Assignment 3: The Quantum Monte Carlo Method

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1 Introduction

In this report, we aim to apply the **Variational Monte Carlo (VMC)** method to compute approximations of the ground state energies for two quantum systems:

A one-dimensional harmonic oscillator and a two-electron system in a two-dimensional harmonic oscillator potential. Optimization of the trial wave function parameter α is performed using a *Golden Section Search* routine. The project focuses on checking the reliability of the VMC method.

2 Theory and Methods

2.1 Problem Description

The objective is to use the **Variational Monte Carlo (VMC)** method to approximate the ground state energies of quantum systems. In VMC the expectation value of the Hamiltonian is evaluated using a trial wave function that depends on variational parameters. The method relies on a stochastic integration via the Metropolis algorithm: we sample configurations according to the probability density given by the square of the trial wave function, compute the local energy at each configuration, and then we average over many samples. By varying the parameters in the trial wave function (in our case denoted by α, and also by λ in the two-electron case) we are able to minimize the energy and obtain an approximation f the ground state.

2.2 One Particle in a One-Dimensional Harmonic Oscillator

For a one-dimensional harmonic oscillator the Hamiltonian is given by:

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \tag{1}$$

As we have seen before, we introduce reduced units to simplify the problem. We define a dimensionless coordinate z ($z = x\sqrt{m\omega/\hbar}$), so that the energy is expressed in units of $\hbar\omega$.

2.2.1 Trial Wave Function and Local Energy

The trial wave function is chosen to be a Gaussian function with a variational parameter α:

$$\psi(z) = e^{-\alpha z^2} \tag{2}$$

The probability density is given by:

$$P(z) = \frac{|\psi(z)|^2}{\mathcal{N}} = \frac{e^{-2\alpha z^2}}{\sqrt{\pi/\alpha}}, \tag{3}$$

where the normalization constant $\sqrt{\pi/\alpha}$ ensures that $\int_{-\infty}^{\infty} P(z)\,dz = 1$. The local energy is computed as:

$$E_{\text{local}}(z) = \frac{H\psi(z)}{\psi(z)} \tag{4}$$

Hence, from equation 4 we obtain the following expression for the local energy:

$$E_{\text{local}}(z) = \alpha + z^2\left(\frac{1}{2} - 2\alpha^2\right) \tag{5}$$

which we use in the code to evaluate the energy at each configuration.

2.2.2 Implementation of the Metropolis Algorithm

We aim to sample the configuration space according to the probability density $P(z)$.

We implement the following Metropolis algorithm:

1. **Choice of Domain:** The trial wave function is a Gaussian. Therefore, the relevant values of z are within a few standard deviations from zero. We choose the range $[-L, L]$ with:

$$L = \frac{3}{\sqrt{2\alpha}} \tag{6}$$

corresponding approximately to three standard deviations.

2. **Markov Chain:** We randomly choose a z in $[-L, L]$ and generate a trial move:

$$z_{\text{trial}} = z + 0.9 * (\text{rand} * 2 * L - L), \tag{7}$$

where 0.9 is a small displacement that controls how much the particle's position changes and rand is a random number uniformly distributed between $[0, 1)$.

3. **Acceptance Criterion:** The new configuration is accepted with probability

$$p = \min\left[1, \frac{P(z_{\text{trial}})}{P(z)}\right]. \tag{8}$$

A uniform random number is used to decide if the move is accepted according to this probability.

At each configuration the local energy $E_{\text{local}}(z)$ is computed. After many iterations the statistical average of the local energy approximates the expectation value $\langle E \rangle$. Moreover, the variance

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \tag{9}$$

is calculated to check how good the approximation of the trial wave function is.

2.2.3 Analytical Energy and Variance for Comparison

For this system the analytical expectation value of the energy is known:

$$\langle E \rangle_{\text{analytical}} = \frac{1}{2}\alpha + \frac{1}{8\alpha}, \tag{10}$$

as well as the one for the variance:

$$\sigma^2_{E_{\text{analytical}}} = \frac{(1 - 4\alpha^2)^2}{32\alpha^2}. \tag{11}$$

These expressions can be compared with the numerical results obtained.

