# Gross Pitaevskii Equation-Simulations

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Under the supervision of
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## 1 Introduction

From the description provided by thermodynamics, all the particles behave in the same manner within a gas. In particular, they occupy certain quantum states, that is, certain eigenstates. If the particles are half spin(fermions), two or more cannot occupy the same energy state without violating the Pauli exclusion principle.

However, if they are integer spin (bosons), any number can occupy the same quantum state. When we put these particles in a given configuration, they will get distributed in the energy levels of such a configuration, with an increasing occupation of the states of minimum energy as we lower the temperature.

For a collection of bosons, and in the limit where the temperature goes to zero, all the particles will occupy the system's ground state. Before achieving this limit, a spectacular accumulation of particles in the ground state can be observed. Therefore, most particles are in the same quantum state for a sufficiently low temperature. Physically for a system, the Bose-Einstein condensation occurs when a gas of bosonic atoms cools to the point at which the de Broglie wavelength $l_B = \frac{\hbar}{mv_T}$ is comparable to the mean interparticle separation $d = n^{-1/3}$.

Here, $v_T$ is the atomic thermal speed, $m$ is the atomic mass, and $n$ is the atomic number density. Under these conditions, the atomic wave packets overlap, and quantum interference between identical particles becomes crucial in determining the statistical behavior.

A diluted gas of bosons in a matter state of Bose-Einstein condensate (BEC) has a significant portion of bosons occupying the lowest quantum state; hence tiny quantum phenomena, in particular wavefunction interference, become apparent. A BEC is created by cooling a gas with an exceedingly low density—about 100,000 times that of ordinary air—to shallow temperatures. The ground state of a quantum system of identical bosons is described by the Gross-Pitaevskii equation (GPE), which incorporates employing the pseudopotential interaction model.

The equation determines the quantum wave function $\psi$(x, t) of gas of bosons in the limit where thermal and quantum fluctuations are negligibly small. Solving the GPE helps us describe a BEC's ground state and its linear and nonlinear excitations and transport properties at ultralow temperatures. Mathematically, the GPE takes the form of a Non-linear Schrödinger equation.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta_{\mathrm{r}}^2\Psi + \frac{\hbar^2\tilde{g}N}{m}|\Psi|^2\Psi + V(\vec{\mathrm{r}})\cdot\Psi \tag{1}$$

where :

- $\Psi = \Psi(\vec{r},t)$ is the single particle wavefunction such that $\int|\Psi|^2 d^2\vec{r} = 1$,
- $m$ is the mass of the particle; for our case, it will be Rubidium 87: $m = 1.44 \times 10^{-25}$kg,
- N is the number of particles in the trap,
- $\tilde{g} = \frac{\sqrt{8\pi}a_s}{l_z}$ quantifies as the inter-atomic interactions,
- $a_s = 5 \times 10^{-9}$ is the scattering length for $^{87}$Rb,
- $l_z = \sqrt{\frac{\hbar}{m\omega_z}}$ is the $|0\rangle$ (**G.S**) width for an harmonic trap with angular trapping frequency $\omega_z$,
- $V(\vec{r})$ is the trapping potential(the external potential).

As pointed out, a Bose-Einstein condensate is obtained from a collection of bosons in the ground at nano-Kelvin temperatures. Therefore, we will look to find the energy of the ground state and use this to provide information about the system, as we can for any other gas. The general Hamiltonian that describes the system is given by:

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta_{\mathrm{r}}^2 + \frac{\hbar^2\tilde{g}N}{m}|\Psi|^2 + V(\vec{\mathrm{r}}) \tag{2}$$

Given a Hamiltonian $\hat{H}$ and a wavefunction $\Psi$, we can obtain the expectation value for Energy by the following relation:

$$E(\Psi) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

The three terms on the right side of the Eq.2 derive the condensate's kinetic energy $E_{\mathrm{k}}$, the energy $E_{\mathrm{int}}$ of atom-atom interactions, and the potential energy $E_{\mathrm{ext}}$ of interaction with the confining potential $V_{\mathrm{ext}}(x)$. The characteristic expression for the energies are as follows:

$$E_{\mathrm{k}} = \frac{N\hbar^2}{2m} \int |\vec{\nabla}\Psi(\vec{\mathrm{r}})|^2 d^2\vec{\mathrm{r}} \qquad\qquad E_{\mathrm{int}} = \frac{N^2\hbar^2}{2m} \int |\vec{\nabla}\Psi(\vec{\mathrm{r}})|^4 d^2\vec{\mathrm{r}}$$

