BOSE EINSTEIN CONDENSATE (BEC) IN HARMONIC TRAP.

Kunal Singh(UID-219114, Roll No.-9)
Tanishka Manjrekar (UID-219128, Roll No.-19)

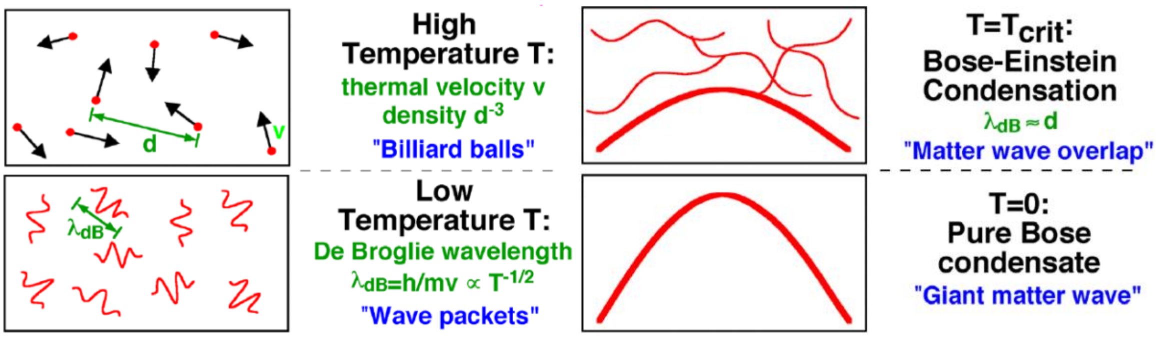
Abstract: *Various models have been developed to calculate the ground state wavefunction of BEC. The Gross-Pitaevskii equation models the ground stave wave function of the interacting system of Bosons at temperature T=0K. In this paper we solve the Time-dependent Gross-Pitaevskii equation using Crank Nicholson Finite Difference method using Python. The results show the variation due to the non-linear term (effect of interaction between the atoms) on the ground state wavefunction.*

Keywords: Crank-Nicholson(CNFD), Bose Einstein Condensate, Gross-Pitaevskii equation(1D), harmonic trap, python, time-dependent.

Theoretical Background and Review of Relevant Literature:

Bose-Einstein condensates were first predicted theoretically by Satyendra Nath Bose in 1894-1974. Bose was working on statistical problems in quantum mechanics, and sent his ideas to Albert Einstein. The first demonstration of Bose–Einstein condensation(BEC) in ultracold atomic gases came in 1995. Cornell and Wieman Bose-condensed 87Rb and Ketterle Bose-condensed 23Na.

Unlike Fermions, Bosons are indistinguishable and their wavefunctions are symmetric i.e., more than one boson can occupy the same state. The De-Broglie wavelength of a molecule varies inversely with the square root of temperature. At high temperatures the De-Broglie wave-length of the atoms is very small, much smaller than interatomic distance and hence they behave as particles. At lower temperatures the wave nature of the atoms can be observed as the De-Broglie wavelength of the particles increases. At the critical temperature the De-Broglie wavelengths become longer than the interatomic distance and the matter waves of the atoms overlap. At temperature T=0K all the matter waves overlap to form a giant matter wave.



(Source: W. Ketterle, MIT)

For given V and T, the total (equilibrium) number of particles in all the excited states taken together is bounded(Statistical Mechanics Third Edition by R. K. Pathria, Paul D. Beale)

$$N_e \leq V\frac{(2\pi mkT)^{3/2}}{h^3}\zeta\left(\frac{3}{2}\right).$$

When the actual number of particles exceeds this limiting value then excited states hold the as many particles as possible (given by the maximum value of the above eq.) and the rest will be pushed into the ground state ε = 0 whose capacity unlimited. Then the particles in ground state is given by

$$N_0 = N - \left\{V\frac{(2\pi mkT)^{3/2}}{h^3}\zeta\left(\frac{3}{2}\right)\right\}.$$