2.3 Golden Section Search for Energy Minimization

To find the optimal variational parameter α that minimizes the energy, we implement the *Golden Section Search* algorithm. The algorithm iteratively narrows the interval $[a, b]$ containing the minimum:

$$c = b - \frac{b-a}{\varphi}, \quad d = a + \frac{b-a}{\varphi}, \tag{12}$$

with the golden ratio $\varphi = \frac{\sqrt{5}+1}{2}$. The function (here the measured local energy) is compared at c and d to decide which part of the interval is discarded. This is repeated until the interval meets a predefined tolerance. The code uses this routine to optimize α by minimizing the average local energy.

2.4 Two Electrons in a Two-Dimensional Harmonic Oscillator

In the second model we consider two interacting electrons confined in a two-dimensional harmonic oscillator potential. The Hamiltonian in reduced units is written as:

$$H = \sum_{i=1}^{2} \left[-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\left(x_i^2 + y_i^2\right) \right] + \frac{\lambda}{r_{12}}, \tag{13}$$

where $r_{12} = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$ is the distance between the two electrons. The parameter λ where:

$$\lambda = \frac{me^2}{4\pi\varepsilon_0\varepsilon_r\hbar^2}\sqrt{\frac{\hbar}{m\omega}} \tag{14}$$

regulates the strength of the Coulomb repulsion. When $\lambda = 0$ the electrons do not interact. Increasing the value of λ, increases the importance of the electron–electron interaction.

2.4.1 Trial Wave Function

The trial wave function is chosen as follows:

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2; \alpha, \lambda) = \underbrace{\exp\left(-\frac{1}{2}\left(\boldsymbol{r}_1^2 + \boldsymbol{r}_2^2\right)\right)}_{\text{Gaussian part}} \times \underbrace{\exp\left(\frac{\lambda\, r_{12}}{1 + \alpha\, r_{12}}\right)}_{\text{Jastrow factor}}, \tag{15}$$

where $\boldsymbol{r}_i^2 = x_i^2 + y_i^2$ for $i = 1, 2$. The first factor is fixed and represents the non-interacting ground state of the harmonic oscillator, while the second

(Jastrow factor) introduces correlations between electrons. Its form has been chosen so that the wave function reproduces the cusp when the electrons coincide. Again, the variational parameter α is optimized via the *Golden Section Search* to minimize the total energy.

2.4.2 Computation of the Local Energy

To compute the local energy for the two-electron system, we need to evaluate the kinetic energy operator in the trial wave function. We need to calculate the second derivatives with respect to our coordinates. In our code, the kinetic energy contribution is computed by defining a derivative factor for each coordinate:

$$\partial_x^2 \equiv \frac{\partial^2 \Psi}{\partial x^2} \Big/ \Psi, \tag{16}$$

with similar definitions for the other derivatives. These derivative factors involve several terms due to the chain rule as the trial wave function contains both the Gaussian part and the Jastrow factor. Once the four second derivatives (two for each electron) are computed, the kinetic energy is obtained via:

$$\mathcal{K} = -\frac{1}{2}\left[\left(\frac{\partial^2 \Psi}{\partial x_1^2} + \frac{\partial^2 \Psi}{\partial y_1^2}\right) + \left(\frac{\partial^2 \Psi}{\partial x_2^2} + \frac{\partial^2 \Psi}{\partial y_2^2}\right)\right] \tag{17}$$

The potential energy includes both the harmonic oscillator potential:

$$\mathcal{V}_{\text{HO}} = \frac{1}{2}(x_1^2 + y_1^2 + x_2^2 + y_2^2) \tag{18}$$

and the Coulomb repulsion term:

$$\mathcal{V}_{\text{Coulomb}} = \frac{\lambda}{r_{12}}. \tag{19}$$

Thus, the local energy is given by

$$E_{\text{local}} = \mathcal{K} + \mathcal{V}_{\text{HO}} + \mathcal{V}_{\text{Coulomb}}. \tag{20}$$

2.4.3 Metropolis Algorithm for Two Electrons in 2D

We use the Metropolis algorithm for the one-dimensional case but now we extend it to a two-particle, two-dimensional problem:

1. **Configuration:** The system is represented in a 2×2 array:

$$\mathbf{r} = \begin{pmatrix} x_1 & y_1 \\ x_2 & y_2 \end{pmatrix}, \tag{21}$$

   where each row contains the coordinates of one electron.

2. **Trial Moves:** A new trial configuration is generated by displacing both electrons simultaneously by a random amount. The displacement is scaled by the parameter **step_size** to control the magnitude of the moves.