For a Harmonic trap, the Harmonic trapping potential energy is:

$$E_{\mathrm{p}} = \frac{N}{2} m\omega^2 \int |\Psi(\vec{\mathrm{r}})|^2 d^2\vec{\mathrm{r}}$$

The report is organized as follows in Sec.2; we will introduce imaginary time to show how the wavefunction is forced to tend towards the ground state once contributions from higher energy eigenfunctions have contributed for a long enough transitory time. Further, in Sec.3, the solutions for the GPE will be found using the Box and Harmonic potential. However, the interactions among the particles will be considered to be minimum. After that, we will introduce the Interactions among the particles and solve the equation under those interactions for Harmonic potential and then Box potential Sec.4 and Sec.5.

## 2 The imaginary time propagation method

Using the substitution $t \to it$, the imaginary time approach for calculating the ground state switches between real and imaginary time. This transforms the GPE into a form similar to a diffusion equation. As a result, a local equilibrium can be found by propagating in time. This can be understood by considering a solution of the form $\Psi(\vec{\mathrm{r}},t) = \sum_n \Psi_n(\vec{\mathrm{r}}) \exp(-iE_n t/\hbar)$, where $\Psi(\vec{\mathrm{r}},t)$ is a superposition of eigenfunctions $\Psi_n(\vec{\mathrm{r}})$ with eigenvalues $E_n$.

Under this substitution of the GPE in imaginary time, the wavefunction exponentially decays;

$$\Psi(\vec{\mathrm{r}}, \quad t) \qquad = \qquad \sum_n \qquad \Psi_n(\vec{\mathrm{r}}) \exp(-E_n t/\hbar) \quad (3)$$

The contributions we get from higher energy eigenfunctions decay the fastest since the wavefunction in Eq.3 decays proportionally to eigenvalues $E_n$. The next step is to renormalize the wavefunction during propagation to prevent the wavefunction's overall decay. The wavefunction is forced to tend towards the ground state once contributions from higher energy eigenfunctions have contributed for a long enough transitory time.

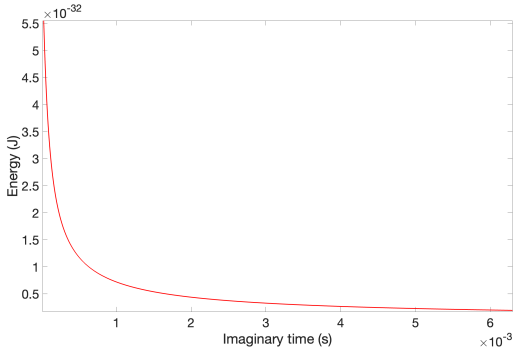



Figure 1: An example of using the imaginary time propagation method converges on the ground state solution.

## 3 Simulations of GPE without interactions

We will be studying the evolution of the eigenstates and eigenfunction for a Bose gas under the condition of zero interaction; in that case, Eq.1 and the Hamiltonian equation, Eq.2 will lose the interaction part. We will have;

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta_{\mathrm{r}}^2 \Psi + V(\vec{\mathrm{r}}) \cdot \Psi \qquad\qquad \hat{H} = -\frac{\hbar^2}{2m} \Delta_{\mathrm{r}}^2 + V(\vec{\mathrm{r}})$$

### 3.1 Particle in a Box potential

The Schrödinger equation for a particle in 1D in a Box potential is given by,

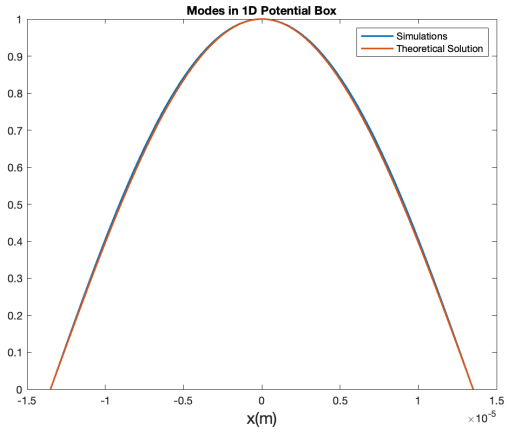



Figure 2: The fundamental mode for the wave function for a Box potential with results from simuluations and theoritical behaviour.