Fugacity z becomes unity for all practical purposes. This accumulation of macroscopically large number of particles in a single quantum state, is referred to as Bose Einstein Condensation.(BEC)

There are various models used to approximate the single particle ground state wavefunction of the BEC

The Gross Pitaevskii equation is one of the models .It uses the Hatree-Fock approximation and a pseudopotential to model a time-dependent non-linear Schrodinger Equation:

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + g|\Psi(\mathbf{r},t)|^2\right)\Psi(\mathbf{r},t).$$

where g is the coupling constant given by $g = \frac{4\pi\hbar^2 a_s}{m}$ (a_s is scattering length)

The magnetic traps used for cooling the system can be approximated using anisotropic harmonic oscillator potential:

$$V(r) = \frac{1}{2}m(w_1^2x^2 + w_2^2y^2 + w_3^2z^2)$$

For a 1D system:

$$V(x) = \frac{1}{2}m(\omega^2x^2)$$

This gives rise to the unperturbed single particle wavefunction:

$$\phi(r) = \frac{1}{\pi^{3/4}\sqrt{a_1a_2a_3}}exp\left[-\frac{1}{2}\left(\frac{x^2}{a_1^2} + \frac{y^2}{a_2^2} + \frac{z^2}{a_3^2}\right)\right]$$

For 1D system:

$$\phi(x) = \frac{1}{\pi^{3/4}\sqrt{a_1}}exp\left[-\frac{1}{2}\left(\frac{x^2}{a_1^2}\right)\right]$$

Where $a_1 = \sqrt{\frac{\hbar}{m\omega_1}}$ is the linear size of the unperturbed harmonic oscillator ground state.

If the scattering length a_s is positive, the interaction is repulsive while if a_s is negative the interaction is attractive.

The exact solutions of the Gross-Pitaevskii equation(GPE) are hard to find since it is a non-linear equation. Various Numerical methods have been employed to solve the GPE. A lot of attempts have been made to solve the GPE using various methods and parameters.

"*Gross-Pitaevskii Equation Using The Crank-Nicholson Scheme" (Fonseca, F. & Martinez, Roberto & (Plinio del Carmen Teherán Sermeño), P. del C. Teherán. 2011)* and "*Time-dependent solution of the nonlinear Schrödinger equation for Bose-condensed trapped neutral atoms"(Ruprecht PA, Holland MJ, Burnett K, Edwards M.*) give numerical solution if time dependent GPE using Crank Nicholson Finite Difference Scheme.

"Interference and Transport of Bose-Einstein Condensates" (Bo Xiong, MSc Thesis submitted to the University of Nottingham for the degree of Doctor of Philosophy, November 2,2009) solves the 3D GPE using Crank Nicholson Finite Difference scheme.

Other methods include Time splitting finite-difference (TSFD) scheme, Time-splitting Runge-Kutta method (TSRK) etc. *"A Primer on Quantum Fluids" (Carlo F. Barenghi and Nick G. Parker. August 26, 2016)* by explores MATLAB codes for 1D GPE using Split-Step Fourier Method, 1D GPE Solver and Imaginary Time Method.

"Numerical solution of the Gross–Pitaevskii equation for Bose–Einstein condensation"(Weizhu Bao a,, Dieter Jaksch b , Peter A. Markowich c)*

And *"Comparison of Splitting Methods for Deterministic/Stochastic Gross–Pitaevskii Equation"(Jürgen Geiser and Amirbahador Nasari)* provide a comparison of various numerical methods and while

"Comparison of finite-difference schemes for the Gross-Pitaevskii equation"(V. A. Trofimov & N. V. Peskov) compares specifically finite difference schemes.

Various codes are available on Fortran, C++ and MATLAB however only a few sources have used python programming to solve the GPE.

In this project we will solve the 1D GPE using Crank-Nicholson Finite Difference Scheme using Python 3.