3. **Acceptance Criterion:** The trial configuration is accepted with probability:

$$p_{\text{accept}} = \min\left[1, \left(\frac{\Psi(\mathbf{r}_{\text{trial}})}{\Psi(\mathbf{r}_{\text{old}})}\right)^2\right]. \tag{22}$$

   As before, a uniform random number is used to decide if the move is accepted according to this probability.

Each visited configuration is used to calculate the local energy. After many iterations the mean energy and its variance help show how good the approximation of the trial wave function is.

3 Results and Discussions

3.1 One Particle in a One-Dimensional Harmonic Oscillator

Here we present and analyse the numerical results obtained for a single particle in a one-dimensional harmonic oscillator potential. Our goal was to validate the trial wave function, check quality of the sampling and compare the computed and analytical energies and variances.

3.1.1 Choice of Sampling Parameters

The number of computed Metropolis steps was of $N = 1 \times 10^6$ so our results converge to an accurate solution. The initial position z was sampled uniformly within the interval $[-L, L]$, where $L = \frac{3}{\sqrt{2\alpha}}$ as mentioned in the previous section. Sampling from this region ensures that the algorithm starts in a physically meaningful range. The choice of multiplying by a factor of 0.9 in our trial move was made to achieve an acceptance ratio close to 40% so the Markov chain samples the probability distribution efficiently.

3.1.2 Comparison of Numerical and Analytical Results

For each chosen α value, the mean energy and its variance were calculated and compared with their corresponding analytical expressions:

Table 1 presents the results for a set of α values.

Table 1: Comparison between numerical and analytical results for different values of α. The acceptance ratio was maintained close to 40%.

α	$\langle E \rangle_{\text{num}}$	$E_{\text{analytical}}$	$\text{Var}(E)_{\text{num}}$	$\text{Var}_{\text{analytical}}$	Acceptance Ratio
0.6348	0.5138	0.5143	0.0293	0.0290	0.4072
0.9652	0.6143	0.6121	0.2457	0.2494	0.4065
0.4787	0.5005	0.5005	0.0010	0.0009	0.4060
0.4971	**0.5000**	**0.5000**	**0.0000**	**0.0000**	**0.4072**
0.3043	0.5625	0.5630	0.1323	0.1339	0.4069

As shown in Table 1, the numerical estimates for both the mean energy and the variance align well with the analytical predictions.

The optimal variational parameter α was found to be:

$$\alpha_{\text{opt}} = 0.5007702765514341$$

using the golden section search algorithm. This result is consistent with theoretical expectations. Additionally, at this point, the variance of the local energy vanishes, confirming that the trial wave function exactly matches the true ground state.

3.1.3 Energy and Variance as a Function of α

Figure 1 illustrates the computed mean local energy as a function of α. The numerical results coincide perfectly with the analytical curve, validating the correctness of the algorithm and the accuracy of the implementation.

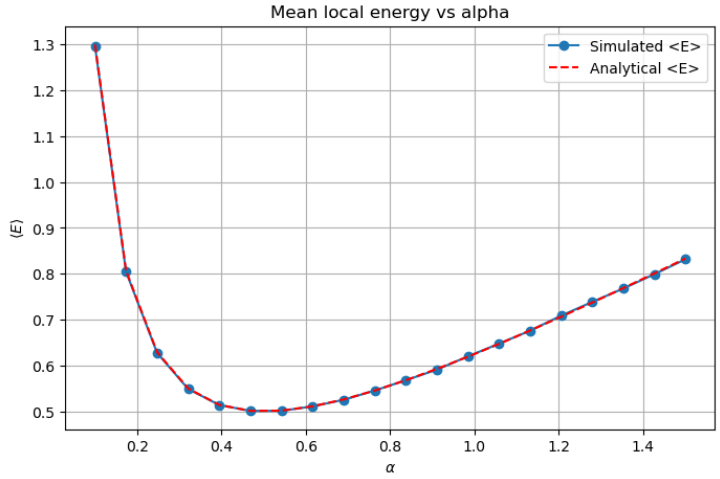


Figure 1: Mean local energy $\langle E \rangle$ as a function of the variational parameter α.

Similarly, the variance of the local energy, shown in Figure 2, illustrates that the variance drops to zero at $\alpha = 0.5$.

