University of Oslo

FYS4411

Computational Physics II: Quantum mechanical systems

Project 2 - Variational Monte Carlo of Fermionic systems

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Abstract

A numerical study of ground-state energies for closed-shell quantum dot systems is presented. Variational Monte Carlo methods have been applied on systems of 2, 6, 12 and 20 electrons trapped in harmonic oscillator potentials. Interactions between the particles and the Jastrow factor has been added for more accurate energy calculations. The steepest descent method has been applied to find the optimal variational parameters for every desired case and blocking has been added for better statistics.

The code as been proved to reproduce Taut's analytical calculations [1] down to 0.02 % deviation from the analytical work.

1 Introduction

A quantum dot can be seen as a zero-dimensional particle or a system of two-dimensional electrons trapped in harmonic oscillator like potentials. This first odd definition gives rise to the property that a quantum dot only has quantum mechanical effects and no classical effects. This includes things like energy, which can only be discrete and never continuous.

The term "quantum dot" was coined already in 1986, in a paper by M. A. Reed et al. [2]. First seen as an exotic quantum mechanical phenomena, quantum dots are today a central theme in nanotechnology and its applications range from LED screens to solar cells to quantum computing and much more. It is therefore essential to study the quantum dots that can make such an impact on society and the technology we use.

In this paper we present our numerical studies of quantum dots. By using Monte Carlo methods we can simulate systems of closed shell quantum dots. Starting with a simple system of two electrons and expanding up to twenty electrons, we have developed a code that calculates the energy of a quantum dot system for a given set of parameters. Using variational Monte Carlo (VMC) methods we have also implemented variational parameters which are used for finding the optimal set of parameters, making us able to accurately determine the ground state energies. Our numerical results will be compared to similar analytical and computational calculations.

The code developed for this project can be found in it's entirety on GitHub, in repository: `https://github.com/wiggoen/FYS4411/tree/master/Project_2`

2 Theory

Quantum dots refer to a two-dimensional system where electrons are trapped in harmonic oscillator like potentials. The Hamiltonian for such a system, at least the idealized version, is

$$\hat{H} = \underbrace{\sum_{k=1}^{N}\left(-\frac{1}{2}\nabla_k^2 + \frac{1}{2}\omega^2 r_k^2\right)}_{\hat{H}_0} + \underbrace{\sum_{k<j}\frac{1}{r_{kj}}}_{\hat{H}_1} = \hat{H}_0 + \hat{H}_1 \tag{1}$$

It is idealized in such a way, that we use natural units ($\hbar = c = e = m_e = 1$). The energy is given in a.u. (atomic units). We will focus on studying closed shell systems, with $N = 2$, 6, 12 or 20 electrons. Electrons have spin 1/2 and are thus fermions. The first sum of the Hamiltonian, $\hat{H}_0$, called the 'unperturbed' Hamiltonian, is the standard harmonic oscillator, while the second sum, $\hat{H}_1$, the 'perturbation', represents the repulsive interaction between the electrons. The electrons moves independently of each other in a net central potential V(r). The potential represents the attraction of the nucleus and in addition a average central repulsive potential due to the other electron [3]. The distance between two electrons i and j is given as $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ when the position of an electron is $r_i = \sqrt{r_{i_x}^2 + r_{i_y}^2}$.

For one particle in the two-dimensional Harmonic Oscillator potential, with wave function

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

the lowest-lying state is given as $n_x = n_y = 0$ and the energy will be $\epsilon_{n_x,n_y} = \omega(n_x + n_y + 1) = \omega$.

For the two-particle system we will start by looking at, both electrons can be in the ground-state assuming that they have opposite spins. In the non-interacting case, the total energy of the system is simply the sum of each particles energy. In other words, the energy for the lowest-lying two-particle state is simply 2ω.

Another note on the ground state is that it is only possible to have both particles in the ground state if their spins are oppositely pointed. Thus it is necessary for the total spin in the ground state to be zero. The total unperturbed wave function,

$$\psi_\Phi(\mathbf{r}_1,\mathbf{r}_2) = C\exp\left(-\frac{\alpha\omega}{2}(r_1^2+r_2^2)\right), \tag{3}$$

will therefore have a total spin zero.

Note that the lowest possible energy will always be the energy given from the pure harmonic oscillator without particle interactions. Adding the repulsion term, $1/r_{12}$, can in other words only raise the unperturbed energy levels. In the two-electron case, the repulsion term $1/r_{12}$ can be treated by perturbation theory, but in the many-particle case, the repulsion term $\sum_{k<j} 1/r_{kj}$ is in general too large to be treated as a perturbation [3].

2.1 The Pauli Principle

One of the most fundamental principles in quantum physics is the famous Pauli principle. According to the Pauli principle, a system of N fermions must have a total wave function, $\psi(q_1, q_2, \ldots, q_N)$, that is antisymmetric. Mathematically this means that if two electrons were to change places (spatially as well as with consideration to spin), $\psi(q_1, q_2, \ldots, q_N)$ must change sign. The exclusion principle introduces a coupling between the space and spin variables of the electrons, and they behave as if they were acted upon by a exchange force whose sign depends on the relative orientation of their spins. The exchange forces are negligible between two electrons, because they will always be far apart. [3].

2.2 Local Energy

The local energy is defined as

$$E_L = \frac{1}{\psi_T} \hat{H} \psi_T \tag{4}$$

where ψ_T is the trial wave function of the system. With the Hamiltonian as defined in (1) and trial wave function

$$\begin{aligned} \psi_T(\mathbf{r}_1, \mathbf{r}_2) &= \psi_\Phi(\mathbf{r}_1, \mathbf{r}_2)\psi_{\mathcal{J}}(\mathbf{r}_1, \mathbf{r}_2) \\ &= \underbrace{C \exp\left(-\frac{\alpha\omega}{2}(r_1^2 + r_2^2)\right)}_{\psi_\Phi(\mathbf{r}_1,\mathbf{r}_2)} \underbrace{\exp\left(\frac{a r_{12}}{(1+\beta r_{12})}\right)}_{\psi_{\mathcal{J}}(\mathbf{r}_1,\mathbf{r}_2)}, \end{aligned} \tag{5}$$

it can be shown that the local energy of our system with two electrons is

$$\begin{aligned} E_L = 2\alpha\omega + \frac{1}{2}\omega^2(1-\alpha^2)(r_1^2 + r_2^2) - \frac{a}{(1+\beta r_{12})^2}\Bigg(&- \alpha\omega r_{12} \\ + \frac{a}{(1+\beta r_{12})^2} + \frac{1-\beta r_{12}}{r_{12}(1+\beta r_{12})}\Bigg) &+ \frac{1}{r_{12}} \end{aligned} \tag{6}$$

where $\frac{1}{r_{12}}$ is the repulsive interaction between the two electrons and

$$a = \begin{cases} 1, & \text{if the two electrons have anti-parallel spins} \\ 1/3, & \text{if the spins are parallel} \end{cases}$$

See section 9.1.2 in Appendix for the full calculation.

Equation (6) is our analytical expression for the local energy. In the code, we implemented this expression as well as a numerical expression for the energy. The numerical calculation of the energy is based on the simple classical expression for kinetic energy, using the derivative of position as the velocity. In the numerical approximations we use central difference approximation formulas for both the first derivative and the second derivative. The first derivative is given by the 'two-point approximation of first derivative'

$$\frac{df(x)}{dx} \approx \frac{f(x+h) - f(x-h)}{2h} \qquad \text{Error: } \mathcal{O}(h^2) \tag{7}$$

and the second derivative is given by the 'three-point approximation of second derivative'

$$\frac{d^2f(x)}{dx^2} \approx \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} \qquad \text{Error: } \mathcal{O}(h^2) \tag{8}$$

where h is a small stepsize ($h \to 0$) and the error goes as $\mathcal{O}(h^2)$. In our code we used $h = 10^{-4}$. Using these two methods with analytical and numerical expressions we expect to get the same result, so our main question about the two methods is a matter of CPU time.

2.3 Adding more electrons

Much of our studies include only two electrons. It is now time to look at bigger systems, namely quantum dots of $N = 6$ and $N = 12$ electrons. Mathematically, extending our calculations to include more electrons means adding a Slater determinant, $Det(\phi)$. The new wave function can then be written as

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_6) = \underbrace{Det\left(\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \ldots, \phi_6(\mathbf{r}_6)\right)}_{\psi_D} \underbrace{\prod_{i<j}^{6} \exp\left(\frac{a_{ij} r_{ij}}{1 + \beta r_{ij}}\right)}_{\psi_J} \tag{9}$$

for $N = 6$. We still keep the single-particle part of the wave function which is the harmonic oscillator, but must now include the states $n_x = 0, 1$ and $ny = 0, 1$, to account for the Pauli principle. Similarly the wave function for twelve electrons is

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{12}) = \underbrace{Det\left(\phi_1(\mathbf{r}_1), \phi_2(\mathbf{r}_2), \ldots, \phi_{12}(\mathbf{r}_{12})\right)}_{\psi_D} \underbrace{\prod_{i<j}^{12} \exp\left(\frac{a_{ij} r_{ij}}{1 + \beta r_{ij}}\right)}_{\psi_J} \tag{10}$$

where we use $n_x = 0, 1, 2$ and $n_y = 0, 1, 2$. The spin parameter is chosen as

$$a_{ij} = \begin{cases} 1, & \text{if two coupled electrons have anti-parallel spins} \\ 1/3, & \text{if the spins are parallel} \end{cases}$$

Splitting this up, we see that the wave function consists of two parts, the Slater determinant and the Jastrow factor. For calculating the local energy, we remember that we need to find an expression for the Laplacian of the wave function. We start with the Jastrow factor, which is more straight forward than the determinant.

It is obvious that the Laplacian of the many-particle closed-shell trial wave function will be calculated as

$$\frac{\nabla^2 \psi_T}{\psi_T} = \frac{\nabla^2 \psi_D}{\psi_D} + \frac{\nabla^2 \psi_{\mathcal{J}}}{\psi_{\mathcal{J}}} + 2 \frac{\nabla \psi_D}{\psi_D} \cdot \frac{\nabla \psi_{\mathcal{J}}}{\psi_{\mathcal{J}}} \tag{11}$$

where $\psi_{\mathcal{J}}$ is the part of the wave function corresponding to the Jastrow factor and ψ_D is the Slater determinant.

We name the exponent of the Jastrow factor

$$f(r_{ij}) = \frac{a_{ij} r_{ij}}{1 + \beta r_{ij}} \tag{12}$$

Using this we find that the gradient and Laplacian of the Jastrow factor are given as

$$\nabla_k \psi_{\mathcal{J}} = \psi_{\mathcal{J}} \sum_{j \neq k} \frac{\mathbf{r}_{kj}}{r_{kj}} \frac{\partial f(r_{kj})}{\partial r_{kj}} \tag{13}$$

and

$$\nabla_k^2 \psi_{\mathcal{J}} = \frac{(\nabla_k \psi_{\mathcal{J}})^2}{\psi_{\mathcal{J}}} + \psi_{\mathcal{J}} \sum_{j \neq k} \left(\frac{1}{r_{kj}} \frac{\partial f(r_{kj})}{\partial r_{kj}} + \frac{\partial^2 f(r_{kj})}{\partial r_{kj}^2} \right) \tag{14}$$

where
$$\frac{\partial f(r_{kj})}{\partial r_{kj}} = \frac{a_{kj}}{(1+\beta r_{kj})^2} \qquad \text{and} \qquad \frac{\partial^2 f(r_{kj})}{\partial r_{kj}^2} = -\frac{2\beta a_{kj}}{(1+\beta r_{kj})^3}. \tag{15}$$

When inserting this for equation (14) we get

$$\frac{\nabla_k^2 \psi_{\mathcal{J}}}{\psi_{\mathcal{J}}} = \sum_{ij\neq k} \frac{(\mathbf{r}_k - \mathbf{r}_i)(\mathbf{r}_k - \mathbf{r}_j)}{r_{ki} r_{kj}} \frac{a_{ki}}{(1+\beta r_{ki})^2} \frac{a_{kj}}{(1+\beta r_{kj})^2} + \sum_{j\neq k} \left(\frac{a_{kj}}{r_{kj}(1+\beta r_{kj})^2} - \frac{2\beta a_{kj}}{(1+\beta r_{kj})^3} \right)$$

as the complete expression for the Laplacian of the Jastrow factor divided by the Jastrow. See section 9.2 for calculations.

Now that we have everything we need in order to calculate the Jastrow-part of the wave function, it is time to take a look at the calculation of the Slater determinant and its derivatives.

2.4 Efficient calculation of the Slater determinant

The theory for this and the next section is gotten from M. Hjorth-Jensen's lecture notes on Variational Monte Carlo methods [4].

Working with big matrices can be a major time-consuming part of the code. With up to 20 electrons, we risk doing several calculations with the 20×20 Slater determinant. Luckily, here there is room for optimization. The biggest one of these is that we chose to move only one electron at the time. In this section we will use $\hat{D}$ to describe the Slater matrix determinant and we will name its elements

$$d_{ij} = \phi_j(x_i) \tag{16}$$

for the i-th column and j-th row, where $\phi_j(\mathbf{r}_i)$ is the single particle wave function. As mentioned earlier, we want to move only one particle at the time, or mathematically update only one row. It is therefore unnecessary to recalculate the determinant for each cycle, as a lot of the calculations will be exactly the same as in the previous cycle. The solution to this problem is to keep track of the inverse of the Slater matrix, which can be expressed in terms by its cofactors C_{ij} and the determinant $|\hat{D}|$. The elements of the inverse Slater determinant matrix is then

$$d_{ij}^{-1} = \frac{C_{ij}}{|\hat{D}|} \tag{17}$$

Note that this is the mathematical definition and that we in the code do not need to find the cofactors. Note also that if $\hat{D}$ is invertible, then we must have $\hat{D}^{-1}\hat{D} = 1$, or

$$\sum_{k=1}^{N} d_{ik} d_{kj}^{-1} = \delta_{ij} \tag{18}$$

In order to use the Metropolis algorithm we must make sure that we can calculate the ratio, R, between the old and new wave function. When this wave function includes $\hat{D}$, it is crucial to find a good expression for how to calculate this. We use

$$R = \frac{|\hat{D}(\mathbf{r}^{new})|}{|\hat{D}(\mathbf{r}^{old})|} = \frac{\Sigma_{j=1}^{N} d_{ij}(\mathbf{r}^{new}) C_{ij}(\mathbf{r}^{new})}{\Sigma_{j=1}^{N} d_{ij}(\mathbf{r}^{old}) C_{ij}(\mathbf{r}^{old})} \tag{19}$$

If we choose to only move one particle at a time, then $\hat{D}(\mathbf{r}^{new})$ and $\hat{D}(\mathbf{r}^{old})$ are equal everywhere except in row number i. As we also have that the i-th row of a cofactor matrix $\hat{C}$ is independent of the i-th row of the corresponding matrix $\hat{D}$ we get $C_{ij}(\mathbf{r}^{new}) = C_{ij}(\mathbf{r}^{old})$ for all i in this particular case. Using this fact, we can redefine R to be

$$R = \frac{\Sigma_{j=1}^{N} d_{ij}(\mathbf{r}^{new}) C_{ij}(\mathbf{r}^{old})}{\Sigma_{j=1}^{N} d_{ij}(\mathbf{r}^{old}) C_{ij}(\mathbf{r}^{old})} = \frac{\Sigma_{j=1}^{N} d_{ij}(\mathbf{r}^{new}) d_{ji}^{-1}(\mathbf{r}^{old})}{\Sigma_{j=1}^{N} d_{ij}(\mathbf{r}^{old}) d_{ji}^{-1}(\mathbf{r}^{old})} \tag{20}$$

This last denominator must be unity and thus we arrive at our final expression for the ratio

$$R = \sum_{j=1}^{N} d_{ij}(\mathbf{r}^{new}) d_{ji}^{-1}(\mathbf{r}^{old}) = \sum_{j=1}^{N} \phi_j(\mathbf{r}_i^{new}) d_{ji}^{-1}(\mathbf{r}^{old}) \tag{21}$$

In other words, the only thing we have to do for a good ratio calculation is to keep the inverse of the Jastrow determinant matrix and to calculate the dot product of the single particle wave functions with $\hat{D}^{-1}$. This is a drastic reduction in number of operations per cycle and with this also the CPU time of the code.