Statement of the Problem:

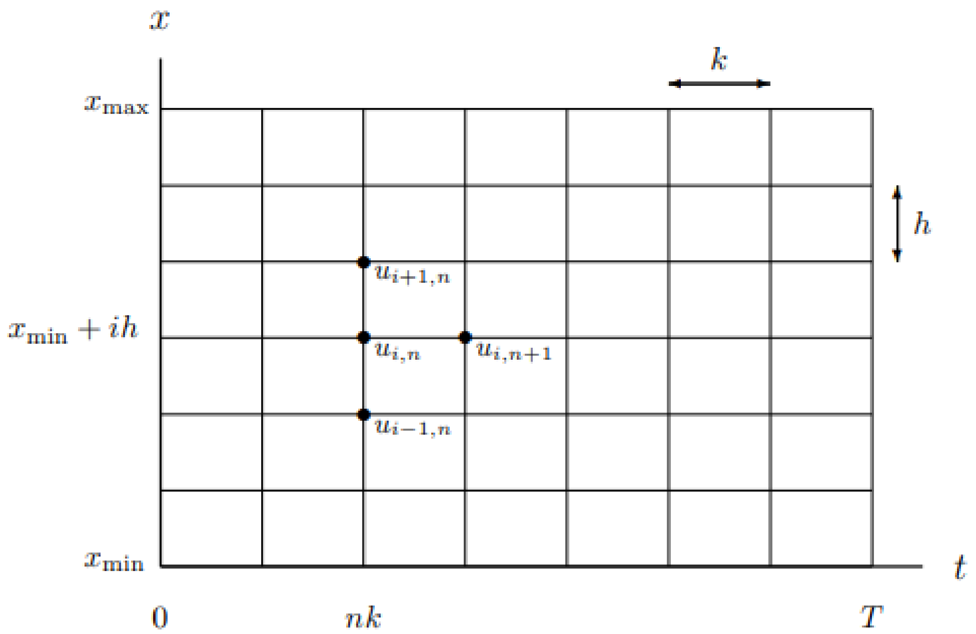
Solution of Bose Einstein Condensate in harmonic trap.

Details of Method of Study:

The Crank-Nicolson method is a well-known finite difference method for the numerical integration of the heat equation and closely related partial differential equations.

In our case, we can resort to this method to solve Time dependent Gross Pitaevskii equation as it fits the form of PDE: $au_{xx} + bu_x + cu - u_t$.

The discretization process is carried out on the spatial and time coordinates of the wave function in an analogous way to the diffusion equation.



In our project we take τ as the time step(instead of k) and h is the spatial discretization which is assumed equal in both directions x and y. Then the derivatives are defined as

$$\frac{\partial \psi}{\partial t} = \frac{\Psi_i^{n+1} - \Psi_i^n}{\tau}$$

$$\frac{\partial \Psi}{\partial x} = \frac{\Psi_{i+1}^{n} - \Psi_{i}^{n}}{h}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{\Psi_{i+1}^{n} - 2\Psi_{i}^{n} + \Psi_{i-1}^{n}}{h^2}$$

$$E\Psi = i\hbar \frac{\Psi_{i}^{n+1} - \Psi_{i}^{n}}{\tau} = -\frac{\hbar^2}{2m}\left[\frac{\Psi_{i+1}^{n} - 2\Psi_{i}^{n} + \Psi_{i-1}^{n}}{h^2}\right] + [g|\Psi_{i}^{n}|^2 + V_i]\Psi_{i}^{n}$$

We can represent this Hamiltonian matrix in the tridiagonal form.