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\Phi(\mathrm{x})}{\mathrm{dx}^2}+V(\mathrm{x})\Phi(\mathrm{x})=E\Phi(\mathrm{x}) \tag{4}$$

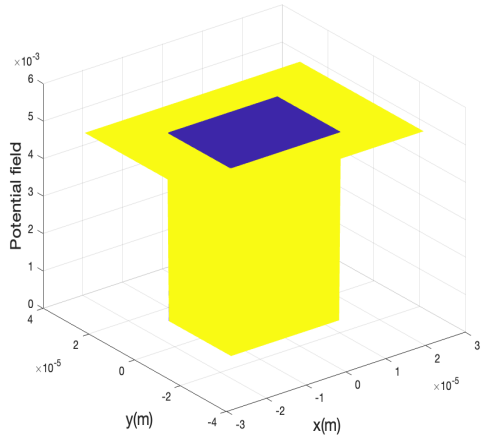
The simplest form of the potential is given by $V(\mathrm{x})=0$ for 0<x<L and $V(\mathrm{x})=\infty$ otherwise. In it's simplest forms the solution to the particle in Box is given by a sinusoidal wavefunction of the form $\Phi(\mathrm{x})=\mathrm{A}\sin(\mathrm{kx})$, where k is calculated from the Boundary conditions and is found to be $\mathrm{k}=\frac{\mathrm{n}\pi}{\mathrm{L}}$ with n=1,2,3.. Our simulations for the case of the 1D box are given and are in excellent agreement with the theoritical behaviuour, as seen from the Fig.2

Further the Eq.4 can be constructed in two dimensions (x , y);

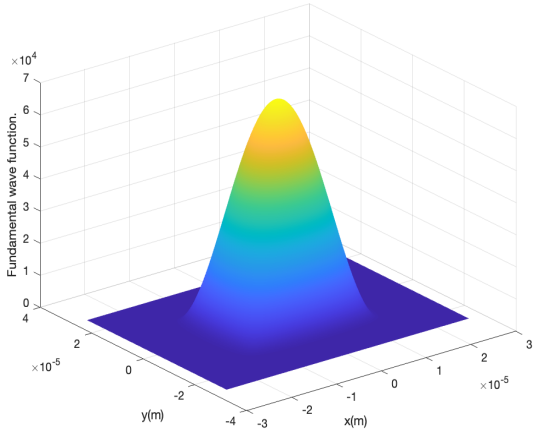
$$\frac{-\hbar^2}{2m}\left[\frac{\mathrm{d}^2\Phi(\mathrm{x,y})}{\mathrm{dx}^2}+\frac{\mathrm{d}^2\Phi(\mathrm{x,y})}{\mathrm{dy}^2}\right]+V(\mathrm{x,y})\Phi(\mathrm{x,y})=E\Phi(\mathrm{x,y}) \tag{5}$$

where, the solution in the normalized form is given by;

$$\Phi_{\mathrm{n_x,n_y}}(\mathrm{x,y})=\frac{2}{\mathrm{L}}\sin\left(\frac{\mathrm{n_x}\pi\mathrm{x}}{\mathrm{L}}\right)\cdot\sin\left(\frac{\mathrm{n_y}\pi\mathrm{x}}{\mathrm{L}}\right)$$




(a) Box potential for a Bose gas without interactions




(b) Evolution of the wavefunction of the BEC in the presence of a Box potential

Figure 3: The cases of the condensate in presence of an external Box potential

### 3.2 Harmonic Potential

We are interested in studying the evolution of the ground state of a Bose gas by implementing an external potential of the form of: $V_{\mathrm{ext}}=\frac{1}{2}m\omega_x x^2$ and $V_{\mathrm{ext}}=\frac{1}{2}m[\omega_x x^2+\omega_y y^2]$ for 1D and 2D cases respectively. To start with the simulations for the Harmonic without interaction, we take a constant wave function at $t$ of the Bose gas; this wavefunction is set to evolve in time$t+dt$, and the evolution is found by:

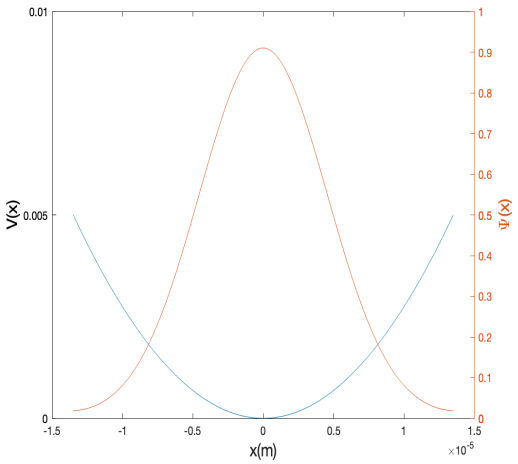
**1D Case**

$$\Psi(x,t+dt)=\Psi(x,t)+dt\left[\frac{\hbar}{2m}\frac{\Psi(x+dx)+\Psi(x-dx)-2\Psi(x,t)}{dx^2}+\ldots-\frac{V(x)}{h}\Psi(x,t)\right] \tag{6}$$

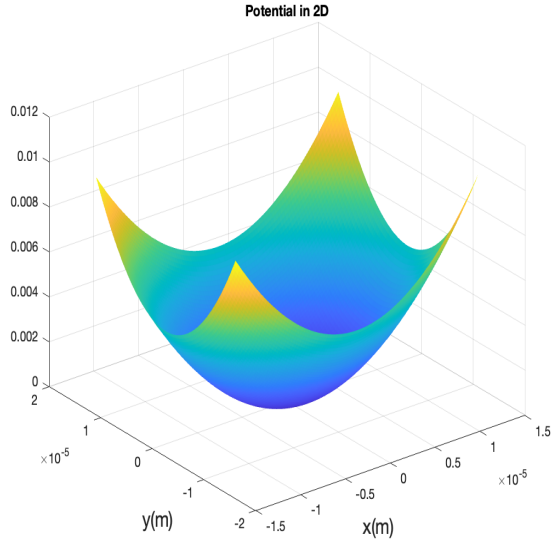
**2-D case**

$$\Psi(x,y,t+dt)=\Psi(x,t)+dt\left[\frac{\hbar}{2m}\frac{\Psi(x+dx)+\Psi(x-dx)-2\Psi(x,y,t)}{dx^2}+\frac{\hbar}{2m}\frac{\Psi(y+dy)+\Psi(y-dy)-2\Psi(x,y,t)}{dx^2}+\ldots-\frac{V(x,y)}{h}\Psi(x,y,t)\right] \quad (7)$$

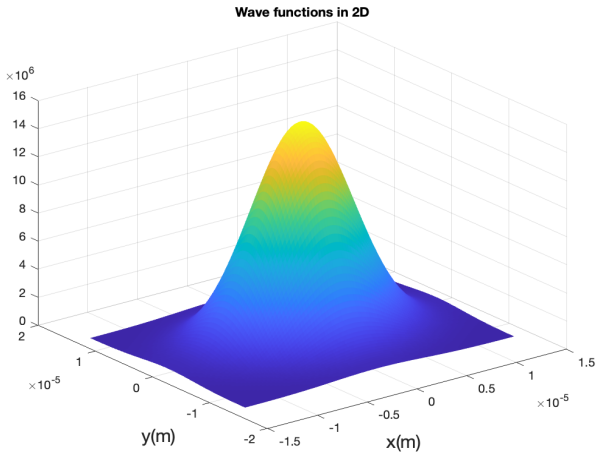
for the respective cases.




(a) (Blue)1D external Harmonic potential applied to a Bose gas (Orange) The evolution of the fun- damental wavefunction through spacetime Harmonic potential field in 2D