Now that we have found a way to keep track of whether or not the new states are accepted, we also need a way to update the Slater determinant matrix with as few operations as possible. We will now present an algorithm for dealing with the Slater and keep it updated.

The first thing we do is to update all columns of $\hat{D}^{-1}$. Then we calculate

$$S_j = (\hat{D}(\mathbf{r}^{new}) \times \hat{D}^{-1}(\mathbf{r}^{old}))_{ij} = \sum_{l=1}^{N} d_{il}(\mathbf{r}^{new}) d_{lj}^{-1}(\mathbf{r}^{old}) \tag{22}$$

which makes the elements of the j-th column of the inverse Slater determinant

$$d_{kj}^{-1}(\mathbf{r}^{new}) = d_{kj}^{-1}(\mathbf{r}^{old}) - \frac{S_j}{R} d_{ki}^{-1}(\mathbf{r}^{old}) \tag{23}$$

for all k from 1 to N except $j = i$. The elements of the i-th column of the inverse Slater determinant is then

$$d_{ki}^{-1}(\mathbf{r}^{new}) = \frac{1}{R} d_{ki}^{-1}(\mathbf{r}^{old}) \tag{24}$$

for all k from 1 to N.

Following from this, it seems as we can use the same approach to calculate the ratios involving derivatives. We then define the gradient and Laplacian of the Slater determinant to be

$$\frac{\vec{\nabla}_i |\hat{D}(\mathbf{r})|}{|\hat{D}(\mathbf{r})|} = \sum_{j=1}^{N} \vec{\nabla}_i d_{ij}(\mathbf{r}) d_{ji}^{-1}(\mathbf{r}) = \sum_{j=1}^{N} \vec{\nabla}_i \phi_j(\mathbf{r}_i) d_{ji}^{-1}(\mathbf{r}) \tag{25}$$

and

$$\frac{\nabla_i^2 |\hat{D}(\mathbf{r})|}{|\hat{D}(\mathbf{r})|} = \sum_{j=1}^{N} \nabla_i^2 d_{ij}(\mathbf{r}) d_{ji}^{-1}(\mathbf{r}) = \sum_{j=1}^{N} \nabla_i^2 \phi_j(\mathbf{r}_i) d_{ji}^{-1}(\mathbf{r}) \tag{26}$$

This has shown us that in reality, we only need the derivatives of the single particle wave functions ($\vec{\nabla}_i \phi_j(\mathbf{r}_i)$ and $\nabla_i^2 \phi_j(\mathbf{r}_i)$) and the elements of its corresponding Slater determinant matrix. The number of floating point operations have been reduced from $O(d \cdot N^4)$ to only $O(d \cdot N^2)$ which is a great reduction when implementing it into our code.

2.5 Slater Determinants

Slater determinants are an essential part of many-particle fermion systems. It is introduced in order to take into consideration the Pauli principle and make sure that the wave function is antisymmetric under exchange of particles. Luckily, this property is exactly the property that can be expressed by a determinant. We thus introduce the Slater determinant

$$\Phi(\mathbf{r}_1, \mathbf{r}_2, , \mathbf{r}_3, \mathbf{r}_4, \alpha, \beta, \gamma, \delta) = \frac{1}{\sqrt{4!}} \begin{vmatrix} \psi_{100\uparrow}(\mathbf{r}_1) & \psi_{100\uparrow}(\mathbf{r}_2) & \psi_{100\uparrow}(\mathbf{r}_3) & \psi_{100\uparrow}(\mathbf{r}_4) \\ \psi_{100\downarrow}(\mathbf{r}_1) & \psi_{100\downarrow}(\mathbf{r}_2) & \psi_{100\downarrow}(\mathbf{r}_3) & \psi_{100\downarrow}(\mathbf{r}_4) \\ \psi_{200\uparrow}(\mathbf{r}_1) & \psi_{200\uparrow}(\mathbf{r}_2) & \psi_{200\uparrow}(\mathbf{r}_3) & \psi_{200\uparrow}(\mathbf{r}_4) \\ \psi_{200\downarrow}(\mathbf{r}_1) & \psi_{200\downarrow}(\mathbf{r}_2) & \psi_{200\downarrow}(\mathbf{r}_3) & \psi_{200\downarrow}(\mathbf{r}_4) \end{vmatrix}.$$

for a four-particle system. Expanding this for more electrons we simply continue on the same pattern which is present in this matrix. However we quickly see that large Slater determinants can be hard to keep track of and use for computation. A solution to this problem is to realize that the up and down oriented spin particles do not swap positions. It is therefore possible to split the determinant into two: one for the up spins and one for the down spins. In other words, we define two new matrices

$$\det\uparrow(1,2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_{100\uparrow}(\mathbf{r}_1) & \psi_{100\uparrow}(\mathbf{r}_2) \\ \psi_{200\uparrow}(\mathbf{r}_1) & \psi_{200\uparrow}(\mathbf{r}_2) \end{vmatrix},$$

and

$$\det\downarrow(3,4) = \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_{100\downarrow}(\mathbf{r}_3) & \psi_{100\downarrow}(\mathbf{r}_4) \\ \psi_{200\downarrow}(\mathbf{r}_3) & \psi_{200\downarrow}(\mathbf{r}_4) \end{vmatrix}.$$

The product of these two determinants will always be the same as the total determinant.

After splitting the determinant into two it is simpler to calculate the ratio R as presented in the last section. The ratio is now

$$R = \frac{|\hat{D}|^{\text{new}}}{|\hat{D}|^{\text{old}}} = \frac{|\hat{D}|^{\text{new}}_{\uparrow}}{|\hat{D}|^{\text{old}}_{\uparrow}} \cdot \frac{|\hat{D}|^{\text{new}}_{\downarrow}}{|\hat{D}|^{\text{old}}_{\downarrow}}$$

Implementing this instead will reduce the CPU time by a constant factor. While the ratio calculation above looks good on paper, what we actually use to calculate the ratio is the expression

$$R = \sum_{j=1}^{N} d_{ij}(\mathbf{r}^{\text{new}})\, d^{-1}_{ji}(\mathbf{r}^{\text{old}}) = \sum_{j=1}^{N} \phi_j(\mathbf{r}^{\text{new}}_i)\, d^{-1}_{ji}(\mathbf{r}^{\text{old}}) \tag{27}$$

To compute the ratios we still have to remember to save the inverse of the Slater determinant matrix for each loop. For each new position, row i is updated and the new inverse has to be calculated. So to save computation time, we will use the expressions

$$d^{-1}_{kj}(\mathbf{x}^{\mathbf{new}}) = \begin{cases} d^{-1}_{kj}(\mathbf{x}^{\mathbf{old}}) - \frac{d^{-1}_{ki}(\mathbf{x}^{\mathbf{old}})}{R}\sum_{l=1}^{N} d_{il}(\mathbf{x}^{\mathbf{new}})d^{-1}_{lj}(\mathbf{x}^{\mathbf{old}}) & \text{if } j \neq i \\ \frac{d^{-1}_{ki}(\mathbf{x}^{\mathbf{old}})}{R}\sum_{l=1}^{N} d_{il}(\mathbf{x}^{\mathbf{old}})d^{-1}_{lj}(\mathbf{x}^{\mathbf{old}}) & \text{if } j = i \end{cases}$$

2.6 Blocking

In statistics we usually talk about correlated and uncorrelated events. If a set of events are uncorrelated, or independent, one measurement does not depend on the previous measurement at all. Throwing a die several times or flipping multiple coins are examples of measurements that are uncorrelated. Measuring the temperature of a system with a few minutes between each measurement is an example of the opposite, where the measurements are indeed correlated. The temperature of measurement i is in fact dependent on the measurement $i-1$, as long as we assume that the time between the measurements is short. To know if a set of measurements are correlated or not is important because if can help us improve our statistics. In our code we calculate the energy of a system with rapid intervals. Close-lying energies will indeed be correlated, which we can exploit to improve our statistics by using the so-called blocking method.

If we have a set of correlated events where we measure a quantity M, we can use the blocking method to obtain better statistics. This is an improvement to the normal standard deviation (STD). While the STD is usually defined as

$$\sigma = \sqrt{\frac{1}{n}(\langle M^2 \rangle - \langle M \rangle^2)}$$

for n samples, we can improve this by using the correlation time, τ, when we have a set of correlated events. The correlation time is the time it takes from one measurement until the next event that is not correlated. If we have this correlation time, τ, we can redefine the STD to be

$$\sigma = \sqrt{\frac{1 + 2\tau/\Delta t}{n}(\langle M^2 \rangle - \langle M \rangle^2)}$$

where Δt is the time between each measurement. The blocking method is then a way of dividing our measurement samples into blocks, finding the STD of each block. The tricky part of this calculation is when the correlation time is unknown, which often is the case. When the correlation time is unknown, then so is the number of blocks we should use. In our calculations we have used a program written by M. Jonsson [5], which finds the optimal number of blocks automatically.

2.7 The Steepest Descent Method

As the name suggests, Variational Monte Carlo (VMC) includes at least one variational parameter. In our case we have two variational parameters, which we will call α and β, that can take different values. Using the steepest descent method, we include an algorithm which calculates the optimal parameters for α and β by trial and error. Calculating the energy and the derivative of the system with a guess on the value of α and β, we can use this to approximate better values for α and β. The new values is set to be

$$\alpha_{new} = \alpha - \eta * \frac{dE_L(\alpha)}{d\alpha} \qquad \beta_{new} = \beta - \eta * \frac{dE_L(\beta)}{d\beta}$$

where η is a small number, corresponding to how exact we want our calculations to be. In other words, we calculate in which direction the descent goes, hence the name "steepest descent". The way we do this in the code is to calculate

$$\overline{E}_\alpha = 2\left(\left\langle \frac{\overline{\psi}_\alpha}{\psi[\alpha]} E_L[\alpha] \right\rangle - \left\langle \frac{\overline{\psi}_\alpha}{\psi[\alpha]} \right\rangle \langle E_L[\alpha] \rangle \right) \tag{28}$$

where the average of ψ with respect to α is really the derivative of ψ with respect to α:

$$\overline{\psi}_\alpha = \frac{d\psi[\alpha]}{d\alpha} \tag{29}$$

and

$$\overline{E}_\alpha = \frac{d\langle E_L[\alpha] \rangle}{d\alpha} \tag{30}$$

and similarly for $\overline{\psi}_\beta$ and $\overline{E}_\beta$. In other words, $\overline{E}_\alpha$ is the derivative of the local energy with respect to α. With multiple variational parameters that are dependent on each other, we add them in the same way and make sure that the new value for each parameter is being calculated for each loops of Monte Carlo cycles. Calculations of $\overline{\psi}_\alpha$ and $\overline{\psi}_\beta$ can be found in section 9.1.5 for two electrons, and in section 9.2.7 for many particles.

2.8 Onebody Density

The onebody density is a fundamental object in quantum mechanics, which presents us with the possibility to optimize wave functions, calculate excitation energies and visualize wave functions. We define the onebody density function as

$$\rho(\mathbf{r}_1) = \int |\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 d\mathbf{r}_2 \cdots d\mathbf{r}_N$$

for wave function, ψ, and the integration is done over all coordinates except one. Physically this tells us the probability of finding a particle in the volume element $d\mathbf{r}_1$ in the position $\mathbf{r}_1$ [6].

In this case we are studying electrons, which are negatively charged fermions. Thinking of them as point-particles, we can easily calculate the distance between them. According to the Pauli principle, they cannot occupy the same state. Luckily, this will never happen in the code as we implement the Coulomb forces between them, making them repulsive to each other.

To calculate the onebody density is to calculate the probability of finding a particle within a distance $|\mathbf{r}|$ from the center. In two dimensions, this means to calculate how many particles are within a circle of varying radius $|\mathbf{r}|$.

2.9 The Virial Theorem

The general Virial theorem[7] used in mechanics

$$\langle T \rangle = -\frac{1}{2}\sum_{k=1}^{N} \langle \mathbf{F}_k \cdot \mathbf{r}_k \rangle \tag{31}$$

relates the time-average of the kinetic energy with the total energy, for a stable system of N particles. We let $\mathbf{F}_k$ and $\mathbf{r}_k$ be the force on particle k and the position of particle k respectively.

Using this theorem it is possible to calculate the average total kinetic energy even for complex systems, such as those we encounter in thermal physics. Unlike other similar energy equations for complex statistical physics problems, the Virial theorem does not depend on the temperature of the system.

The Virial theorem has a quantum mechanical extension, which is much more connected to our project. In this version we instead of the force consider the potential surrounding our particles. This is defined as

$$2\langle T \rangle = -\frac{1}{2}\sum_{n} \left\langle X_n \frac{dV}{dX_n} \right\rangle \tag{32}$$

where V is the potential, which for a simple harmonic oscillator is $V = \frac{1}{2}kx^2$.

3 Methods and algorithms

3.1 Variational Monte Carlo

Variational Monte Carlo (VMC) is Monte Carlo methods applied to quantum mechanical systems, where variational methods are applied to approximate the ground state energy. This means that we will find the best possible values for given variational parameters, in our case α and β, and find the smallest energy possible.

The general expression for the expectation value of the energy using this method is

$$\langle E\rangle = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \tag{33}$$

In our case, we will start by looking at a system of two electrons. With a given trial wave function the expectation value for the energy is

$$\langle E\rangle = \frac{\int d\mathbf{r}_1 d\mathbf{r}_2 \psi_T^*(\mathbf{r}_1,\mathbf{r}_2)\hat{H}(\mathbf{r}_1,\mathbf{r}_2)\psi_T(\mathbf{r}_1,\mathbf{r}_2)}{\int d\mathbf{r}_1 d\mathbf{r}_2 \psi_T^*(\mathbf{r}_1,\mathbf{r}_2)\psi_T(\mathbf{r}_1,\mathbf{r}_2)} \tag{34}$$

Note that if the wave function is normalized, the integral in the numerator is simply just equal to 1. It so happens that our trial wave function in equation (5) indeed does include a normalization factor, C. Equation (34) is then reduced to

$$\langle E\rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_T^*(\mathbf{r}_1,\mathbf{r}_2)\hat{H}(\mathbf{r}_1,\mathbf{r}_2)\psi_T(\mathbf{r}_1,\mathbf{r}_2) \tag{35}$$

We will in our studies mainly use two Monte Carlo algorithms, one we like to call the brute force (standard) Metropolis algorithm and one that is based on importance sampling. A more thorough description of the two can be found in our previous report [8], but the algorithms are presented in Algorithm 1 and 2.