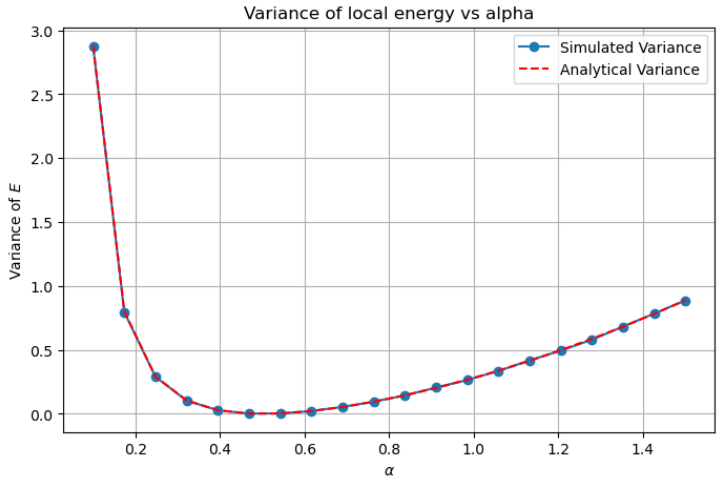


Figure 2: Variance of the local energy as a function of α. The minimum, corresponding to zero variance, is found at $\alpha = 0.5$.

3.1.4 Histogram Analysis

To validate the quality of the sampling, the visited positions z were recorded during the Monte Carlo run. The resulting histogram was compared against

the square of the trial wave function, which represents the theoretical probability density.

Figure 3 shows that the histogram of sampled positions follows the shape of the trial wave function. Although with some fluctuations, we achieve a probability density around $\alpha = 0.5$. This confirms a correct sample.

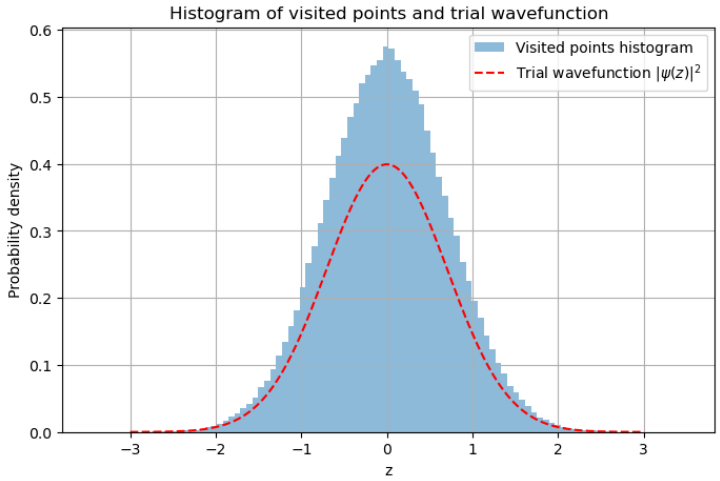


Figure 3: Histogram of visited positions during the Metropolis random walk, compared with the theoretical probability density $|\psi(z)|^2$ for $\alpha = 0.5$.

3.2 Two Electrons in a Two-Dimensional Harmonic Oscillator

Here we present and analyse the results of our Variational Monte Carlo (VMC) simulation for two electrons in a two-dimensional harmonic oscillator potential.

3.2.1 Simulation Details

The Monte Carlo sampling was performed using the Metropolis-Hastings algorithm. The random trial moves for the two electrons were proposed as follows:

$$r_{\text{trial}} = r + \texttt{step\_size} \cdot (\texttt{np.random.rand}(2, 2) - 0.5),$$

where r represents the current positions of the two electrons, and `step_size` controls the magnitude of the displacement. We chose `step_size` $= 2.2$ in order to obtain an acceptance ratio of approximately 40%. A lower `step_size`

would lead to very correlated samples, while a higher `step_size` would decrease the acceptance ratio and slow down the simulation. Each simulation was carried out for 2×10^6 Monte Carlo steps. After every accepted or rejected move, the local energy was computed and stored to evaluate the mean energy and its variance.

3.2.2 Optimization of the Variational Parameter

For each value of λ, the variational parameter α was optimized using the Golden Section Search algorithm. This optimization aimed to minimize the expectation value of the total energy:

$$\langle E \rangle = \frac{1}{N} \sum_{i=1}^{N} E_{\text{local}}(r_i), \tag{23}$$

where $E_{\text{local}}(r)$ is the local energy for a given electron configuration and N is the total number of samples.