First define a tridiagonal matrix with the main and off diagonal elements as 1, then multiply the main diagonal with $-\frac{\hbar^2}{2m}$*(-2/h^2) +V +g$|\Psi_{i}^{n}|^2$ and the upper diagonal and lower diagonal with $-\frac{\hbar^2}{2m}$*(1/h^2)

$$\Psi_{i}^{n+1} = \Psi_{i}^{n} - \frac{i\tau}{\hbar}\left(\frac{\hbar^2}{2m}\left[\frac{\Psi_{i+1}^{n} - 2\Psi_{i}^{n} + \Psi_{i-1}^{n}}{h^2}\right]\right) + [g|\Psi_{i}|^2 + V_i]\Psi_{i}^{n}$$

$$\Psi_{i}^{n+1} = (1 - \frac{i\tau}{\hbar}\left(\frac{\hbar^2}{2m}\left[\frac{\Psi_{i+1}^{n} - 2\Psi_{i}^{n} + \Psi_{i-1}^{n}}{h^2\Psi_{i}^{n}}\right]\right) + \frac{[g|\Psi_{i}|^2 + V_i]}{\Psi_{i}^{n}})\,\Psi_{i}^{n}$$

$$H = \frac{\hbar^2}{2m}\left[\frac{\Psi_{i+1}^{n} - 2\Psi_{i}^{n} + \Psi_{i-1}^{n}}{h^2\Psi_{i}^{n}}\right] + \frac{[g|\Psi_{i}|^2 + V_i]}{\Psi_{i}^{n}}$$

$$\Psi_{i}^{n+1} = \left(I - \frac{i\tau}{\hbar H}\right)\Psi_{i}^{n}$$

$$\Psi_{i}^{n+1} = \Psi_{i}^{n} - \frac{i\tau H}{2}(\Psi_{i}^{n+1} + \Psi_{i}^{n})$$

$$\Psi_{i}^{n+1} = \frac{(1 - \frac{i\tau H}{2})}{\left(1 + \frac{i\tau H}{2}\right)}\Psi_{i}^{n}$$

Defining a new term,

$$\frac{(1 - \frac{i\tau H}{2})}{\left(1 + \frac{i\tau H}{2}\right)} = Q^{-1} - 1$$

Which gives,

$$Q = \frac{1}{2}\left(1 + \frac{i\tau}{2\hbar}H\right)$$

We can form the Q matrix with the help of the H matrix discussed before.

$$Q = \begin{pmatrix} \beta_1 & \gamma_1 & 0 & \dots & 0 & 0 & \alpha_N \\ \alpha_1 & \beta_2 & \gamma_2 & \dots & 0 & 0 & 0 \\ . & . & . & \dots & . & . & . \\ . & . & . & \dots & . & . & . \\ . & . & . & \dots & . & . & . \\ 0 & 0 & 0 & \dots & \alpha_{N-2} & \beta_{N-1} & \gamma_{N-1} \\ \gamma_N & 0 & 0 & \dots & 0 & \alpha_{N-1} & \beta_N \end{pmatrix}$$

$$\beta_i = \frac{1}{2} + \frac{i\tau\hbar}{4mh^2} + \frac{i\tau V_i}{4\hbar} + \frac{i\tau g|\Psi_i^n|^2}{4\hbar}$$

$$\alpha_i = \gamma_i = -i\tau\hbar/8mh^2$$

We can now use the Q matrix to find the time evolution of our wave function by following this method.