Algorithm 1 The brute force Metropolis algorithm.

```
1: Create an $N \times \mathrm{dim}$ matrix where $N$ is the number of particles and dim is the
   number of dimensions.
2: Draw a random new position for a particle
3: Calculate the new value of the wave function
4: Calculate the acceptance weight, $w = \psi^2_{\mathrm{new}}/\psi^2_{\mathrm{old}}$
5: Pick random uniform number $r$ between 0 and 1
6: If $r \leq w$:
7: Keep new position, else:
8: Go back to old position
9: Repeat from step 3
```

Algorithm 2 The importance sampling algorithm.

```
1: Create an $N \times \mathrm{dim}$ matrix where $N$ is the number of particles and dim is the number of dimensions.
2: Draw a random new position for a particle influenced by the quantum force
3: Calculate the new value of the wave function
4: Calculate the greens ratio, $G$
5: Calculate the acceptance weight, $w = G\ \psi^2_{\mathrm{new}}/\psi^2_{\mathrm{old}}$
6: Pick a random number $r$ Gaussianly distributed between 0 and 1
7: If $r \leq w$:
8: Keep new position, else:
9: Go back to old position
10: Repeat from step 3
```

The main differenced between the algorithms is that the importance sampling method is slightly more tailored to our problem. It is based on that we know which way the electron is most likely to move, which is calculated by the drift term, or the quantum force.

4 Implementation

The code is structured into classes where the VMC class is where the most action happens. It is from this class that we call functions from other classes, like `hamiltonian.cpp` to calculate the energies of our system or `wavefunction.cpp` when calculating the ratios. There is also one Hermite class, based on A. A. Mariadason's Hermite header code which is available at GitHub[1].

To get more accurate calculations of the various expectation energies we wanted to wait calculating them until the system was somewhat stable. The way we did this was to introduce a ”terminalization factor”, which is an estimate of how many cycles the system needs to reach stability. What this does is to throw away the first number of cycles corresponding to the terminalization factor. When using the code it is important to take this into account, as it throws away the 10,000 first cycles, unless a different number is specified. Whenever we in this text mention a number of cycles, we run the code for this number of cycles plus the terminalization factor, throwing away the first ones. The terminalization factor leads to an artificially high acceptance ratio, especially for the brute force sampling, since the system has come to a more optimal distribution.

[1] https://github.com/Oo1Insane1oO/Hermite

We were supposed to parallelize our program using Open MPI[2], but in the program MPI only runs the same parameters on all processors specified. That means we get double of similar information in the same time we could without parallelizing the program. Open MPI is an open source Message Passing Interface used for parallelizing processes. Since the calculations is by Markov chains, we cannot split the chains without loosing information. However, a proper implementation of MPI would have helped a lot for running steepest descent for the different particle systems.

5 Code Validation

To make sure our code works for simple cases we could compare with literature. As explained earlier, the energy for a system of two electrons, no interactions and no Jastrow-factor, should be exactly 2 au and have a variance of zero. This is if we put $\alpha = \omega = 1$. Indeed, these values are returned when running the program with the mentioned conditions. Adding the Jastrow factor and fermion interaction however, the energy should become 3 au, according to M. Taut [1], [9]. As shown in table 3, our code returns an energy of 3.00061 which is very good considering that the steepest descent method returns the "almost perfect" optimal variational parameters, but will fluctuate slightly after reaching them.

When testing for more than 2 particles, we have that the unperturbed ground state energies should return 10ω for $N = 6$, 28ω for $N = 12$ and 60ω for $N = 20$. This is also something we tested our code against.

To test the mentioned ground state values we made tests using CATCH2[3], a testing framework designed for C++. With this framework it is easy to make tests. When running these, we check that we can reproduce the known values. For example, one test is to make sure that the analytically achieved value for the energy of two particles without Jastrow, interactions and with $\alpha = 1$ is obtained. Another test is to make sure that for any couple of variational parameters, we do not obtain energies lower than the analytically obtained minimum values.

Table 1 contains some reference values for the energies, and is a great help when trying to figure out what energies to expect. It is also great for comparison and testing the code.

[2] https://www.open-mpi.org
[3] https://github.com/catchorg/Catch2

Table 1: Reference values of the energy. H denotes VMC values from [10] and L denotes DMC values from [9]. All energies are given in atomic units (au). [VMC = Variational Monte Carlo & DMC = Diffusion Monte Carlo]

N	ω	$\langle E \rangle^{\mathrm{H}}_{\mathrm{reference}}$	$\langle E \rangle^{\mathrm{L}}_{\mathrm{reference}}$
2	1	3.00030	3.000000
	0.5	1.66021	1.659772
	0.1	0.44130	
	0.01	0.07406	
6	1	20.1902	20.1597
	0.5	11.8103	11.7888
	0.1	3.5690	
12	1	65.7905	65.700
	0.5	39.2343	39.159
	0.1	12.3162	
20	1	156.062	155.868
	0.5	94.0236	93.867
	0.1	30.0729	

5.1 Energy bug

We found a bug a little too late to fix it while rigorously testing the program. We believe it could be dependent of ω (and maybe the number of particles), because while testing the energy for different $\omega \neq 1$ values without Jastrow and interaction, we found out that the energy overshoots a little bit. What is strange is how this only happens for $N \in \{6, 12, 20\}$. This is why it was a little hard to detect the bug. Implications from this means that we can not entirely trust the energies for $\omega \neq 1$ and $N \in \{6, 12, 20\}$. However, we do get energies close to what we expect and we therefore believe they are not too far away from the real energies. We do not yet know exactly the impact of this, but we know that the energy overshoots for some tested values with $\omega \neq 1$.

We feel like this should be known to users or others evaluating the code and we therefore did not want to keep it a secret. If we find the bug, we will surely fix it.

6 Results

6.1 Two electrons

Step one was to check that the simple case of two electrons and no Jastrow factor or particle interactions returned an energy of exactly 2 au. We also performed a timing analysis consisting of running and timing the code several times and find the time-averages for each case. The result is shown in table 2 below.

Table 2: Expectation value of the energy in two dimensions using both the analytical expressions ($\mathcal{A}$) for the local energy and numerical derivation ($\mathcal{N}$). Also included the numerical derivation of the kinetic energy. The run time (Δt) is an average of 10 tests with 2^{20} ($= 1048576$) cycles each. The step length was set to 0.5 (BF), time step to 0.001 (IS) and $\alpha = \omega = 1$. For these calculations we used the brute force Metropolis algorithm (BF) and the importance sampling (IS) without the Jastrow factor and interaction. The local energy is $\langle E \rangle$, the local energy squared $\langle E^2 \rangle$ and the kinetic energy $\langle E_k \rangle$. The variance is denoted by σ^2 and the acceptance ratio with A_{ratio}.

$\mathcal{A}$ or $\mathcal{N}$	$\boldsymbol{N}$	**Sampling**	$\boldsymbol{\Delta t}$ [s]	$\langle \boldsymbol{E} \rangle$	$\langle \boldsymbol{E}^2 \rangle$	$\langle \boldsymbol{E}_k \rangle$	$\boldsymbol{\sigma}^2$	$\boldsymbol{A}_{ratio}$
$\mathcal{A}$	2	BF	0.714642	2	4	0.9997	0	0.892637
$\mathcal{N}$	2	BF	3.00048	2	4	0.999033	$-9.13 \cdot 10^{-20}$	0.892587
$\mathcal{A}$	2	IS	1.38728	2	4	0.998676	0	1
$\mathcal{N}$	2	IS	5.9908	2	4	1.01009	$-1.41 \cdot 10^{-19}$	1

Varying the frequency parameter ω we ran a steepest descent test for each case to then calculate the energy and mean distance between the two electrons. The variance and kinetic and potential energy is also calculated for each case. The results are presented in table 3.

Table 3: Using the steepest descent method to find the optimal variational parameters α and β for $N = 2$ electrons. For these calculations we used importance sampling with the Jastrow factor ($\boldsymbol{J}$) on and off, time step = 0.001, with fermion interaction and 2^{20} Monte Carlo cycles.

$\boldsymbol{J}$	$\boldsymbol{\omega}$	$\boldsymbol{\alpha}$	$\boldsymbol{\beta}$	$\langle \boldsymbol{E} \rangle$	$\langle \boldsymbol{E}^2 \rangle$	$\boldsymbol{\sigma}^2$	$\langle \boldsymbol{E}_k \rangle$	$\langle \boldsymbol{E}_p \rangle$	$\boldsymbol{A}_{ratio}$	$\langle r_{12} \rangle$
On	1	0.980576	0.434712	3.00061	9.00549	$1.75 \cdot 10^{-9}$	0.845629	2.15498	1	1.606668
Off	1	0.774883	-	3.22115	15.3859	$4.78 \cdot 10^{-6}$	0.781533	2.43962	1	1.441230
On	0.5	0.971146	0.367442	1.66228	2.76509	$1.82 \cdot 10^{-9}$	0.445082	1.2172	1	2.438865
Off	0.5	0.698815	-	1.78376	4.96023	$1.7 \cdot 10^{-6}$	0.355059	1.4287	1	2.088399
On	0.1	0.969692	0.348249	0.449168	0.206141	$4.19 \cdot 10^{-9}$	0.097915	0.351253	1	5.441428
Off	0.1	0.622226	-	0.567382	0.624137	$2.88 \cdot 10^{-7}$	0.077020	0.490362	1	5.104186
On	0.05	0.977588	0.236799	0.2661	0.072176	$1.3 \cdot 10^{-9}$	0.048221	0.21788	1	7.979479
Off	0.05	0.715507	-	0.390182	0.507832	$3.39 \cdot 10^{-7}$	0.050884	0.339298	1	6.717634
On	0.01	0.930168	0.159622	0.088095	0.008002	$2.3 \cdot 10^{-10}$	0.010781	0.077315	1	17.308266
Off	0.01	0.766969	-	0.163628	0.178317	$1.45 \cdot 10^{-7}$	0.010933	0.152695	1	10.465978

To achieve better statistics we performed a blocking analysis for the two-particle case. This reduced the STD, as shown in table 4 below. As the brute-force and importance sampling gave so similar results, they have the same STD's as each other.

Table 4: Blocking analysis for optimal parameters, $\alpha = 0.980576$ and $\beta = 0.434712$ as found with the steepest descent method and shown in table 3. This illustrates how much the uncertainty is reduced when using the blocking method. It also shows us how the importance sampling is slightly more stable than the brute force Metropolis after reaching terminalization.

Sampling	**STD without Blocking**	**STD with Blocking**
BF	$4.280 \cdot 10^{-2}$	$1.474 \cdot 10^{-3}$
IS	$4.144 \cdot 10^{-2}$	$3.387 \cdot 10^{-4}$

One thing we wanted to compute was the so-called one body density, as presented in section 2.8. We computed the one body density with and without the Jastrow factor and also with and without the interaction term. The result is the figure shown in figure 1.

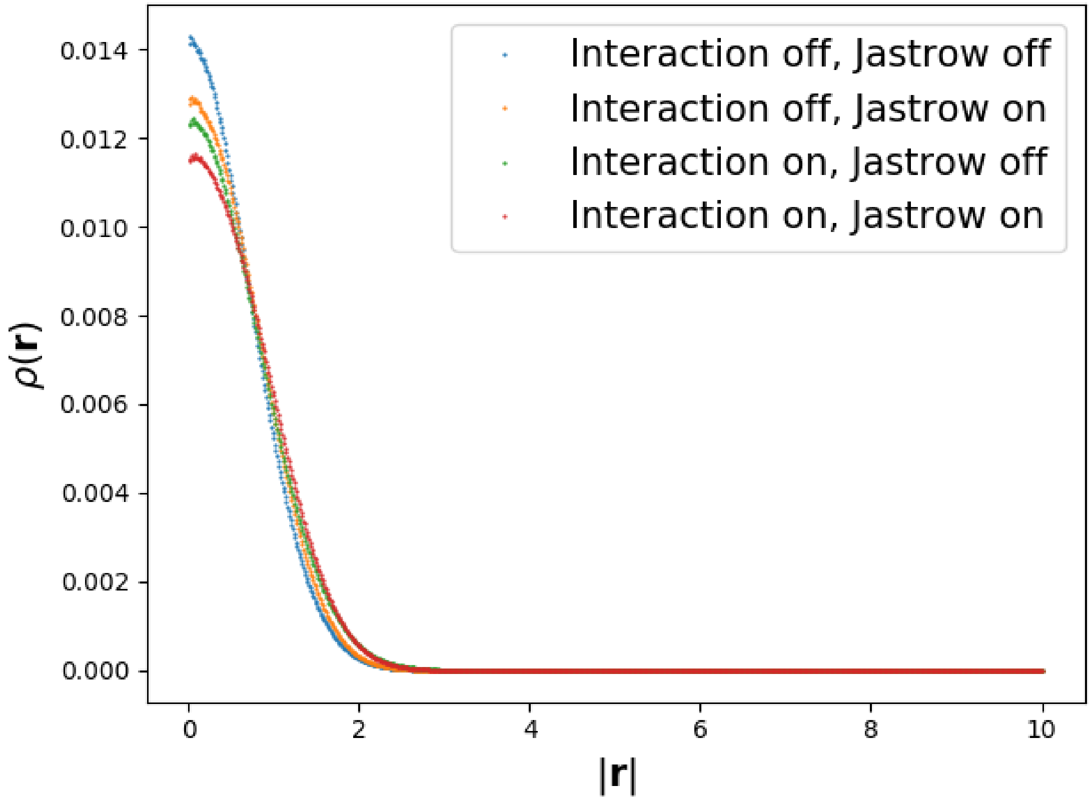

Figure 1: One body density computed for two particles with optimal parameters following from steepest descent for $\omega = 1$. According to this figure, the interaction term seems to have a much bigger effect on the one body density than the Jastrow factor. The green curve (with interaction, without Jastrow) was calculated by the optimal parameters $\alpha = 1.10529$ and $\beta = 0.623213$ found by the steepest descent method. We wanted to see the effect of the interaction as well.

6.2 N particles

In this section we present the results obtained when using more than only two electrons. We start with a presentation of our obtained lowest energy. We note here that the energy was calculated for a number of combination of parameters α and β as the steepest descent method is very time-consuming for many particles. The obtained best parameters along with energy and blocking STD is listed in table 5. In table 6 we present the obtained energy with the same parameters but this time without the Jastrow factor. Figure 2 shows the one body density for $N = 6$ electrons.