The system was investigated for four values of λ:

$$\lambda = 0, 1, 2, 8$$

For each λ, the optimal α was determined and both the energy and the variance were evaluated over a range of α values. The results were visualized in Figure 4, Figure 5, Figure 6 and Figure 7 where the behaviour of the energy and its variance as a function of α are compared.

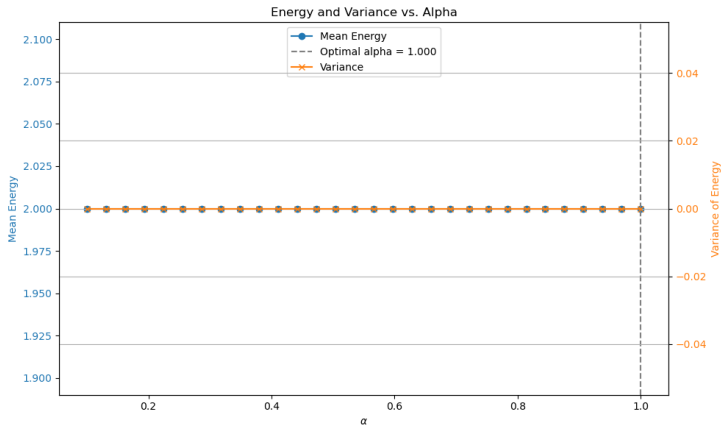


Figure 4: Mean local energy and variance as a function of α for $\lambda = 0$. Optimal α given at $\alpha = 1$. The literature result is $E = 2\hbar\omega$.

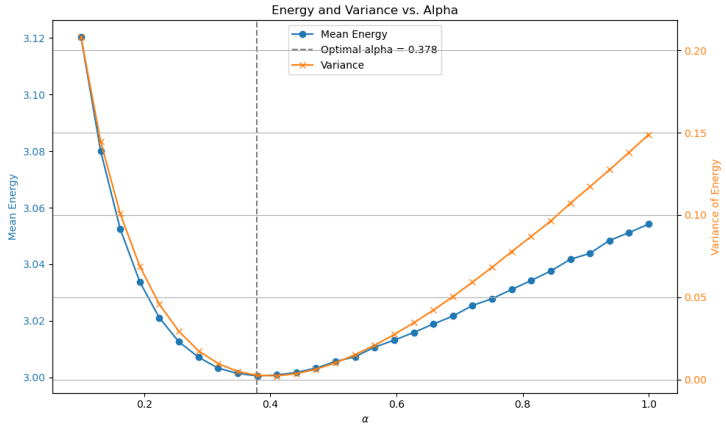


Figure 5: Mean local energy and variance as a function of α for $\lambda = 1$. Optimal α given at $\alpha = 0.378$. The literature result is $E = 3\hbar\omega$.

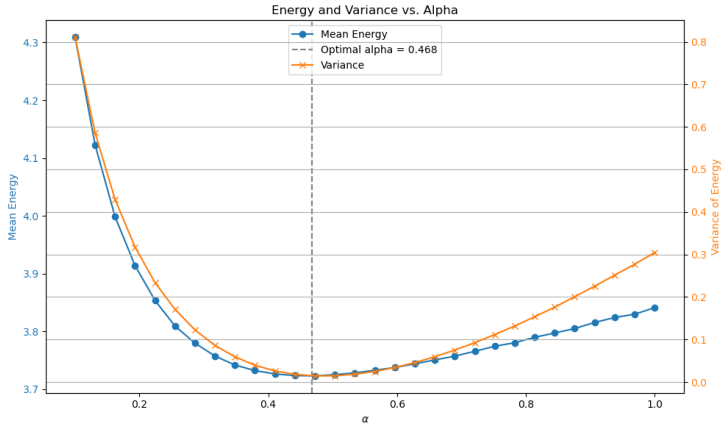


Figure 6: Mean local energy and variance as a function of α for $\lambda = 2$. Optimal α given at $\alpha = 0.4675$. The literature result is $E = 3.729...\hbar\omega$.