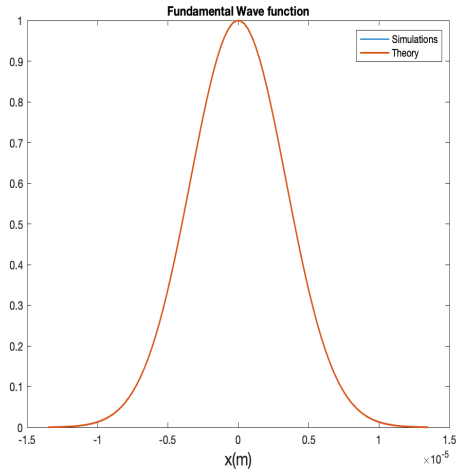

(b) Harmonic potential field in 2-Dimensions



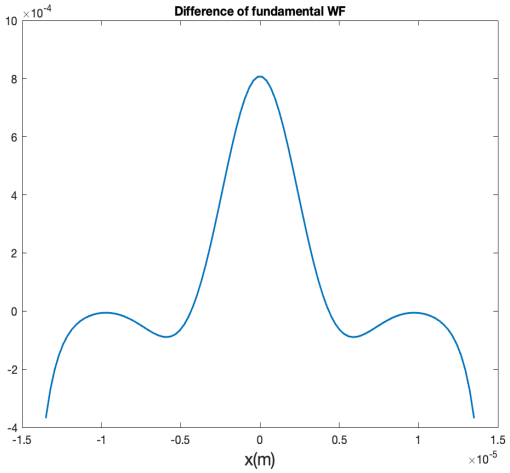

(c) The evolution of the wavefunction in a 2D-Harmonic potential.

Figure 4: The evolution of the WF and the external Harmonic potential in (a)1D and (b) 2D cases respectively.

To check that the ground state evolution of the from GPE is a Gaussian function, we estimated simulations for a gaussian function and compared the results of these two simulations with the results obtained in Eq.6.




(a) Theoretical Gaussian function and the plot of WF obtained in 1D Harmonic potential.




(b) Difference of the fundamental WF from theory and simulations.

Figure 5: The comparisons between the fundamental WF for theoretical and simulated value from the Imaginary time method in the presence of a Harmonic potential in 1D.

## 4 Introduction of interactions between atoms in a Harmonic potential

### 4.1 Interaction Hamiltonian

In the previous part, we did all our calculations neglecting the interactions between atoms in the Bose gas. We now have to contribute to the Hamiltonian corresponding to that phenomenon. We admit that this contribution takes the form of a new term in the Hamiltonian that is :

$$\hat{H}_{int} = -\frac{\hbar^2 \tilde{g} N}{m} |\Psi|^2 \tag{8}$$

This leads to the writing of the GPE presented in the introduction :

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta_{\mathrm{r}}^2 \Psi + \frac{\hbar^2 \tilde{g} N}{m} |\Psi|^2 \Psi + V(\vec{\mathrm{r}}) \cdot \Psi \tag{9}$$

The next calculations will be done in presence of a harmonic potential in the trap.

### 4.2 Transitioning to the interaction case

The addition of the interaction term between the gas atoms is expected to be accompanied by a spatial broadening of the fundamental mode. Indeed, the entire state must now consider the atoms' mutual repulsions. Therefore, the gas is expected to occupy more space in the trap effectively.

#### 4.2.1 1D case

Let us apply a harmonic potential in the trap and increase the number of interacting atoms N until the interaction terms become significant. From N = 0 to N = $10^7$, there is no change in the wave function in the trap. It may be because we have this regime :

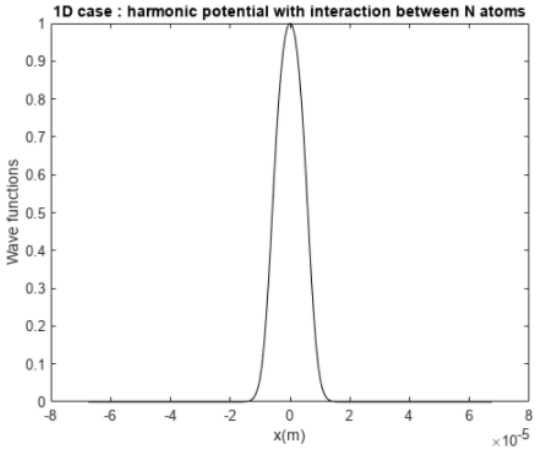
$$|-\frac{\hbar^2}{2m} \Delta_{\mathrm{r}}^2 \Psi + V(\overrightarrow{\mathrm{r}}) \cdot \Psi| \ll |\frac{\hbar^2 \tilde{g} N}{m} |\Psi|^2 \Psi|$$

Starting from N = $10^7$, we can clearly observe the broadening of the wave function.