Table 5: The optimal parameters found by using a grid of different values for α and β. The energy is given for a specific value of ω. In this case, both Jastrow and particle interactions were set to be on.

N	$\boldsymbol{\omega}$	$\boldsymbol{\alpha}$	$\boldsymbol{\beta}$	$\langle \boldsymbol{E} \rangle$	$\langle \boldsymbol{E}_k \rangle$	$\langle \boldsymbol{E}_p \rangle$	$\boldsymbol{\sigma}_{\text{blocking}}$
6	1	0.99	0.50	20.1975	3.78107	16.4065	0.0149061
	0.5	1.05	0.25	12.2483	2.3585	10.2184	0.0197107
	0.1	0.85	0.20	3.93513	0.680717	3.36291	0.0163244
	0.05	0.80	0.15	2.45893	0.345778	2.14912	0.105884
	0.01	0.90	0.05	0.79870	-0.0854131	0.747683	0.103566
12	1	1.20	0.40	65.3095	9.32701	56.0638	0.0761
	0.5	1.10	0.50	40.7454	6.32845	34.6387	0.0829
	0.1	0.80	0.20	13.6928	1.71112	12.6098	0.113
	0.05	0.70	0.15	8.61596	0.732984	8.24489	0.248
	0.01	0.80	0.05	2.77648	-1.38523	2.80174	0.808
20	1	1.05	0.45	154.851	16.6564	138.194	0.220196

Table 6: Same as in table 5, but here without the Jastrow factor.

N	$\boldsymbol{\omega}$	$\boldsymbol{\alpha}$	$\langle \boldsymbol{E} \rangle$	$\langle \boldsymbol{E}_k \rangle$	$\langle \boldsymbol{E}_p \rangle$	$\boldsymbol{\sigma}_{\text{blocking}}$
6	1	0.7	21.4258	4.05949	17.3663	0.0269185
	0.5	0.5	13.3661	2.23272	11.1334	0.0233816
	0.1	0.3	4.47424	0.718956	3.75529	0.0226434
	0.05	0.3	2.83252	0.504699	2.32783	0.0184238
	0.01	0.1	1.04857	0.127475	0.921092	0.0192965
12	1	0.6	69.9328	11.2908	58.6421	0.1396160
	0.5	0.5	44.3943	7.51153	36.8827	0.10284
	0.1	0.3	15.2599	2.7553	12.5443	0.0873433
	0.05	0.2	9.63926	1.57807	8.06119	0.0711009
	0.01	0.1	3.36411	0.508175	2.85594	0.0754827
20	1	0.60	164.544	21.7614	142.783	0.280845

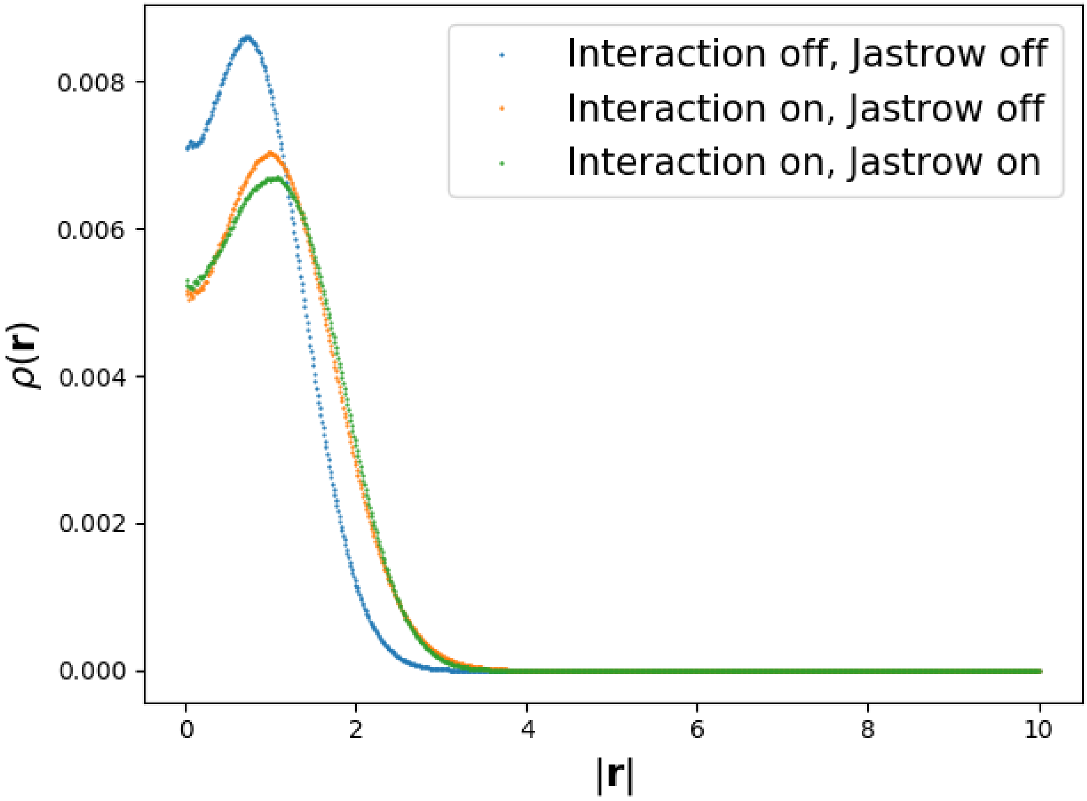

Figure 2: One body density computed for six particles with optimal parameters following from a grid of different α and β values for $\omega = 1$.

6.3 Performance analysis

The last thing we did was to run a performance analysis of our code. What we mean by this is that we ran a set of tests for different compilation flags in order to get a good timing of the code. The result of this is presented below in table 7. This performance analysis was performed for $N = 6$ and 2^{20} cycles.

Table 7: Performance analysis using compile flags -O0 (including -O1 and -O2) which is without vectorization and -O3 which is with vectorization. The run time (Δt) is an average of 10 tests with 2^{20} Monte Carlo cycles (effectively 2^{20} + 10000 cycles since the terminalization factor was included). For sampling we used brute force Metropolis. MPI is not properly implemented, but can run the same parameter file on different processors, leading to double the results in the same time as a regular -O3 run without MPI. Effectively this gives a factor 1/2 in run time. More information about the compile flags can be found at `https://gcc.gnu.org/onlinedocs/gcc/Optimize-Options.html`

Compile flags	$\mathbf{\Delta t}$ [s]
-O0	83.5621
-O1	14.2776
-O2	12.946
-O3	12.1866
MPI (with -O3)	12.3616

7 Discussion

7.1 Two electrons

One of the first things done with our code was to show that we get analytically expected values. A benchmark we did was to make sure that a simple system of two electrons without the Jastrow factor returned an energy of 2 au and a variance of exactly zero. We found that this was indeed the case for the code when using brute force Metropolis and the analytical expression. Adding instead the numerical calculation, we get the same energy but obtain a variance of $9.13 \cdot 10^{-20}$, which is practically zero when keeping numerical precision in mind. The major difference between the two energy calculations was definitely the timing. While the code ran at 0.71 s with the analytic energy expression, it was more than four times as slow with 3.0 s when using numerical energy calculation.

Adding importance sampling makes the code a little slower compared to the brute-force (BF) results. It is however faster than the numerical energy calculation done with BF. Here we must remind ourselves that we only look at two electrons. We have previously found [8] that the importance sampling algorithm first becomes faster than the brute force Metropolis when studying big systems of many particles.

Table 4 shows us the results of using the blocking method when running with the Jastrow factor and optimal parameters. Our original plan was to study the effect of blocking for the system without Jastrow and $\alpha = 1$. However, after implementing the terminalization factor, the variance for this case was of course always zero and thus the STD with and without blocking would also become zero. Because of this we instead decided to study the effects of blocking when running for the two-particles system with the Jastrow factor and optimal parameters. When doing this we achieve the results as presented in table 4, which shows us that using blocking makes the STD reduce by more than a factor of ten. This is a major improvement to the statistics. We also see that the importance sampling algorithm gives more stable results after reaching stability compared to the brute force Metropolis algorithm.

To find the optimal variational parameters, we chose to use the steepest descent method. As expected, we found this to return $\alpha = 1$ when running without the Jastrow factor. When running the steepest descent method with the Jastrow factor we get two variational parameters, α and β, which the energy of the system depends on. What we have found from this is that there are several combinations of α and β that can give the minimum energy for a system. How effective the steepest descent method was had a lot to do with what we chose as initial α and β and how close they were to the optimal values. Another factor that has a lot to do with how fast the steepest descent method was is the step-size η. A bigger η makes the steepest descent faster but will with lower accuracy hit the exact variational parameters that we are looking for.

The minimum energies obtained for the two electrons after running steepest descent are all presented in table 3. For $\omega = 1$ we have from Taut's article [1] that we should obtain 3 au when running with the Jastrow factor and interaction. In our calculations we obtain 3.00061 which deviated only 0.02 % from Taut's value. Considering how the steepest descent will fluctuate slightly around the minimum energy we see this as very good agreement with the analytical calculations.

We also computed the mean distance between the particles, which showed to be very dependent on the frequency ω. Decreasing the value of ω by a factor of 100 made the particle distance increase by more than a factor of 10. Table 3 also shows us the correlation between the energy and particle distance. Higher energies allow the particles to be much closer to each other than the low energies.

When computing the onebody densities for two electrons we get the results shown in figure 1. Comparing the pure harmonic oscillator (HO) potential with that of a HO system including interaction, we see that we gain some small differences. The blue data corresponds to the system without interaction and the Jastrow factor. This is the case where the particles are closest to each other, making the onebody density biggest for small r and dropping quickest of all the cases. We see that the interaction term is what makes the biggest difference, but the Jastrow term also adds to the onebody density.

We see that the Jastrow factor has a great importance especially when studying the minimum energy. While the minimum energy becomes 2 au without the Jastrow factor and the interaction term, the energy is increased by 10 % to ~ 2.2 au when adding Jastrow. For an accurate result energy wise, including the Jastrow therefore appears to be crucial. If we on top of this adds interaction, we get 3.00061 au, increasing the energy by 36 %. Together this shows us that in order to get a good understanding and accurate results of quantum dot systems, the Jastrow factor is indeed an important part.

In table 3 we study the dependence of ω for the kinetic and potential energy. As the harmonic oscillator energy steps $\frac{1}{2}\hbar\omega$ are dependent on the frequency ω we expect the energy to increase as we choose higher frequencies. This is indeed what we saw was the case.

Comparing the result with what we obtain analytically using the Virial theorem we see that the results vary quite a lot. This is probably because (at least the simple Virial theorem we used) does not consider the interaction between the particles. When computing the Virial theorem we find kinetic energies which are in the same order of magnitude as the ones calculated in the code. Comparing with the Virial theorem does not help us much to determine whether our numerical calculations are good or not, but only gives us the order of magnitude the energies should be.

7.2 More electrons

Table 5 shows the results obtained for 6 and 12 particles when using blocking and importance sampling. We added the steepest descent method for for N particles, but found that it was very slow, because we didn't have a proper implementation of MPI to use parallelization. We instead chose to run normal energy calculation with a grid of α and β pairs. Around the optimal parameters we found that the exact values for the variational parameters did not change the energies too much. We therefore feel that the time we saved by running the grid of parameters was worth it, even though we might have been able to reduce the energies slightly more if we had used the steepest descent method.

Table 5 also shows us how the different expectation values changes with ω. We see that the energy is heavily dependent on choice of ω, where the potential energy has the most effect on the total energy, while the kinetic energy also changes a little.

When repeating the energy calculation for many particles and varying ω but without the Jastrow factor, we get the results presented in table 6. This shows us that the energy becomes slightly higher (about ten percent) when running without Jastrow. For accurate energy calculations, it is therefore necessary to run with the Jastrow factor on. The timing is however bigger for many particles, so if the only thing wanted is a rough estimate of the energy, running without the Jastrow is enough.

Calculating the onebody density for many particles gives different curves than for just two particles. It looks almost like a Gaussian to the right, but close to zero the Gaussian shape disappears. Here we again see that the density is greatest at low distances when interaction and Jastrow are turned off. Adding them give slightly lower results.

Table 7 shows us the effects of running with different optimization flags. We see that the -O3 flag gives the fastest calculations, with -O2 and -O1 slightly behind. -O0 gives terrible timing results and we strongly recommend that this is not used for our code. We note that using MPI will give approximately the same timing for each run of the code, but when using MPI we have the ability to run several calculations at the same time. It is only here the parallelization comes in. As it is implemented now, running only one experiment once will not have any affect from using MPI.

8 Conclusion

We have written a VMC code that lets us calculate the energy, mean distance between particles, one body density and other values for closed shell quantum dot systems of $N = 2$, 6, 12 and 20 particles. The code includes features like variational parameters optimization methods (steepest descent) and blocking. It has been benchmarked to analytical and computational calculations of the energy, both simple calculations done by ourselves and calculations from papers. Built into the code is a numerical and an analytical calculation of the energy, which both give the same result. The major difference between the two energy calculation algorithms is that the analytical expression are much faster than the numerical. We strongly recommend users of the code to avoid the numerical energy calculation if it is not used for specific studies that require the numerical calculation.

There are two different sampling algorithms to use, namely a brute-force Metropolis algorithm and one algorithm where we have implemented importance sampling. For the two-electron case we found that the brute force method was slightly faster than using importance sampling. It is known from earlier projects [8] that importance sampling really only start shining for many particles where the CPU times gets significantly improved from importance sampling.

In our system we have two variational parameters, α and β. Given that we have two variational parameters it is hard to get only one pair of parameters which yield the lowest energy. Instead we have found that there are a number of combinations that yield the lowest possible energy.

In our code we have implemented a feature which makes the user able to run all calculations with or without the Jastrow factor. We wanted to explore how important this factor was for the calculations or if calculations of the various properties could be done efficiently and correctly without it. For the mean distance, we found that the distance with Jastrow was 1.1 times bigger than without it. There was a factor 1.07 times larger energy without the Jastrow factor compared to with it. The difference when studying the one body density was the greatest. Looking at figure 1 we see that the Jastrow factor gives a big difference in the result. From all this we can conclude that the Jastrow factor definitely is important for as accurate calculations as possible. However, if the user wants a quick estimate of a system and the precision is not crucial then running the code with a slight speedup by excluding the Jastrow factor might be ideal.

We have found that the expectation value for the different number of particles we use is very dependent on the frequency, or ω. When changing this value it is mostly the potential energy which changes and affects the total energy the most, although the kinetic energy also is affected.

As a final remark, we would like to remind the user about optimization flags, where -O3 is optimal for fast running of the code.