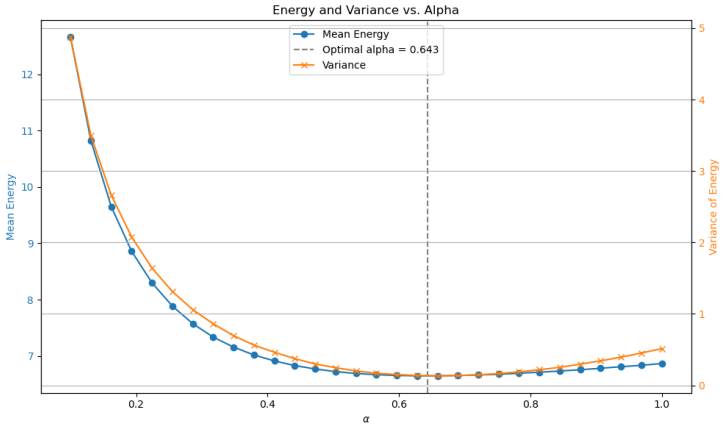


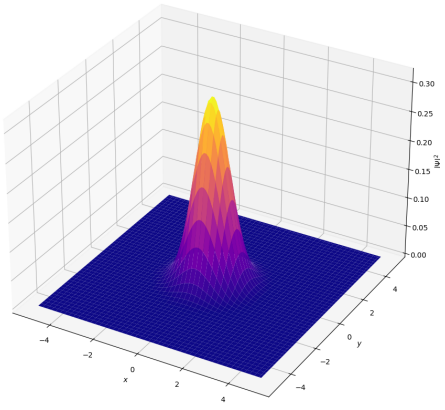
Figure 7: Mean local energy and variance as a function of α for $\lambda = 8$. Optimal α given at $\alpha = 0.6434$. The literature result is $E = 6.618...\hbar\omega$.

In all four plots, the mean energy reached a minimum at an optimal α value while the variance showed a corresponding minimum as well. The results obtained align well with the literature values. Varying λ allowed us to explore how the strength of the electron-electron interaction influences the energy landscape, ranging from the non-interacting case at $\lambda = 0$ to increasingly stronger repulsive interactions as λ is increased.

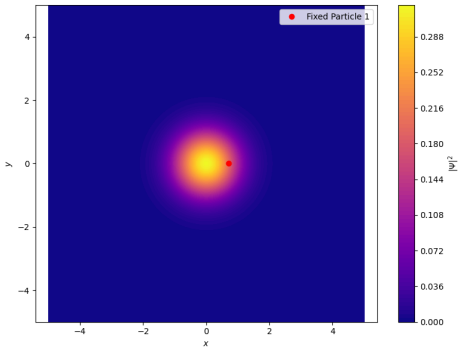
We note that as λ increases, the electron-electron repulsion grows stronger and the system is less dominated by the external harmonic potential. This reduces the dependence of the total energy on α, leading to a flattening of the energy curve around its minimum. When the interaction is strong ($\lambda = 8$), the repulsion between electrons is the most responsible for obtaining the optimal wave function, making the energy less sensitive to α and resulting in a less pronounced U-shaped plot.

3.2.3 Probability Distribution of Particle 2

To better see how the system is arranged in space, we fixed the position of particle 1 at $r_1 = (0.7, 0.0)$ and computed the probability density $|\Psi(r_1, r_2)|^2$ for particle 2 on a two-dimensional grid. The results are presented in Figure 8, Figure 9, Figure 10 and Figure 11:

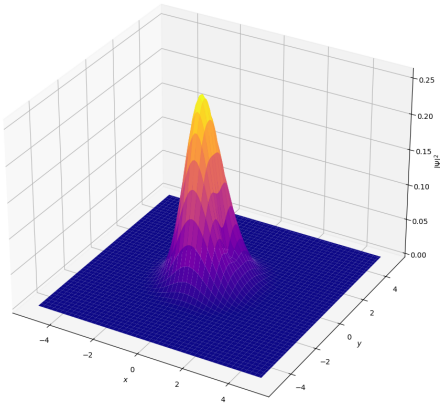


(a) Probability Distribution of Particle 2 (Particle 1 fixed)

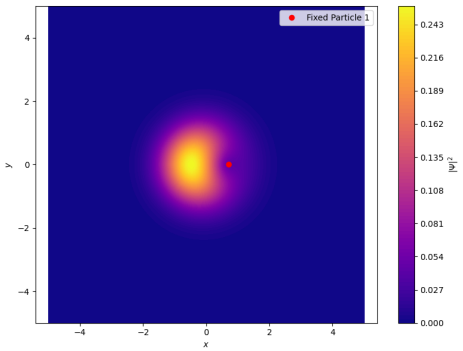


(b) Heat map of $|\Psi|^2$ for Particle 2 (Particle 1 fixed)

Figure 8: Probability Distribution of Particle 2 with fixed Particle 1 for $\lambda = 0$ and optimal α.