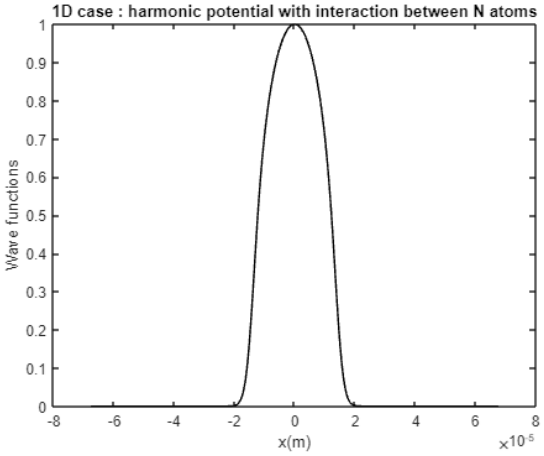
There is an apparent widening of the width of the wave function at the center, which is accompanied by a change in the shape of the wave function. Indeed, it is not simply a Gaussian wave function whose width at mid-height increases but a change to another function.

We expected this wave function. In the case of strong interactions, the kinetic energy can be neglected in the GPE. The shape of the ground state that we expect is :

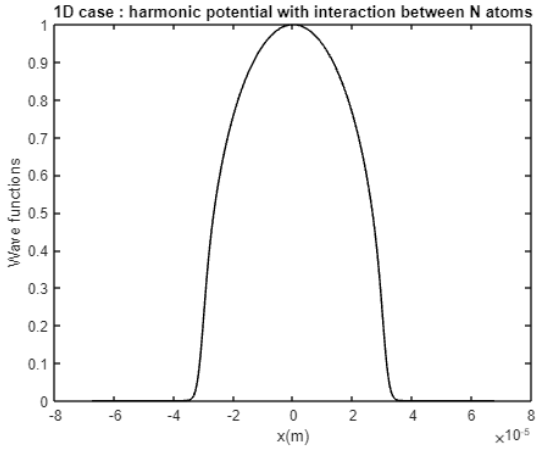
$$\Psi(\vec{r}) = \max\left(0, \left(m \frac{\mathrm{E} - \mathrm{V}(\tilde{\mathrm{r}})}{\hbar^2 \mathrm{g} \tilde{N}}\right)^{1/2}\right)$$



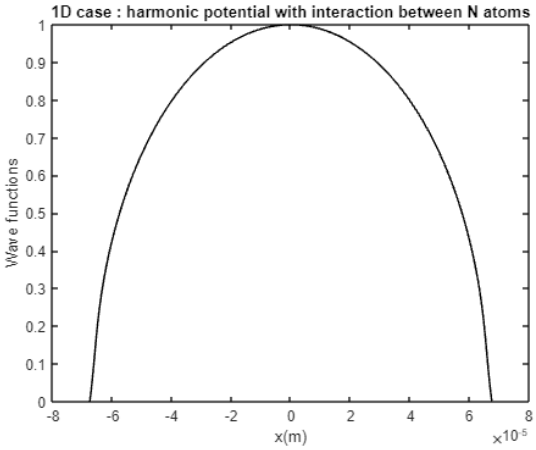

(a) Number of atoms $N = 10^7$




(b) Number of atoms $N = 10^8$



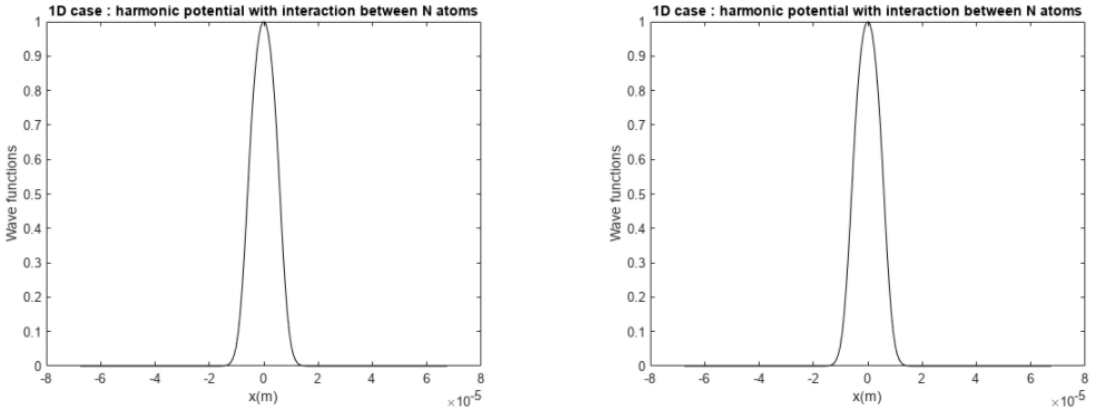

(c) Number of atoms $N = 10^9$




(d) Number of atoms $N = 10^{10}$

Figure 6: Observation of the broadening of the fundamental mode with the number of atoms in interaction

