 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[2]. 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] E.g. $(0, 0, \uparrow)$, $(2, 1, \downarrow)$, etc.

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:

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

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 **??**, the local energy for a two-fermion system is:

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

The numerical local (kinetic) energy is calculated using the derivitive 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

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

Δx is the stepsize which we let run towards zero. The error is proportional to (Δx^2).

2.4 Quantum Force

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

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

as shown in Appendix B.1.

2.5 Slater determinant

The slater determinant is a crucial, time consuming part of the trail wavefunction and hence the metropolis algorithm, in evaluating the quantum force, and when computing the local energy and other observebales. Standard Gaussian elimination determinant calculation for a $N \times N$ matrix is in the ordrer of N^3. Our gradient and Laplacien requiers $N \cdot dim$ determinant calculations. Hence, it is important to optimize.

Calcutating the trasition probability of the trial wavefunction $\Psi_{old}(\mathbf{R})/\Psi_{new}(\mathbf{R})$ requieres a computation of the ratio of the determinants $det(D_{old}(\mathbf{R}))/det(D_{new}(\mathbf{R}))$. Insted of recalculate 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.

Chapter 3

Method

3.1 Variational Monte Carlo

Our variational Monte Carlo approach is as explained by our previous work (Aasrud et al., 2021). 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 in Aasrud et al. (2021). From the states $\mathbf{R}$ and $\mathbf{R}'$, and the trial wave function Ψ_T, we evaluate an acceptance factor, that determines whether or not we accept the proposed changed system.

Regardless of whether the new step is accepted or not, the desired quantities - in our case the energy, it's gradient and their composites - are sampled in Monte Carlo integration. The integrated values are then used in steepest gradient descent (Aasrud et al., 2021) to find the optimal variational parameters.

3.2 Optimization of 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 Nukala & Kent (2009), 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 aquire D_0^{-1}, we can iteratively find the succeeding inversions by using a special case of the *Sherman-Morrison-Woodbury formula*[1] (Golub & Van Loan, 2013), which states:

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

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} (Nukala & Kent, 2009), we can simplify this to the iterative statement

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

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

3.3 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

[1] Which, confusingly, is just called the *Sherman-Morrison formula*.

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 (Rust-Docs, 2021).

3.4 Parallelization

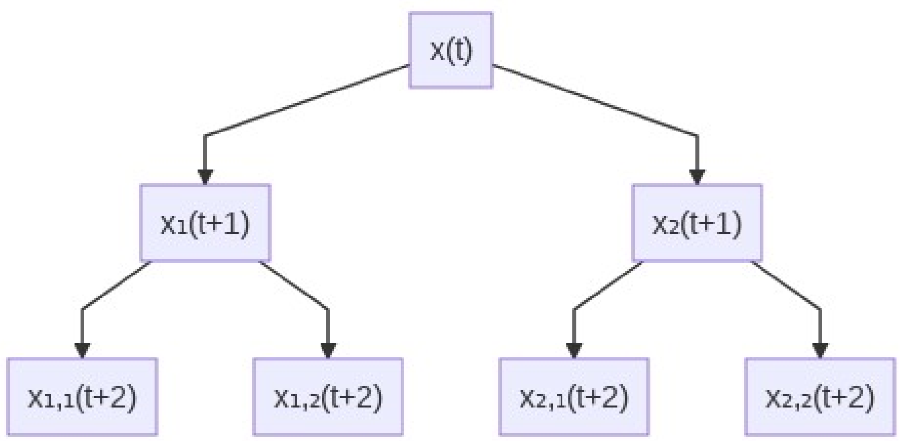

Figure 3.1: Temporary diagram for visualization

Chapter 4

Results

Chapter 5

Discussion

Chapter 6

Conclusion

Appendix A

Definitions and notation

A.1 Hermite polynomials

The Hermite polynomials are the solutions to the following contour integral (Arfken & Weber, 2005):

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

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

$$H_n(x) = c_{n+m}x^n + c_{n-1+m}x^{n-1} ... + c_m x^0, \qquad m = \sum_{i=1}^{n} i$$

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

$$c_i = 1, 0, 2, -2, 0, 4, 0, -12, 0, 8, 12, 0, -48, ... \tag{A.1}$$

This is just a a selection of the sequence, more can be found from the work by Jovovic (2001).

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

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

as defined in theory section 2.3.

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 twodimensional 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.

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

where

$$\begin{aligned} f =& C \exp\left(-\alpha\omega(r_1^2 + r_2^2)/2\right) \\ g =& \exp\left(\frac{a r_{12}}{1 + \beta r_{12}}\right) \end{aligned}$$

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

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

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

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

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

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

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

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

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

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

And the second term, g.

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

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

With this, we get

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

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

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

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:

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

And then, we insert the double derivatives.

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

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

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

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