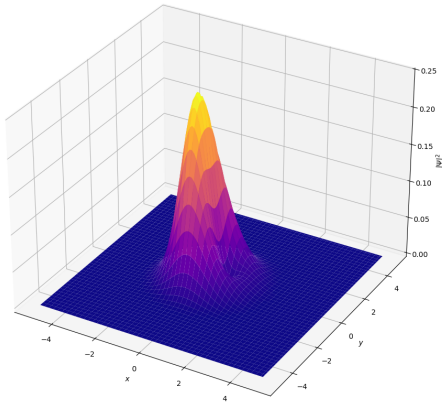


(a) Probability Distribution of Particle 2 (Particle 1 fixed)

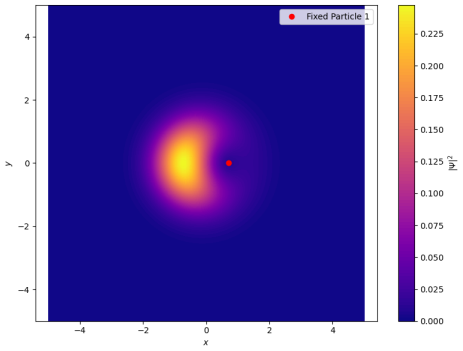


(b) Heat map of $|\Psi|^2$ for Particle 2 (Particle 1 fixed)

Figure 9: Probability Distribution of Particle 2 with fixed Particle 1 for $\lambda = 1$ and optimal α.

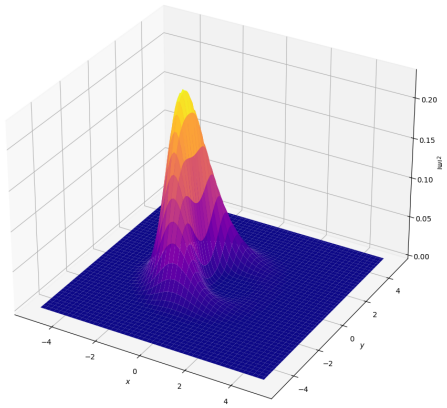


(a) Probability Distribution of Particle 2 (Particle 1 fixed)

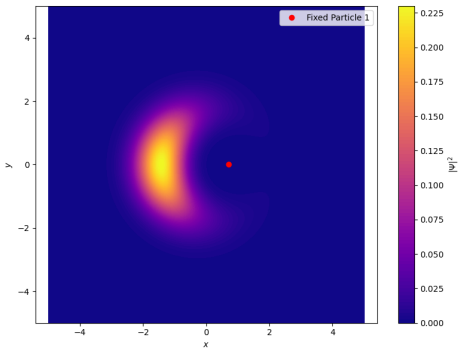


(b) Heat map of $|\Psi|^2$ for Particle 2 (Particle 1 fixed)

Figure 10: Probability Distribution of Particle 2 with fixed Particle 1 for $\lambda = 2$ and optimal α.



(a) Probability Distribution of Particle 2 (Particle 1 fixed)



(b) Heat map of $|\Psi|^2$ for Particle 2 (Particle 1 fixed)

Figure 11: Probability Distribution of Particle 2 with fixed Particle 1 for $\lambda = 8$ and optimal α.

As we can observe, the probability distribution of particle 2 is very much affected by λ.

For the non-interacting case ($\lambda = 0$), the distribution is located around the origin, as expected. Fixing the position of particle 1 does not affect the probability distribution of particle 2, which is centered at the minimum.

When the electron-electron interaction is introduced ($\lambda > 0$), the probability density of particle 2 starts to deform. The most noticeable effect is the development of a well at the position of particle 1 and how a ring-like structure is formed at its surroundings. This reflects the repulsive nature of the Coulomb interaction: particle 2 is less likely to be found near particle 1 and instead prefers positions at a finite distance.

As λ is increased, the peak of the distribution moves farther out and the empty area around particle 1 becomes more pronounced. The interaction makes it very unlikely for the two particles to be close to each other.