9 Appendix

9.1 Calculations for two electrons

9.1.1 Local energy without the Jastrow factor

For two electrons, $N = 2$, the unperturbed part of the Hamiltonian becomes

$$\hat{H}_0 = \sum_{k=1}^{2} \left(-\frac{1}{2}\nabla_k^2 + \frac{1}{2}\omega^2 r_k^2 \right) = \left(-\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}\omega^2 (r_1^2 + r_2^2) \right)$$

where the Laplacian for $k = \{1, 2\}$ in two dimensions is

$$\nabla_k^2 = \nabla_1^2 + \nabla_2^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2}$$

and the repulsive interaction between the electrons becomes

$$\hat{H}_1 = \sum_{k<j} \frac{1}{r_{kj}} = \sum_{1<2} \frac{1}{r_{12}} = \frac{1}{r_{12}}$$

The trial wave function without the Jastrow factor is given as

$$\begin{aligned} \psi_T(\mathbf{r}_1, \mathbf{r}_2) &= \psi_\Phi(\mathbf{r}_1, \mathbf{r}_2) \\ &= C \exp\left(-\frac{\alpha\omega}{2}(r_1^2 + r_2^2) \right) \end{aligned}$$

Since

$$r_i = \sqrt{r_{ix}^2 + r_{iy}^2} = \sqrt{x_i^2 + y_i^2} \qquad \Longrightarrow \qquad r_1^2 = x_1^2 + y_1^2 \qquad \text{and} \qquad r_2^2 = x_2^2 + y_2^2$$

the first derivative of the wave function with respect to x_1 becomes

$$\begin{aligned} \frac{\partial}{\partial x_1}\psi_\Phi &= \psi_\Phi \frac{\partial}{\partial x_1} \left[-\frac{\alpha\omega}{2}(r_1^2 + r_2^2) \right] \\ &= \psi_\Phi \left[-\frac{\alpha\omega}{2}(2x_1) \right] \\ &= \psi_\Phi \left[-\alpha\omega x_1 \right] \end{aligned}$$

and similarly for y_1, x_2 and y_2 we get

$$\begin{aligned}
\frac{\partial}{\partial y_1}\psi_\Phi &= \psi_\Phi\left[-\alpha\omega y_1\right] \\
\frac{\partial}{\partial x_2}\psi_\Phi &= \psi_\Phi\left[-\alpha\omega x_2\right] \\
\frac{\partial}{\partial y_2}\psi_\Phi &= \psi_\Phi\left[-\alpha\omega y_2\right]
\end{aligned}$$

Which means the gradient of the trial wave function is

$$\begin{aligned}
\nabla_k\psi_\Phi &= (\nabla_1 + \nabla_2)\psi_\Phi \\
&= \left(\frac{\partial}{\partial x_1}\hat{e}_x + \frac{\partial}{\partial y_1}\hat{e}_y + \frac{\partial}{\partial x_2}\hat{e}_x + \frac{\partial}{\partial y_2}\hat{e}_y\right)\psi_\Phi \\
&= \frac{\partial}{\partial x_1}\psi_\Phi\hat{e}_x + \frac{\partial}{\partial y_1}\psi_\Phi\hat{e}_y + \frac{\partial}{\partial x_2}\psi_\Phi\hat{e}_x + \frac{\partial}{\partial y_2}\psi_\Phi\hat{e}_y \\
&= \psi_\Phi\left[-\alpha\omega x_1\right]\hat{e}_x + \psi_\Phi\left[-\alpha\omega y_1\right]\hat{e}_y + \psi_\Phi\left[-\alpha\omega x_2\right]\hat{e}_x + \psi_\Phi\left[-\alpha\omega y_2\right]\hat{e}_y \\
&= \psi_\Phi(-\alpha\omega(\mathbf{r}_1 + \mathbf{r}_2))
\end{aligned}$$

The second derivative of the wave function with respect to x_1 becomes

$$\begin{aligned}
\frac{\partial^2}{\partial x_1^2}\psi_\Phi &= \frac{\partial}{\partial x_1}\cdot\frac{\partial}{\partial x_1}\psi_\Phi \\
&= \frac{\partial}{\partial x_1}(\psi_\Phi\left[-\alpha\omega x_1\right]) \\
&= \left(\frac{\partial}{\partial x_1}\psi_\Phi\right)\left[-\alpha\omega x_1\right] + \psi_\Phi\left(\frac{\partial}{\partial x_1}\left[-\alpha\omega x_1\right]\right) \\
&= \psi_\Phi\left[-\alpha\omega x_1\right])\left[-\alpha\omega x_1\right] + \psi_\Phi(-\alpha\omega) \\
&= \psi_\Phi(\alpha^2\omega^2 x_1^2 - \alpha\omega)
\end{aligned}$$

and similarly for y_1, x_2, and y_2 we get

$$\begin{aligned}
\frac{\partial^2}{\partial y_1^2}\psi_\Phi &= \psi_\Phi(\alpha^2\omega^2 y_1^2 - \alpha\omega) \\
\frac{\partial^2}{\partial x_2^2}\psi_\Phi &= \psi_\Phi(\alpha^2\omega^2 x_2^2 - \alpha\omega) \\
\frac{\partial^2}{\partial y_2^2}\psi_\Phi &= \psi_\Phi(\alpha^2\omega^2 x_2^2 - \alpha\omega)
\end{aligned}$$

The Laplacian used on the trial wave function gives

$$\begin{aligned}
\nabla_k^2\psi_\Phi &= (\nabla_1^2+\nabla_2^2)\psi_\Phi \\
&= \left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial y_2^2}\right)\psi_\Phi \\
&= \frac{\partial^2}{\partial x_1^2}\psi_\Phi+\frac{\partial^2}{\partial y_1^2}\psi_\Phi+\frac{\partial^2}{\partial x_2^2}\psi_\Phi+\frac{\partial^2}{\partial y_2^2}\psi_\Phi \\
&= \psi_\Phi\left[\alpha^2\omega^2(x_1^2+y_1^2+x_2^2+y_2^2)-4\alpha\omega\right] \\
&= \psi_\Phi\left[\alpha^2\omega^2(r_1^2+r_2^2)-4\alpha\omega\right]
\end{aligned}$$

The local energy for two electrons without the Jastrow factor is then

$$\begin{aligned}
E_L &= \frac{1}{\psi_\Phi}\hat{H}\psi_\Phi \\
&= \frac{1}{\psi_\Phi}(\hat{H}_0+\hat{H}_1)\psi_\Phi \\
&= \frac{1}{\psi_\Phi}(\hat{H}_0\psi_\Phi+\hat{H}_1\psi_\Phi) \\
&= \frac{1}{\psi_\Phi}\left(-\frac{1}{2}(\nabla_1^2+\nabla_2^2)+\frac{1}{2}\omega^2(r_1^2+r_2^2)\right)\psi_\Phi+\frac{1}{\psi_\Phi}\frac{1}{r_{12}}\psi_\Phi \\
&= \frac{1}{\psi_\Phi}\left(-\frac{1}{2}(\nabla_1^2+\nabla_2^2)\psi_\Phi+\frac{1}{2}\omega^2(r_1^2+r_2^2)\psi_\Phi\right)+\frac{1}{r_{12}} \\
&= \frac{1}{\psi_\Phi}\left(-\frac{1}{2}\psi_\Phi\left[\alpha^2\omega^2(r_1^2+r_2^2)-4\alpha\omega\right]+\frac{1}{2}\omega^2(r_1^2+r_2^2)\psi_\Phi\right)+\frac{1}{r_{12}} \\
&= -\frac{1}{2}\alpha^2\omega^2(r_1^2+r_2^2)+2\alpha\omega+\frac{1}{2}\omega^2(r_1^2+r_2^2)+\frac{1}{r_{12}} \\
&= 2\alpha\omega+\frac{1}{2}\omega^2(1-\alpha^2)(r_1^2+r_2^2)+\frac{1}{r_{12}}
\end{aligned}$$

where $\frac{1}{r_{12}}$ is the repulsive interaction between the two electrons.

9.1.2 Local energy with the Jastrow factor

We use the same Hamiltonian and derivatives of ψ_Φ as in Section 9.1.1.

The trial wave function including the Jastrow factor is given as

$$\begin{aligned}\psi_T(\mathbf{r}_1,\mathbf{r}_2) &= \psi_\Phi(\mathbf{r}_1,\mathbf{r}_2)\psi_\mathcal{J}(\mathbf{r}_1,\mathbf{r}_2)\\ &= C\exp\left(-\frac{\alpha\omega}{2}(r_1^2+r_2^2)\right)\exp\left(\frac{ar_{12}}{1+\beta r_{12}}\right)\end{aligned}$$

where

$$\begin{aligned}r_{12} &= |\mathbf{r}_1-\mathbf{r}_2|\\ &= |(r_{1x}-r_{2x})\hat{e}_x+(r_{1y}-r_{2y})\hat{e}_y|\\ &= |(x_1-x_2)\hat{e}_x+(y_1-y_2)\hat{e}_y|\\ &= \sqrt{(x_1-x_2)^2+(y_1-y_2)^2}\end{aligned}$$

The first derivative of the Jastrow factor with respect to x_1 becomes

$$\begin{aligned}\frac{\partial}{\partial x_1}\psi_\mathcal{J} &= \psi_\mathcal{J}\frac{\partial}{\partial x_1}\left[\frac{ar_{12}}{1+\beta r_{12}}\right]\\ &= \psi_\mathcal{J}\left[\frac{a\frac{1}{2r_{12}}\cdot 2(x_1-x_2)(1+\beta r_{12})-ar_{12}(\beta\frac{1}{2r_{12}}\cdot 2(x_1-x_2))}{(1+\beta r_{12})^2}\right]\\ &= \psi_\mathcal{J}\left[\frac{ar_{12}^{-1}(x_1-x_2)(1+\beta r_{12}-\beta r_{12})}{(1+\beta r_{12})^2}\right]\\ &= \psi_\mathcal{J}\left[\frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right]\end{aligned}$$

Similarly for y_1 we get

$$\frac{\partial}{\partial y_1}\psi_\mathcal{J} = \psi_\mathcal{J}\left[\frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right]$$

For x_2 and y_2 we get a change in sign when we differentiate r_{12}, giving

$$\begin{aligned}\frac{\partial}{\partial x_2}\psi_\mathcal{J} &= \psi_\mathcal{J}\left[-\frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right]\\ \frac{\partial}{\partial y_2}\psi_\mathcal{J} &= \psi_\mathcal{J}\left[-\frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right]\end{aligned}$$

The first derivative of the wave function with respect to x_1 becomes

$$\begin{aligned}
\frac{\partial}{\partial x_1}\psi_T(\mathbf{r}_1,\mathbf{r}_2) &= \frac{\partial}{\partial x_1}(\psi_\Phi\psi_{\mathcal{J}}) \\
&= \left(\frac{\partial}{\partial x_1}\psi_\Phi\right)\psi_{\mathcal{J}} + \psi_\Phi\left(\frac{\partial}{\partial x_1}\psi_{\mathcal{J}}\right) \\
&= \left(\psi_\Phi\left[-\alpha\omega x_1\right]\right)\psi_{\mathcal{J}} + \psi_\Phi\left(\psi_{\mathcal{J}}\left[\frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right]\right) \\
&= \psi_T\underbrace{\left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)}_{X_1} \\
&= \psi_T X_1
\end{aligned}$$

Similarly for y_1 we get

$$\frac{\partial}{\partial y_1}\psi_T(\mathbf{r}_1,\mathbf{r}_2) = \psi_T\underbrace{\left(-\alpha\omega y_1 + \frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right)}_{Y_1} = \psi_T Y_1$$

For x_2 and y_2 we get a change in sign for the second term when we differentiate r_{12}, giving

$$\begin{aligned}
\frac{\partial}{\partial x_2}\psi_T(\mathbf{r}_1,\mathbf{r}_2) &= \psi_T\underbrace{\left(-\alpha\omega x_2 - \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)}_{X_2} = \psi_T X_2 \\
\frac{\partial}{\partial y_2}\psi_T(\mathbf{r}_1,\mathbf{r}_2) &= \psi_T\underbrace{\left(-\alpha\omega y_2 - \frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right)}_{Y_2} = \psi_T Y_2
\end{aligned}$$

Which means the gradient of the trial wave function is

$$\begin{aligned}
\nabla_k \psi_T &= (\nabla_1 + \nabla_2)\psi_T \\
&= \left(\frac{\partial}{\partial x_1}\hat{e}_x + \frac{\partial}{\partial y_1}\hat{e}_y + \frac{\partial}{\partial x_2}\hat{e}_x + \frac{\partial}{\partial y_2}\hat{e}_y\right)\psi_T \\
&= \frac{\partial}{\partial x_1}\psi_T\hat{e}_x + \frac{\partial}{\partial y_1}\psi_T\hat{e}_y + \frac{\partial}{\partial x_2}\psi_T\hat{e}_x + \frac{\partial}{\partial y_2}\psi_T\hat{e}_y \\
&= \psi_T\Bigg[\left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)\hat{e}_x + \left(-\alpha\omega y_1 + \frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right)\hat{e}_y \\
&\quad + \left(-\alpha\omega x_2 - \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)\hat{e}_x + \left(-\alpha\omega y_2 - \frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right)\hat{e}_y\Bigg] \\
&= \psi_T\Bigg[\left(-\alpha\omega(x_1\hat{e}_x + y_1\hat{e}_y) + \frac{a[(x_1-x_2)\hat{e}_x + (y_1-y_2)\hat{e}_y]}{r_{12}(1+\beta r_{12})^2}\right) \\
&\quad + \left(-\alpha\omega(x_2\hat{e}_x + y_2\hat{e}_y) - \frac{a[(x_1-x_2)\hat{e}_x - (y_1-y_2)\hat{e}_y]}{r_{12}(1+\beta r_{12})^2}\right)\Bigg] \\
&= \psi_T\left[\left(-\alpha\omega\mathbf{r}_1 + \frac{a(\mathbf{r}_1-\mathbf{r}_2)}{r_{12}(1+\beta r_{12})^2}\right) + \left(-\alpha\omega\mathbf{r}_2 - \frac{a(\mathbf{r}_1-\mathbf{r}_2)}{r_{12}(1+\beta r_{12})^2}\right)\right]
\end{aligned}$$

The second derivative of the wave function with respect to x_1 can be calculated by

$$\begin{aligned}
\frac{\partial^2}{\partial x_1^2}\psi_T(\mathbf{r}_1,\mathbf{r}_2) &= \frac{\partial}{\partial x_1}\cdot\frac{\partial}{\partial x_1}\psi_T(\mathbf{r}_1,\mathbf{r}_2) \\
&= \frac{\partial}{\partial x_1}(\psi_T X_1) \\
&= \left(\frac{\partial}{\partial x_1}\psi_T\right)X_1 + \psi_T\left(\frac{\partial}{\partial x_1}X_1\right) \\
&= (\psi_T X_1)X_1 + \psi_T\left(\frac{\partial}{\partial x_1}X_1\right) \\
&= \psi_T\left[X_1^2 + \frac{\partial}{\partial x_1}X_1\right]
\end{aligned}$$

where

$$\begin{aligned}
X_1^2 &= \left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)\left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right) \\
&= \left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)^2
\end{aligned}$$

and

$$
\begin{aligned}
\frac{\partial}{\partial x_1} X_1 = & \frac{\partial}{\partial x_1}\left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)\\
= & -\alpha\omega + \frac{a r_{12}(1+\beta r_{12})^2}{r_{12}^2(1+\beta r_{12})^4}\\
& - \frac{a(x_1-x_2)[\frac{1}{2r_{12}}\cdot 2(x_1-x_2)(1+\beta r_{12})^2 + r_{12}\cdot 2(1+\beta r_{12})(\beta\frac{1}{2r_{12}}\cdot 2(x_1-x_2))]}{r_{12}^2(1+\beta r_{12})^4}\\
= & -\alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{\frac{a}{r_{12}}(x_1-x_2)^2(1+\beta r_{12})[(1+\beta r_{12})+2\beta r_{12}]}{r_{12}^2(1+\beta r_{12})^4}\\
= & -\alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(x_1-x_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}
\end{aligned}
$$