First of all, we check if the term of interaction is negligible in Fig.6a .We must compare the wave function obtained in Fig.6a with N = 0. Calculations on Matlab give a relative error of less than 0.1% RMS. That justifies the choice of N made in the beginning to give a visual representation of the transition between the harmonic potential with and without interactions between atoms and the possibility of skipping the plotting of the wave function with N being between all the powers of 10 between 0 and 7.




(a) WF with N = 0

(b) WF with N = $10^7$

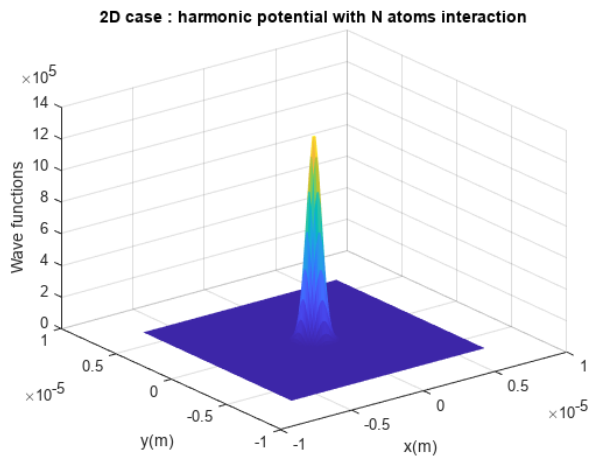
Figure 7: Comparison of the WF in the case N = 0 and N = $10^7$

In the same way, we also obtain the exact Fig.6d by plotting the wave function when we neglect the kinetic energy. We can verify that the final form of the wave function is no longer a Gaussian; it can be observed on the edges of the wave function: the drop at 0 loses its $C^\infty$ property due to the Gaussian shape, and becomes much steeper.

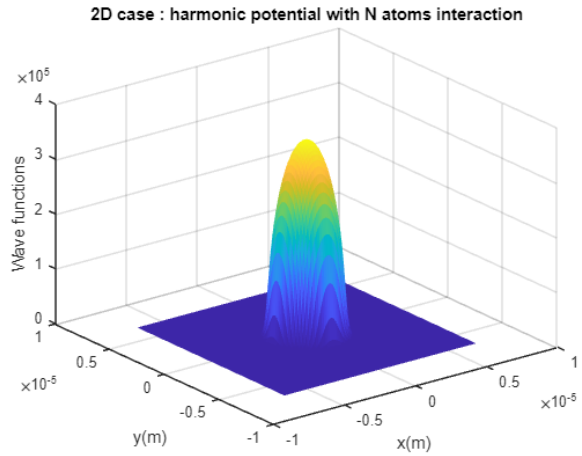
### 4.2.2 2D case

The implementation of the transition to a regime of interactions between atoms is very similar to what was done previously in the 1D case, with the difference that this time the transition is done for much fewer atoms.

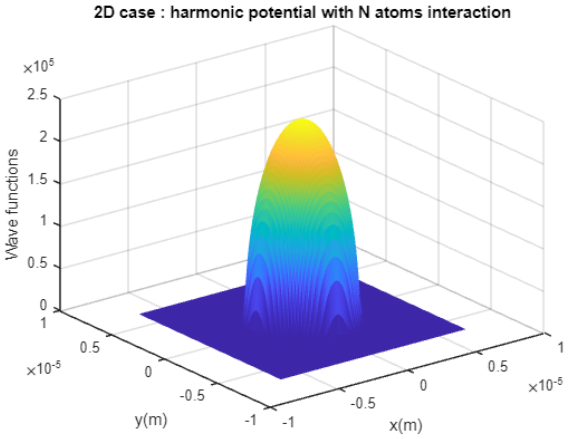
This can be explained by the fact that in order to speed up the calculations, we have reduced the size of the trap without touching the other parameters. The atoms "see" each other much more.