$$\Psi_i^{n+1} = (Q^{-1} - 1)\,\Psi_i^n$$

Defining an auxiliary function Ξ

$$Q\Xi = \Psi_i^n \longrightarrow \Xi = Q^{-1}\Psi_i^n$$

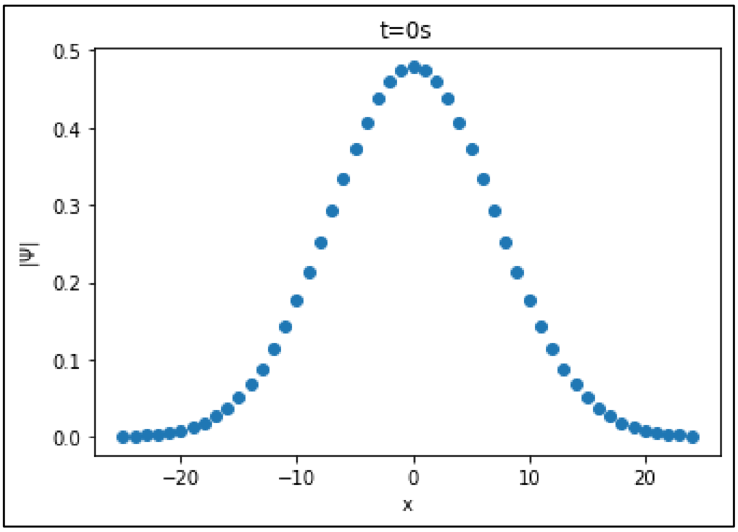
$$\Psi_i^{n+1} = \Xi - \Psi_i^n$$

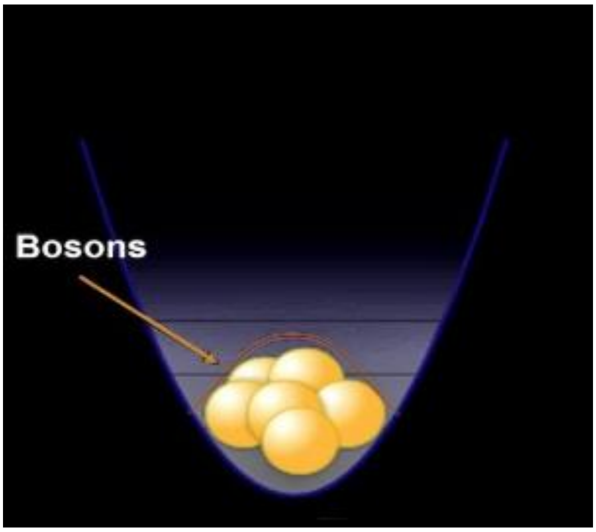
We use the Neumann Boundary conditions and specify that the derivative of the wavefunction w.r.t. the spatial coordinates at the boundaries is zero.

These are the exact steps to solve Gross Pitaevskii equation with the help of Crank Nicolson method

Results and Discussions:

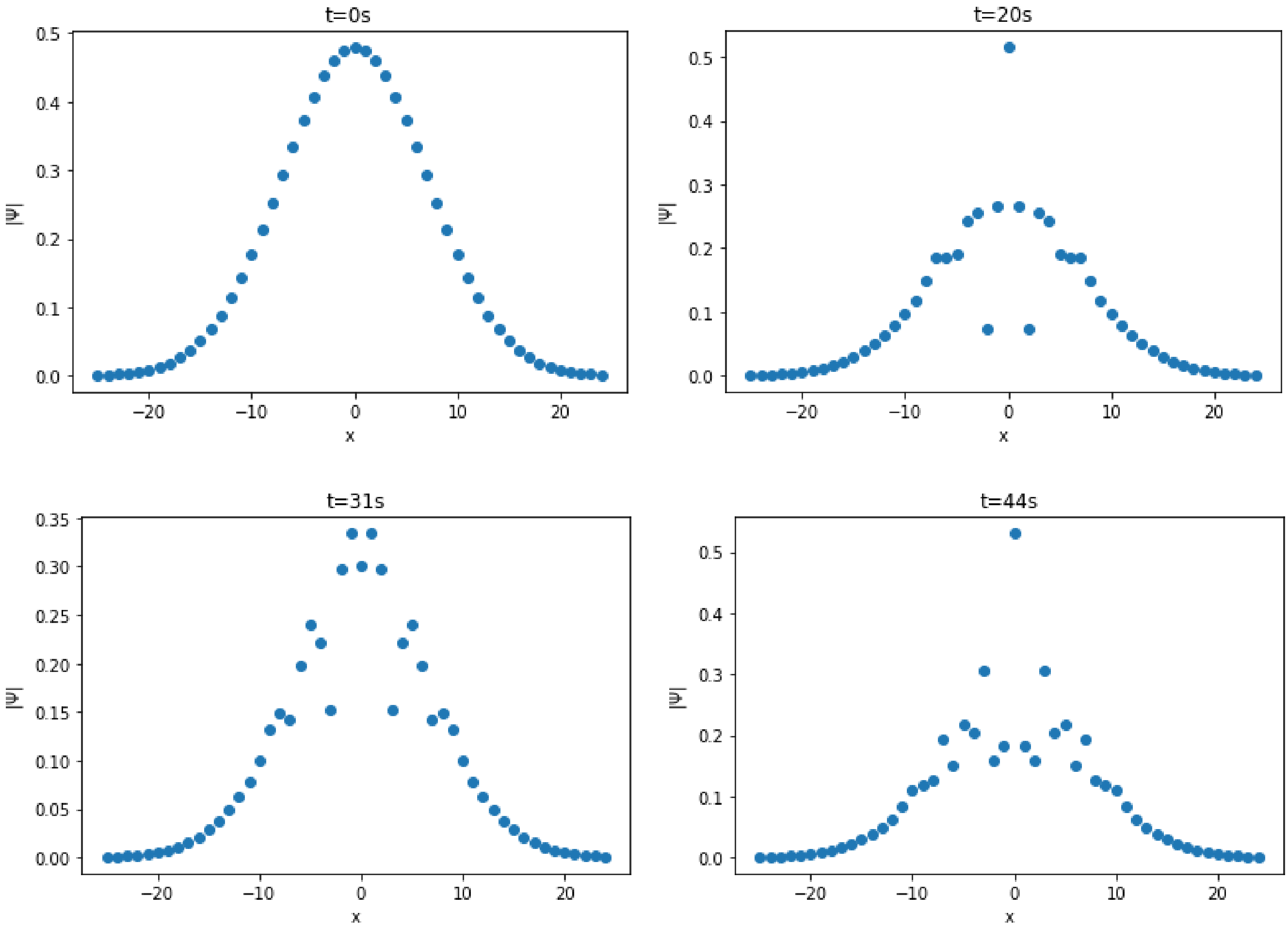
The solution of the Gross-Pitaevskii equation gives us the ground state single particle wavefunction at a time t.