The second derivative of the wave function with respect to x_1 then becomes

$$
\begin{aligned}
\frac{\partial^2}{\partial x_1^2}\psi_T(\mathbf{r}_1,\mathbf{r}_2) = & \psi_T\Bigg[\left(-\alpha\omega x_1 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)^2 - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2}\\
& - \frac{a(x_1-x_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg]\\
= & \psi_T\Bigg[\alpha^2\omega^2 x_1^2 - \frac{2\alpha\omega x_1 a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2} + \frac{a^2(x_1-x_2)^2}{r_{12}^2(1+\beta r_{12})^4}\\
& - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(x_1-x_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg]
\end{aligned}
$$

Similarly for y_1 we get

$$
\begin{aligned}
\frac{\partial^2}{\partial y_1^2}\psi_T(\mathbf{r}_1,\mathbf{r}_2) = & \psi_T\Bigg[\left(-\alpha\omega y_1 + \frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right)^2 - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2}\\
& - \frac{a(y_1-y_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg]\\
= & \psi_T\Bigg[\alpha^2\omega^2 y_1^2 - \frac{2\alpha\omega y_1 a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2} + \frac{a^2(y_1-y_2)^2}{r_{12}^2(1+\beta r_{12})^4}\\
& - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(y_1-y_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg]
\end{aligned}
$$

For x_2 and y_2 we get a change in sign each time we differentiate r_{12}, giving

$$\begin{aligned}\frac{\partial^2}{\partial x_2^2}\psi_T(\mathbf{r}_1,\mathbf{r}_2) &= \psi_T\Bigg[\left(-\alpha\omega x_2 - \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)^2 - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} \\ &\quad - \frac{a(x_1-x_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg] \\ &= \psi_T\Bigg[\left(\alpha\omega x_2 + \frac{a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2}\right)^2 - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} \\ &\quad - \frac{a(x_1-x_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg] \\ &= \psi_T\Bigg[\alpha^2\omega^2x_2^2 + \frac{2\alpha\omega x_2 a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2} + \frac{a^2(x_1-x_2)^2}{r_{12}^2(1+\beta r_{12})^4} \\ &\quad - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(x_1-x_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg]\end{aligned}$$

$$\begin{aligned}\frac{\partial^2}{\partial y_2^2}\psi_T(\mathbf{r}_1,\mathbf{r}_2) &= \psi_T\Bigg[\left(-\alpha\omega y_2 - \frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right)^2 - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} \\ &\quad - \frac{a(y_1-y_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg] \\ &= \psi_T\Bigg[\left(\alpha\omega y_2 + \frac{a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2}\right)^2 - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} \\ &\quad - \frac{a(y_1-y_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg] \\ &= \psi_T\Bigg[\alpha^2\omega^2y_2^2 + \frac{2\alpha\omega y_2 a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2} + \frac{a^2(y_1-y_2)^2}{r_{12}^2(1+\beta r_{12})^4} \\ &\quad - \alpha\omega + \frac{a}{r_{12}(1+\beta r_{12})^2} - \frac{a(y_1-y_2)^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg]\end{aligned}$$

The Laplacian used on the trial wave function gives

$$
\begin{aligned}
\nabla_k^2\psi_T &= (\nabla_1^2 + \nabla_2^2)\psi_T \\
&= \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2}\right)\psi_T \\
&= \frac{\partial^2}{\partial x_1^2}\psi_T + \frac{\partial^2}{\partial y_1^2}\psi_T + \frac{\partial^2}{\partial x_2^2}\psi_T + \frac{\partial^2}{\partial y_2^2}\psi_T \\
&= \psi_T\Bigg[\left(\alpha^2\omega^2x_1^2 - \frac{2\alpha\omega x_1 a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2} + \frac{a^2(x_1-x_2)^2}{r_{12}^2(1+\beta r_{12})^4}\right) \\
&\quad + \left(\alpha^2\omega^2y_1^2 - \frac{2\alpha\omega y_1 a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2} + \frac{a^2(y_1-y_2)^2}{r_{12}^2(1+\beta r_{12})^4}\right) \\
&\quad + \left(\alpha^2\omega^2x_2^2 + \frac{2\alpha\omega x_2 a(x_1-x_2)}{r_{12}(1+\beta r_{12})^2} + \frac{a^2(x_1-x_2)^2}{r_{12}^2(1+\beta r_{12})^4}\right) \\
&\quad + \left(\alpha^2\omega^2y_2^2 + \frac{2\alpha\omega y_2 a(y_1-y_2)}{r_{12}(1+\beta r_{12})^2} + \frac{a^2(y_1-y_2)^2}{r_{12}^2(1+\beta r_{12})^4}\right) \\
&\quad - 4\alpha\omega + \frac{4a}{r_{12}(1+\beta r_{12})^2} - \frac{2a[(x_1-x_2)^2+(y_1-y_2)^2](1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg] \\
&= \psi_T\Bigg[\alpha^2\omega^2(x_1^2+y_1^2+x_2^2+y_2^2) - \frac{2\alpha\omega a[(x_1-x_2)^2+(y_1-y_2)^2]}{r_{12}(1+\beta r_{12})^2} \\
&\quad + \frac{2a^2[(x_1-x_2)^2+(y_1-y_2)^2]}{r_{12}^2(1+\beta r_{12})^4} - 4\alpha\omega + \frac{4a}{r_{12}(1+\beta r_{12})^2} \\
&\quad - \frac{2a[(x_1-x_2)^2+(y_1-y_2)^2](1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg]
\end{aligned}
$$

Since

$$r_{12}^2 = (x_1 - x_2)^2 + (y_1 - y_2)^2$$

we get

$$\begin{aligned}(\nabla_1^2 + \nabla_2^2)\psi_T = \psi_T \Bigg[& \alpha^2\omega^2(r_1^2 + r_2^2) - \frac{2\alpha\omega a r_{12}^2}{r_{12}(1+\beta r_{12})^2} + \frac{2a^2 r_{12}^2}{r_{12}^2(1+\beta r_{12})^4} \\ & - 4\alpha\omega + \frac{4a}{r_{12}(1+\beta r_{12})^2} - \frac{2a r_{12}^2(1+3\beta r_{12})}{r_{12}^3(1+\beta r_{12})^3}\Bigg] \\ = \psi_T \Bigg[& \alpha^2\omega^2(r_1^2 + r_2^2) - \frac{2\alpha\omega a r_{12}}{(1+\beta r_{12})^2} + \frac{2a^2}{(1+\beta r_{12})^4} \\ & - 4\alpha\omega + \frac{4a}{r_{12}(1+\beta r_{12})^2} - \frac{2a(1+3\beta r_{12})}{r_{12}(1+\beta r_{12})^3}\Bigg] \\ = \psi_T \Bigg[& \alpha^2\omega^2(r_1^2 + r_2^2) - 4\alpha\omega + \frac{2a}{(1+\beta r_{12})^2}\Bigg(- \alpha\omega r_{12} \\ & + \frac{a}{(1+\beta r_{12})^2} + \frac{2}{r_{12}} - \frac{(1+3\beta r_{12})}{r_{12}(1+\beta r_{12})}\Bigg)\Bigg]\end{aligned}$$

The last two terms can be put on a common denominator

$$\frac{2}{r_{12}} - \frac{(1+3\beta r_{12})}{r_{12}(1+\beta r_{12})} = \frac{2(1+\beta r_{12})}{r_{12}(1+\beta r_{12})} - \frac{(1+3\beta r_{12})}{r_{12}(1+\beta r_{12})} = \frac{2 + 2\beta r_{12} - 1 - 3\beta r_{12}}{r_{12}(1+\beta r_{12})} = \frac{1-\beta r_{12}}{r_{12}(1+\beta r_{12})}$$

which leads to

$$\begin{aligned}(\nabla_1^2 + \nabla_2^2)\psi_T = \psi_T \Bigg[& \alpha^2\omega^2(r_1^2 + r_2^2) - 4\alpha\omega + \frac{2a}{(1+\beta r_{12})^2}\Bigg(- \alpha\omega r_{12} \\ & + \frac{a}{(1+\beta r_{12})^2} + \frac{1-\beta r_{12}}{r_{12}(1+\beta r_{12})}\Bigg)\Bigg]\end{aligned}$$

The local energy for two electrons with the Jastrow factor is then

$$\begin{aligned}
E_L &= \frac{1}{\psi_T}\hat{H}\psi_T \\
&= \frac{1}{\psi_T}(\hat{H}_0 + \hat{H}_1)\psi_T \\
&= \frac{1}{\psi_T}(\hat{H}_0\psi_T + \hat{H}_1\psi_T) \\
&= \frac{1}{\psi_T}\left(-\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}\omega^2(r_1^2 + r_2^2)\right)\psi_T + \frac{1}{\psi_T}\sum_{i<j}\frac{1}{r_{ij}}\psi_T \\
&= \frac{1}{\psi_T}\left(-\frac{1}{2}(\nabla_1^2 + \nabla_2^2)\psi_T + \frac{1}{2}\omega^2(r_1^2 + r_2^2)\psi_T\right) + \sum_{1<2}\frac{1}{r_{12}} \\
&= \frac{1}{\psi_T}\Bigg(-\frac{1}{2}\psi_T\Bigg[\alpha^2\omega^2(r_1^2 + r_2^2) - 4\alpha\omega + \frac{2a}{(1+\beta r_{12})^2}\Bigg(- \alpha\omega r_{12} \\
&\quad + \frac{a}{(1+\beta r_{12})^2} + \frac{1-\beta r_{12}}{r_{12}(1+\beta r_{12})}\Bigg)\Bigg] + \frac{1}{2}\omega^2(r_1^2 + r_2^2)\psi_T\Bigg) + \frac{1}{r_{12}} \\
&= -\frac{1}{2}\alpha^2\omega^2(r_1^2 + r_2^2) + 2\alpha\omega - \frac{a}{(1+\beta r_{12})^2}\Bigg(- \alpha\omega r_{12} \\
&\quad + \frac{a}{(1+\beta r_{12})^2} + \frac{1-\beta r_{12}}{r_{12}(1+\beta r_{12})}\Bigg) + \frac{1}{2}\omega^2(r_1^2 + r_2^2) + \frac{1}{r_{12}} \\
&= 2\alpha\omega + \frac{1}{2}\omega^2(1-\alpha^2)(r_1^2 + r_2^2) - \frac{a}{(1+\beta r_{12})^2}\Bigg(- \alpha\omega r_{12} \\
&\quad + \frac{a}{(1+\beta r_{12})^2} + \frac{1-\beta r_{12}}{r_{12}(1+\beta r_{12})}\Bigg) + \frac{1}{r_{12}}
\end{aligned}$$

where $\frac{1}{r_{12}}$ is the repulsive interaction between the two electrons.

9.1.3 Quantum force without the Jastrow factor

The gradient of the wave function without the Jastrow factor is given by

$$\nabla_k \psi_\Phi = \psi_\Phi(-\alpha\omega(\mathbf{r}_1 + \mathbf{r}_2))$$

which leads to the quantum force

$$F = \frac{2\nabla_k \psi_\Phi}{\psi_\Phi} = \frac{2\psi_\Phi(-\alpha\omega(\mathbf{r}_1 + \mathbf{r}_2))}{\psi_\Phi} = -2\alpha\omega(\mathbf{r}_1 + \mathbf{r}_2)$$

9.1.4 Quantum force with the Jastrow factor

The gradient of the wave function with the Jastrow factor is given by

$$\nabla_k \psi_T = \psi_T \left[\left(-\alpha\omega\mathbf{r}_1 + \frac{a(\mathbf{r}_1 - \mathbf{r}_2)}{r_{12}(1+\beta r_{12})^2} \right) + \left(-\alpha\omega\mathbf{r}_2 - \frac{a(\mathbf{r}_1 - \mathbf{r}_2)}{r_{12}(1+\beta r_{12})^2} \right) \right]$$

which leads to the quantum force

$$\begin{aligned} F &= \frac{2\nabla_k \psi_T}{\psi_T} \\ &= \frac{2}{\psi_T}\psi_T \left[\left(-\alpha\omega\mathbf{r}_1 + \frac{a(\mathbf{r}_1 - \mathbf{r}_2)}{r_{12}(1+\beta r_{12})^2} \right) + \left(-\alpha\omega\mathbf{r}_2 - \frac{a(\mathbf{r}_1 - \mathbf{r}_2)}{r_{12}(1+\beta r_{12})^2} \right) \right] \\ &= 2 \left[\left(-\alpha\omega\mathbf{r}_1 + \frac{a(\mathbf{r}_1 - \mathbf{r}_2)}{r_{12}(1+\beta r_{12})^2} \right) + \left(-\alpha\omega\mathbf{r}_2 - \frac{a(\mathbf{r}_1 - \mathbf{r}_2)}{r_{12}(1+\beta r_{12})^2} \right) \right] \end{aligned}$$

9.1.5 Steepest descent

The trial wave function with the Jastrow factor is given by

$$\psi_T = \psi_\phi \psi_{\mathcal{J}} = \underbrace{C \exp\left(-\frac{\alpha\omega}{2}(r_1^2 + r_2^2)\right)}_{\psi_\alpha} \underbrace{\exp\left(\frac{ar_{12}}{1+\beta r_{12}}\right)}_{\psi_\beta}$$

The derivative of the wave function with respect to α is

$$\overline{\psi}_\alpha = \frac{d\psi_T[\alpha]}{d\alpha} = \psi_T \left(-\frac{\omega}{2}(r_1^2 + r_2^2)\right)$$

making

$$\frac{\overline{\psi}_\alpha}{\psi_T} = -\frac{\omega}{2}(r_1^2 + r_2^2)$$

The derivative of the wave function with respect to β is

$$\overline{\psi}_\beta = \frac{d\psi_T[\beta]}{d\beta} = \psi_T \left(-\frac{ar_{12}^2}{(1+\beta r_{12})^2}\right)$$

making

$$\frac{\overline{\psi}_\beta}{\psi_T} = -\frac{ar_{12}^2}{(1+\beta r_{12})^2}$$

9.2 Calculations for many-particle systems

9.2.1 Gradient of the single particle wave function

The wave fuction for one particle is given by

$$\phi_{n_x,n_y}(x_i,y_i) = AH_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)$$