(a) N = 0




(b) N = 10



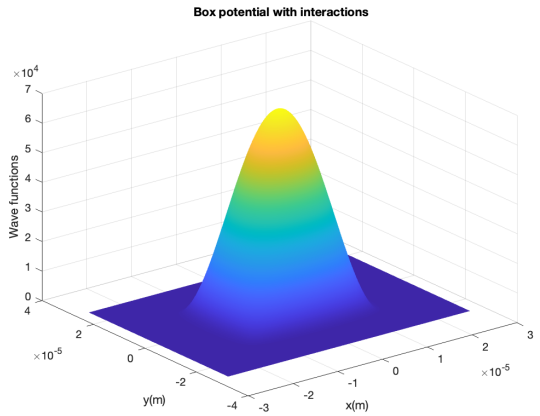

(c) N = 50

Figure 8: Observation of the broadening of the wave function in 2D when introducing more and more interactions between atoms in GPE

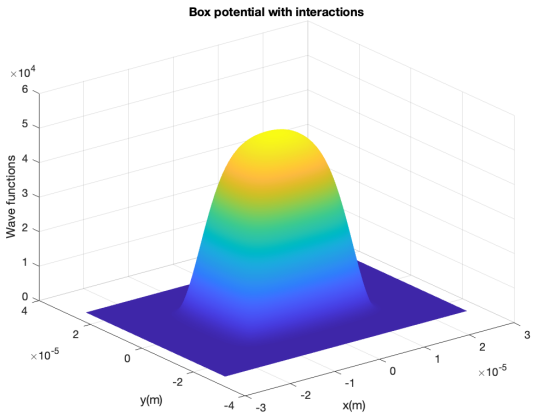
We also observe a broadening of the wave function: the atoms occupy more space in the trap due to the fact that they repel each other.

## 5 Interaction in Box potential

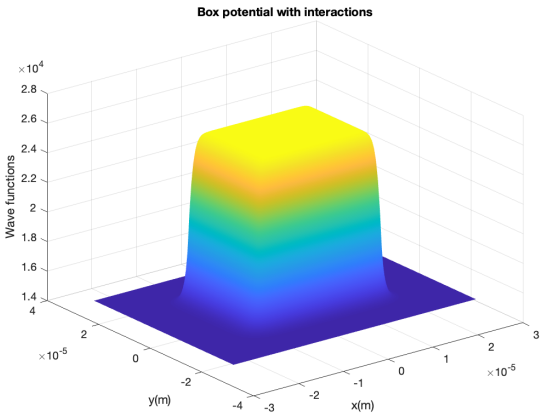
Moving ahead, having demonstrated in the preceding section that when we introduce interactions in the system, this leads to broadening of the WF, we will try to simulate the results for a Box potential under interactions and compare the modification of the wavefunction. Keeping in the Box potential given by Fig.3a, we obtained the results in Fig.9




(a) N = 0




(b) N = 100




(c) N = $10^4$

Figure 9: Observation of the broadening of the wave function in 2D when introducing more and more interactions between atoms in GPE for Box potential

The behavior of the WF under any interaction now is quite intuitive; we have already seen that in the case of the Harmonic potential, there is a broadening in WF, and this generalization is extended to the Box potential further.

## 6 Conclusion

We studied the Gross–Pitaevskii equation (GPE) that describes the ground state of a quantum system of identical bosons. We used the identity of the imaginary time to manipulate the damping of the excited eigenstates of condensate into a ground state via a decaying exponential. We introduced the harmonic and box potential to study the ground state of condensate in the regime where there is a no or little interaction between the atoms and the encompassed interaction into our simulations through the Non-Linear schröndinger equation.

We were able to plot the evolution of the ground state of condensate under a state of negligible interactions and strong interactions by using first and second differential formulas of the limits and derivatives for a function $f(x)$, which was used to find the evolution in 1d and 2d. Further, we could see that when the interactions became dominant, the WF started to broaden, which was one of the objectives of this work. We also studied the Thomas fermi regime, where the kinetic energy is neglected, and the leftover is potential energy.

Now moving ahead, the final part of the project would involve the sudden removal of the Box-Potential, and the introduction of Harmonic potential again and transform the imaginary time with real-time. However, sadly, we have not yet manipulated that part of our code.