The gradient of the wave function is

$$\begin{aligned}\nabla_k\phi_{n_x,n_y}(x_i,y_i) &= \left(\frac{\partial}{\partial x_i}\hat{e}_x + \frac{\partial}{\partial y_i}\hat{e}_y\right)\phi_{n_x,n_y}(x_i,y_i)\\ &= \frac{\partial}{\partial x_i}\phi_{n_x,n_y}(x_i,y_i)\hat{e}_x + \frac{\partial}{\partial y_i}\phi_{n_x,n_y}(x_i,y_i)\hat{e}_y\end{aligned}$$

where

$$\begin{aligned}\frac{\partial}{\partial x_i}\phi_{n_x,n_y}(x_i,y_i) &= \frac{\partial}{\partial x_i}\left(AH_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\right)\\ &= A\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]H_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\\ &\quad + AH_{n_x}(\sqrt{\alpha\omega}x_i)\underbrace{\left[\frac{\partial}{\partial x_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right]}_{=0}\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\\ &\quad + AH_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)\underbrace{\left[\frac{\partial}{\partial x_i}\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\right]}_{-\alpha\omega x_i\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)}\\ &= AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left(\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] - H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega x_i\right)\end{aligned}$$

and similarly

$$\frac{\partial}{\partial y_i}\phi_{n_x,n_y}(x_i,y_i) = AH_{n_x}(\sqrt{\alpha\omega}x_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left(\left[\frac{\partial}{\partial y_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right] - H_{n_y}(\sqrt{\alpha\omega}y_i)\alpha\omega y_i\right)$$

In the quantum force we need the gradient divided by the single particle wave function, which is

$$\begin{aligned}
\frac{\nabla_k \phi_{n_x,n_y}(x_i,y_i)}{\phi_{n_x,n_y}(x_i,y_i)} &= \frac{AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left(\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] - H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega x_i\right)\hat{e}_x}{AH_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)} \\
&+ \frac{AH_{n_x}(\sqrt{\alpha\omega}x_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left(\left[\frac{\partial}{\partial y_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right] - H_{n_y}(\sqrt{\alpha\omega}y_i)\alpha\omega y_i\right)\hat{e}_y}{AH_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)} \\
&= \left(\frac{1}{H_{n_x}(\sqrt{\alpha\omega}x_i)}\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] - \alpha\omega x_i\right)\hat{e}_x \\
&+ \left(\frac{1}{H_{n_y}(\sqrt{\alpha\omega}y_i)}\left[\frac{\partial}{\partial y_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right] - \alpha\omega y_i\right)\hat{e}_y
\end{aligned}$$

9.2.2 Laplacian of the single particle wave function

The Laplacian can be calculated by

$$\begin{aligned}
\nabla_k^2 \phi_{n_x,n_y}(x_i,y_i) &= \left(\frac{\partial}{\partial x_i^2} + \frac{\partial}{\partial y_i^2}\right)\phi_{n_x,n_y}(x_i,y_i) \\
&= \frac{\partial}{\partial x_i^2}\phi_{n_x,n_y}(x_i,y_i) + \frac{\partial}{\partial y_i^2}\phi_{n_x,n_y}(x_i,y_i)
\end{aligned}$$

where

$$
\begin{aligned}
\frac{\partial}{\partial x_i^2}\phi_{n_x,n_y}(x_i,y_i) &= \frac{\partial}{\partial x_i}\cdot\frac{\partial}{\partial x_i}\phi_{n_x,n_y}(x_i,y_i) \\
&= \frac{\partial}{\partial x_i}\cdot\Bigg[AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\Bigg(\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&\quad - H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega x_i\Bigg)\Bigg] \\
&= \frac{\partial}{\partial x_i}\cdot\Bigg[AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&\quad - AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega x_i\Bigg] \\
&= A\underbrace{\left[\frac{\partial}{\partial x_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right]}_{=0}\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&\quad + AH_{n_y}(\sqrt{\alpha\omega}y_i)\underbrace{\left[\frac{\partial}{\partial x_i}\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\right]}_{-\alpha\omega x_i\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)}\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&\quad + AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{\partial}{\partial x_i^2}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&\quad - A\underbrace{\left[\frac{\partial}{\partial x_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right]}_{=0}\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega x_i \\
&\quad - AH_{n_y}(\sqrt{\alpha\omega}y_i)\underbrace{\left[\frac{\partial}{\partial x_i}\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\right]}_{-\alpha\omega x_i\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)}H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega x_i \\
&\quad - AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]\alpha\omega x_i \\
&\quad - AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega\underbrace{\left[\frac{\partial}{\partial x_i}x_i\right]}_{=1}
\end{aligned}
$$

factorizing gives

$$
\begin{aligned}
\frac{\partial}{\partial x_i^2}\phi_{n_x,n_y}(x_i,y_i) =& -AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]\alpha\omega x_i \\
&+ AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{\partial}{\partial x_i^2}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&+ AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)H_{n_x}(\sqrt{\alpha\omega}x_i)(\alpha\omega x_i)^2 \\
&- AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]\alpha\omega x_i \\
&- AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega \\
=& AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{\partial}{\partial x_i^2}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&- 2AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]\alpha\omega x_i \\
&+ AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)H_{n_x}(\sqrt{\alpha\omega}x_i)(\alpha\omega x_i)^2 \\
&- AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega \\
=& AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\Bigg(\left[\frac{\partial}{\partial x_i^2}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&- 2\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]\alpha\omega x_i + H_{n_x}(\sqrt{\alpha\omega}x_i)(\alpha\omega x_i)^2 - H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega\Bigg)
\end{aligned}
$$

Simlilarly we have

$$
\begin{aligned}
\frac{\partial}{\partial y_i^2}\phi_{n_x,n_y}(x_i,y_i) =& AH_{n_x}(\sqrt{\alpha\omega}x_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\Bigg(\left[\frac{\partial}{\partial y_i^2}H_{n_y}(\sqrt{\alpha\omega}y_i)\right] \\
&- 2\left[\frac{\partial}{\partial y_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right]\alpha\omega y_i + H_{n_y}(\sqrt{\alpha\omega}y_i)(\alpha\omega y_i)^2 - H_{n_y}(\sqrt{\alpha\omega}y_i)\alpha\omega\Bigg)
\end{aligned}
$$

This leads to the Laplacian

$$
\begin{aligned}
\nabla_k^2 \phi_{n_x,n_y}(x_i,y_i) = &\left(\frac{\partial}{\partial x_i^2} + \frac{\partial}{\partial y_i^2}\right)\phi_{n_x,n_y}(x_i,y_i) \\
&= \frac{\partial}{\partial x_i^2}\phi_{n_x,n_y}(x_i,y_i) + \frac{\partial}{\partial y_i^2}\phi_{n_x,n_y}(x_i,y_i) \\
&= AH_{n_y}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\Bigg(\left[\frac{\partial}{\partial x_i^2}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&- 2\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]\alpha\omega x_i + H_{n_x}(\sqrt{\alpha\omega}x_i)(\alpha\omega x_i)^2 - H_{n_x}(\sqrt{\alpha\omega}x_i)\alpha\omega\Bigg) \\
&+ AH_{n_x}(\sqrt{\alpha\omega}x_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\Bigg(\left[\frac{\partial}{\partial y_i^2}H_{n_y}(\sqrt{\alpha\omega}y_i)\right] \\
&- 2\left[\frac{\partial}{\partial y_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right]\alpha\omega y_i + H_{n_y}(\sqrt{\alpha\omega}y_i)(\alpha\omega y_i)^2 - H_{n_y}(\sqrt{\alpha\omega}y_i)\alpha\omega\Bigg) \\
&= A\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\Bigg(H_{n_y}(\sqrt{\alpha\omega}y_i)\left[\frac{\partial}{\partial x_i^2}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&- 2H_{n_y}(\sqrt{\alpha\omega}y_i)\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]\alpha\omega x_i + H_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)(\alpha\omega x_i)^2 \\
&- H_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)\alpha\omega\Bigg) \\
&+ A\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\Bigg(H_{n_x}(\sqrt{\alpha\omega}x_i)\left[\frac{\partial}{\partial y_i^2}H_{n_y}(\sqrt{\alpha\omega}y_i)\right] \\
&- 2H_{n_x}(\sqrt{\alpha\omega}x_i)\left[\frac{\partial}{\partial y_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right]\alpha\omega y_i + H_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)(\alpha\omega y_i)^2 \\
&- H_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)\alpha\omega\Bigg) \\
&= A\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\Bigg(H_{n_y}(\sqrt{\alpha\omega}y_i)\left[\frac{\partial}{\partial x_i^2}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&+ H_{n_x}(\sqrt{\alpha\omega}x_i)\left[\frac{\partial}{\partial y_i^2}H_{n_y}(\sqrt{\alpha\omega}y_i)\right] \\
&- 2\alpha\omega\left(H_{n_y}(\sqrt{\alpha\omega}y_i)\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]x_i + H_{n_x}(\sqrt{\alpha\omega}x_i)\left[\frac{\partial}{\partial y_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right]y_i\right) \\
&+ H_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)\alpha\omega\left[\alpha\omega(x_i^2+y_i^2)-2\right]\Bigg)
\end{aligned}
$$

and

$$\begin{aligned}
\frac{\nabla_k^2 \phi_{n_x,n_y}(x_i,y_i)}{\phi_{n_x,n_y}(x_i,y_i)} &= \frac{A\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)}{AH_{n_x}(\sqrt{\alpha\omega}x)H_{n_y}(\sqrt{\alpha\omega}y)\exp\left(-\frac{\alpha\omega}{2}(x^2+y^2)\right)}\Bigg(H_{n_y}(\sqrt{\alpha\omega}y_i)\left[\frac{\partial}{\partial x_i^2}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] \\
&\quad + H_{n_x}(\sqrt{\alpha\omega}x_i)\left[\frac{\partial}{\partial y_i^2}H_{n_y}(\sqrt{\alpha\omega}y_i)\right] \\
&\quad - 2\alpha\omega\left(H_{n_y}(\sqrt{\alpha\omega}y_i)\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]x_i + H_{n_x}(\sqrt{\alpha\omega}x_i)\left[\frac{\partial}{\partial y_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right]y_i\right) \\
&\quad + H_{n_x}(\sqrt{\alpha\omega}x_i)H_{n_y}(\sqrt{\alpha\omega}y_i)\alpha\omega\left[\alpha\omega(x_i^2+y_i^2)-2\right]\Bigg) \\
&= \frac{1}{H_{n_x}(\sqrt{\alpha\omega}x_i)}\left[\frac{\partial}{\partial x_i^2}H_{n_x}(\sqrt{\alpha\omega}x_i)\right] + \frac{1}{H_{n_y}(\sqrt{\alpha\omega}y_i)}\left[\frac{\partial}{\partial y_i^2}H_{n_y}(\sqrt{\alpha\omega}y_i)\right] \\
&\quad - 2\alpha\omega\left(\frac{1}{H_{n_x}(\sqrt{\alpha\omega}x_i)}\left[\frac{\partial}{\partial x_i}H_{n_x}(\sqrt{\alpha\omega}x_i)\right]x_i + \frac{1}{H_{n_y}(\sqrt{\alpha\omega}y_i)}\left[\frac{\partial}{\partial y_i}H_{n_y}(\sqrt{\alpha\omega}y_i)\right]y_i\right) \\
&\quad + (\alpha\omega)^2(x_i^2+y_i^2) - 2\alpha\omega
\end{aligned}$$

9.2.3 Gradient of the Jastrow factor

By substituting $r_{kj} = |\mathbf{r}_k - \mathbf{r}_j|$ we can write the gradient ∇_k as

$$\nabla_k = \nabla_k \frac{\partial r_{kj}}{\partial r_{kj}} = \nabla_k r_{kj}\frac{\partial}{\partial r_{kj}} = \frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}}\frac{\partial}{\partial r_{kj}} = \frac{\mathbf{r}_{kj}}{r_{kj}}\frac{\partial}{\partial r_{kj}}$$

where $\mathbf{r}_{kj} = \mathbf{r}_k - \mathbf{r}_j$.

The Jastrow wave function is given by

$$\psi_{\mathcal{J}} = \prod_{i<j}^{N} g(r_{ij}) = \exp\left(\sum_{i<j}^{N} f(r_{ij})\right) = \exp\left(\sum_{i<j}^{N}\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}\right)$$

The gradient of the Jastrow factor then becomes

$$\begin{aligned}
\nabla_k \psi_{\mathcal{J}} &= \nabla_k \exp\left(\sum_{i<j}^{N} f(r_{ij})\right) \\
&= \exp\left(\sum_{i<j}^{N} f(r_{ij})\right) \nabla_k \left(\sum_{i<j}^{N} f(r_{ij})\right) \\
&= \exp\left(\sum_{i<j}^{N} f(r_{ij})\right) \sum_{j\neq k} \nabla_k f(r_{kj}) \\
&= \psi_{\mathcal{J}} \sum_{j\neq k} \frac{\mathbf{r}_{kj}}{r_{kj}} \frac{\partial}{\partial r_{kj}} f(r_{kj}) \\
&= \psi_{\mathcal{J}} \sum_{j\neq k} \frac{\mathbf{r}_{kj}}{r_{kj}} f'(r_{kj})
\end{aligned}$$

where

$$f'(r_{kj}) = \frac{\partial}{\partial r_{kj}} f(r_{kj}) = \frac{\partial}{\partial r_{kj}} \frac{a_{kj} r_{kj}}{(1+\beta r_{kj})} = \frac{a_{kj}(1+\beta r_{kj}) - a_{kj} r_{kj}(0+\beta)}{(1+\beta r_{kj})^2} = \frac{a_{kj} + \beta a_{kj} r_{kj} - \beta a_{kj} r_{kj}}{(1+\beta r_{kj})^2} = \frac{a_{kj}}{(1+\beta r_{kj})^2}$$

9.2.4 Laplacian of the Jastrow factor

The Laplacian of the Jastrow factor can be calculated by

$$\begin{aligned}
\nabla_k^2 \psi_{\mathcal{J}} &= \nabla_k \cdot (\nabla_k \psi_{\mathcal{J}}) \\
&= \nabla_k \cdot \left(\psi_{\mathcal{J}} \sum_{j\neq k} \frac{\mathbf{r}_{kj}}{r_{kj}} f'(r_{kj})\right) \\
&= (\nabla_k \psi_{\mathcal{J}}) \left(\sum_{j\neq k} \frac{\mathbf{r}_{kj}}{r_{kj}} f'(r_{kj})\right) + \psi_{\mathcal{J}} \left[\nabla_k \left(\sum_{j\neq k} \nabla_k f(r_{kj})\right)\right] \\
&= \psi_{\mathcal{J}} \sum_{i\neq k} \frac{\mathbf{r}_{ki}}{r_{ki}} f'(r_{ki}) \sum_{j\neq k} \frac{\mathbf{r}_{kj}}{r_{kj}} f'(r_{kj}) + \psi_{\mathcal{J}} \left(\sum_{j\neq k} \nabla_k^2 f(r_{kj})\right) \\
&= \psi_{\mathcal{J}} \left(\sum_{ij\neq k} \frac{\mathbf{r}_{ki} \cdot \mathbf{r}_{kj}}{r_{ki}} f'(r_{ki}) f'(r_{kj}) + \sum_{j\neq k} \nabla_k^2 f(r_{kj})\right)
\end{aligned}$$

where

$$\begin{aligned}
\nabla_k^2 f &= \nabla_k \cdot \nabla_k f & f &= f(r_{kj}) \\
&= \nabla_k \cdot \frac{\mathbf{r}_{kj}}{r_{kj}} \frac{\partial f}{\partial r_{kj}} & \nabla_k f &= \frac{\mathbf{r}_{kj}}{r_{kj}} \frac{\partial f}{\partial r_{kj}} \\
&= \sum_d \frac{\partial}{\partial x_k^{(d)}} \left(\frac{x_{kj}^{(d)}}{r_{kj}} \frac{\partial f}{\partial r_{kj}} \right) & x_{kj} &= x_k - x_j \\
&= \sum_d \left[\left(\frac{\partial}{\partial x_k^{(d)}} \frac{x_{kj}^{(d)}}{r_{kj}} \right) \frac{\partial f}{\partial r_{kj}} + \frac{x_{kj}^{(d)}}{r_{kj}} \frac{\partial}{\partial x_k^{(d)}} \frac{\partial f(r_{kj})}{\partial r_{kj}} \right] \\
&= \sum_d \left[\left(\frac{r_{kj} - x_{kj}^{(d)2} r_{kj}^{-1}}{r_{kj^2}} \right) \frac{\partial f}{\partial r_{kj}} + \frac{x_{kj}^{(d)}}{r_{kj}} \frac{\partial r_{kj}}{\partial x_k^{(d)}} \frac{\partial^2 f}{\partial r_{kj}^2} \right] & \frac{\partial r_{kj}}{\partial x_k^{(d)}} &= \frac{x_{kj}^{(d)}}{r_{kj}} \\
&= \sum_d \left[\left(\frac{1}{r_{kj}} - \frac{x_{kj}^{(d)2}}{r_{kj^3}} \right) \frac{\partial f}{\partial r_{kj}} + \frac{x_{kj}^{(d)2}}{r_{kj}^2} \frac{\partial^2 f}{\partial r_{kj}^2} \right] \\
&= \left(\frac{\text{dim}}{r_{kj}} - \frac{1}{r_{kj}} \right) \frac{\partial f}{\partial r_{kj}} + \frac{\partial^2 f}{\partial r_{kj}^2} \\
&= \frac{\text{dim} - 1}{r_{kj}} \frac{\partial f}{\partial r_{kj}} + \frac{\partial^2 f}{\partial r_{kj}^2}
\end{aligned}$$

Since we operate in two dimensions (dim = 2), we get

$$\nabla_k^2 f = \frac{2-1}{r_{kj}} \frac{\partial f}{\partial r_{kj}} + \frac{\partial^2 f}{\partial r_{kj}^2} = \frac{1}{r_{kj}} \frac{\partial f}{\partial r_{kj}} + \frac{\partial^2 f}{\partial r_{kj}^2} = \frac{1}{r_{kj}} f'(r_{kj}) + f''(r_{kj})$$

where

$$\frac{1}{r_{kj}} f'(r_{kj}) = \frac{1}{r_{kj}} \frac{a_{kj}}{(1+\beta r_{kj})^2} = \frac{a_{kj}}{r_{kj}(1+\beta r_{kj})^2}$$

and

$$f''(r_{kj}) = \frac{\partial}{\partial r_{kj}} f'(r_{kj}) = \frac{\partial}{\partial r_{kj}} \frac{a_{kj}}{(1+\beta r_{kj})^2} = \frac{0 - a_{kj} \cdot 2(1+\beta r_{kj})\beta}{(1+\beta r_{kj})^4} = -\frac{2\beta a_{kj}}{(1+\beta r_{kj})^3}$$

The Laplacian of the Jastrow factor is thus

$$\begin{aligned}\nabla_k^2 \psi_{\mathcal{J}} &= \psi_{\mathcal{J}} \left(\sum_{ij\neq k} \frac{\mathbf{r}_{ki}\cdot\mathbf{r}_{kj}}{r_{ki}} f'(r_{ki}) f'(r_{kj}) + \sum_{j\neq k} \nabla_k^2 f(r_{kj}) \right) \\ &= \psi_{\mathcal{J}} \left[\sum_{ij\neq k} \frac{\mathbf{r}_{ki}\cdot\mathbf{r}_{kj}}{r_{ki}} f'(r_{ki}) f'(r_{kj}) + \sum_{j\neq k} \left(\frac{1}{r_{kj}} f'(r_{kj}) + f''(r_{kj}) \right) \right] \\ &= \psi_{\mathcal{J}} \left[\sum_{ij\neq k} \frac{\mathbf{r}_{ki}\cdot\mathbf{r}_{kj}}{r_{ki}} \frac{a_{ki}}{(1+\beta r_{ki})^2} \frac{a_{kj}}{(1+\beta r_{kj})^2} + \sum_{j\neq k} \left(\frac{a_{kj}}{r_{kj}(1+\beta r_{kj})^2} - \frac{2\beta a_{kj}}{(1+\beta r_{kj})^3} \right) \right]\end{aligned}$$

where $\mathbf{r}_{ki} = \mathbf{r}_k - \mathbf{r}_i$ and $\mathbf{r}_{kj} = \mathbf{r}_k - \mathbf{r}_j$.

9.2.5 Quantum force without the Jastrow factor

The quantum force without the Jastrow factor is given by

$$F = 2\frac{\nabla_k \phi_{n_x,n_y}}{\phi_{n_x,n_y}}$$

where

$$\begin{aligned}\frac{\nabla_k \phi_{n_x,n_y}}{\phi_{n_x,n_y}} &= \sum_k^N \frac{\nabla_k \phi_{n_x,n_y}(x_i,y_i)}{\phi_{n_x,n_y}(x_i,y_i)} \\ &= \sum_k^N \left[\left(\frac{1}{H_{n_x}(\sqrt{\alpha\omega}x_k)} \left[\frac{\partial}{\partial x_k} H_{n_x}(\sqrt{\alpha\omega}x_k) \right] - \alpha\omega x_k \right) \hat{e}_x \right. \\ &\quad \left. + \left(\frac{1}{H_{n_y}(\sqrt{\alpha\omega}y_k)} \left[\frac{\partial}{\partial y_k} H_{n_y}(\sqrt{\alpha\omega}y_k) \right] - \alpha\omega y_k \right) \hat{e}_y \right]\end{aligned}$$

9.2.6 Quantum force with the Jastrow factor

The quantum force with the Jastrow factor is given by

$$F = 2\frac{\nabla\psi_T}{\psi_T} = 2\frac{\nabla(\phi\psi_J)}{\phi\psi_J} = 2\frac{\nabla(\phi\psi_J)}{\phi\psi_J} = 2\left(\frac{(\nabla\phi)\psi_J}{\phi\psi_J} + \frac{\phi(\nabla\psi_J)}{\phi\psi_J} \right) = 2\left(\frac{\nabla\phi}{\phi} + \frac{\nabla\psi_J}{\psi_J} \right)$$

where $\phi = \phi_{n_x,n_y}$,

$$
\begin{aligned}
\frac{\nabla_k \phi_{n_x,n_y}}{\phi_{n_x,n_y}} &= \sum_k^N \frac{\nabla_k \phi_{n_x,n_y}(x_i, y_i)}{\phi_{n_x,n_y}(x_i, y_i)} \\
&= \sum_k^N \left[\left(\frac{1}{H_{n_x}(\sqrt{\alpha\omega} x_k)} \left[\frac{\partial}{\partial x_k} H_{n_x}(\sqrt{\alpha\omega} x_k) \right] - \alpha\omega x_k \right) \hat{e}_x \right. \\
&\quad \left. + \left(\frac{1}{H_{n_y}(\sqrt{\alpha\omega} y_k)} \left[\frac{\partial}{\partial y_k} H_{n_y}(\sqrt{\alpha\omega} y_k) \right] - \alpha\omega y_k \right) \hat{e}_y \right]
\end{aligned}
$$

and

$$
\frac{\nabla_k \psi_{\mathcal{J}}}{\psi_{\mathcal{J}}} = \sum_{j \neq k} \frac{\mathbf{r}_{kj}}{r_{kj}} \frac{a_{kj}}{(1 + \beta r_{kj})^2}
$$

9.2.7 Steepest descent

The wave fuction for one particle in the determinant can be written as

$$
\phi_j(\mathbf{r}_i) = A H_{jx}(\sqrt{\alpha\omega} x_i) H_{jy}(\sqrt{\alpha\omega} y_i) \exp\left(-\frac{\alpha\omega}{2}(x_i^2 + y_i^2) \right)
$$

The derivative of the wave function with respect to α is then

$$
\begin{aligned}
\overline{\psi}_\alpha &= \frac{\partial}{\partial\alpha}\phi_j \\
&= A\left[\frac{\partial}{\partial\alpha}H_{jx}(\sqrt{\alpha\omega}x_i)\right]H_{jy}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right) \\
&\quad + AH_{jx}(\sqrt{\alpha\omega}x_i)\left[\frac{\partial}{\partial\alpha}H_{jy}(\sqrt{\alpha\omega}y_i)\right]\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right) \\
&\quad + AH_{jx}(\sqrt{\alpha\omega}x_i)H_{jy}(\sqrt{\alpha\omega}y_i)\left[\frac{\partial}{\partial\alpha}\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\right] \\
&= A\left[\frac{\omega x_i}{2\sqrt{\alpha\omega}}\frac{\partial}{\partial\alpha}H_{jx}(\sqrt{\alpha\omega}x_i)\right]H_{jy}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right) \\
&\quad + AH_{jx}(\sqrt{\alpha\omega}x_i)\left[\frac{\omega y_i}{2\sqrt{\alpha\omega}}\frac{\partial}{\partial\alpha}H_{jy}(\sqrt{\alpha\omega}y_i)\right]\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right) \\
&\quad + AH_{jx}(\sqrt{\alpha\omega}x_i)H_{jy}(\sqrt{\alpha\omega}y_i)\left[\left(-\frac{\omega}{2}(x_i^2+y_i^2)\right)\frac{\partial}{\partial\alpha}\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\right] \\
&= A\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)\left[\frac{1}{2}\sqrt{\frac{\omega}{\alpha}}\left(\left[x_i\frac{\partial}{\partial\alpha}H_{jx}(\sqrt{\alpha\omega}x_i)\right]H_{jy}(\sqrt{\alpha\omega}y_i)\right.\right. \\
&\quad \left.\left. + H_{jx}(\sqrt{\alpha\omega}x_i)\left[y_i\frac{\partial}{\partial\alpha}H_{jy}(\sqrt{\alpha\omega}y_i)\right]\right) - H_{jx}(\sqrt{\alpha\omega}x_i)H_{jy}(\sqrt{\alpha\omega}y_i)\right]
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\overline{\psi}_\alpha}{\psi_\alpha} &= \frac{\frac{\partial}{\partial\alpha}\phi_j}{\phi_j} \\
&= \frac{1}{2}\sqrt{\frac{\omega}{\alpha}}\frac{A\left[x_i\frac{\partial}{\partial\alpha}H_{jx}(\sqrt{\alpha\omega}x_i)\right]H_{jy}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)}{AH_{jx}(\sqrt{\alpha\omega}x_i)H_{jy}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)} \\
&\quad + \frac{1}{2}\sqrt{\frac{\omega}{\alpha}}\frac{AH_{jx}(\sqrt{\alpha\omega}x_i)\left[y_i\frac{\partial}{\partial\alpha}H_{jy}(\sqrt{\alpha\omega}y_i)\right]\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)}{AH_{jx}(\sqrt{\alpha\omega}x_i)H_{jy}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)} \\
&\quad - \frac{AH_{jx}(\sqrt{\alpha\omega}x_i)H_{jy}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)}{AH_{jx}(\sqrt{\alpha\omega}x_i)H_{jy}(\sqrt{\alpha\omega}y_i)\exp\left(-\frac{\alpha\omega}{2}(x_i^2+y_i^2)\right)} \\
&= \frac{1}{2}\sqrt{\frac{\omega}{\alpha}}\frac{x_i}{H_{jx}(\sqrt{\alpha\omega}x_i)}\left[\frac{\partial}{\partial\alpha}H_{jx}(\sqrt{\alpha\omega}x_i)\right] + \frac{1}{2}\sqrt{\frac{\omega}{\alpha}}\frac{y_i}{H_{jy}(\sqrt{\alpha\omega}y_i)}\left[\frac{\partial}{\partial\alpha}H_{jy}(\sqrt{\alpha\omega}y_i)\right] - 1
\end{aligned}
$$

The wave function with respect to β is

$$\begin{aligned}\overline{\psi}_\beta &= \frac{\partial}{\partial\beta}\psi_J \\ &= \frac{\partial}{\partial\beta}\exp\left(\sum_{i<j}\frac{a_{ij}r_{ij}}{1+\beta r_{ij}}\right) \\ &= \psi_J\sum_{j\neq k}\frac{\partial}{\partial\beta}\left(\frac{a_{kj}r_{kj}}{1+\beta r_{kj}}\right) \\ &= \psi_J\sum_{j\neq k}\left(-\frac{a_{kj}r_{kj}^2}{(1+\beta r_{kj})^2}\right)\end{aligned}$$

and

$$\frac{\overline{\psi}_\beta}{\psi_\beta} = \frac{\frac{\partial}{\partial\beta}\psi_J}{\psi_J} = \sum_{j\neq k}\left(-\frac{a_{kj}r_{kj}^2}{(1+\beta r_{kj})^2}\right)$$

9.3 Derivatives of the Hermite polynomials with respect to alpha

The first five Hermite polynomials is

$$\begin{aligned}H_0 &= 1 \\ H_1 &= 2x \\ H_2 &= 4x^2-2 \\ H_3 &= 8x^3-12x \\ H_4 &= 16x^4-48x^2+12\end{aligned}$$

Sending in $\sqrt{\alpha\omega}x$ as the function variable in the Hermite polynomials, we find that they are

$$\begin{aligned}H_0 &= 1 \\ H_1 &= 2\sqrt{\alpha\omega}x \\ H_2 &= 4\alpha\omega x^2-2 \\ H_3 &= 8(\alpha\omega)^{3/2}x^3-12\sqrt{\alpha\omega}x \\ H_4 &= 16\alpha^2\omega^2x^4-48\alpha\omega x^2+12\end{aligned}$$

Taking the derivatives of these with respect to α we end up with

$$\begin{aligned}
\frac{\partial H_0}{\partial \alpha} &= 0 \\
\frac{\partial H_1}{\partial \alpha} &= \sqrt{\frac{\omega}{\alpha}}x \\
\frac{\partial H_2}{\partial \alpha} &= 4\omega x^2 \\
\frac{\partial H_3}{\partial \alpha} &= 12\sqrt{\alpha\omega}\omega x^3 - 6\sqrt{\frac{\omega}{\alpha}}x \\
\frac{\partial H_4}{\partial \alpha} &= 32\alpha\omega^2 x^4 - 48\omega x^2
\end{aligned}$$

These were implemented into the code in order to use it for the steepest descent for many particles.

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