At T=0K all the atoms in the system accumulate into the ground state.

The atoms in the condensate expand very little because they are in the lowest energy state and we observe a sharp peak at the centre of the harmonic trap. The centre of the harmonic trap was taken to be at the origin in our system. Hence at x=0 we observe a sharp peak in the ground state wavefunction.



For negative scattering lengths(a_{sc}), the forces between the atoms are attractive. The condensate grows in number until they reach a critical value and then their number decreases. Following the decrease, the number begins to grow again and the growth and collapse cycle is repeated as atoms are fed into the condensate from the large thermal cloud that is always present.

	Energy	spatial grid point	Ψ at t=0	Ψ at t=10s
0	-1.388420-0.000000j	-5	0.372901	0.224324
1	-1.388420-0.000000j	-4	0.408019	0.314142
2	-1.388420-0.000000j	-3	0.437604	0.235841
3	-1.388420-0.000000j	-2	0.460040	0.278428
4	-1.388420-0.000000j	-1	0.474051	0.407485
5	-1.388420-0.000000j	0	0.478815	0.477489
6	-1.388420-0.000000j	1	0.474051	0.407485
7	-1.388420-0.000000j	2	0.460040	0.278428
8	-1.388420-0.000000j	3	0.437604	0.235841
9	-1.388420-0.000000j	4	0.408019	0.314142

The above table shows the Energy eigenvalues of wavefunctions of different points on the spatial grid.

Limitations:

1. The Gross-Pitaevskii equation models the ground state wavefunction of the Bose Einstein Condensate only at temperature T=0K. In practical applications T=0K is not achievable. We use nanokelvins of temperature to study the BEC. Hence, we cannot study the variation in the wavefunction at different temperatures using the Gross-Pitaevskii equation.
2. The Gross-Pitaevskii is limited to weaky interacting systems and produces incorrect results for strong interaction. To get the correct ground state wavefunction for strong interactions we need to implement corrections to like the Lee-Huang-Yang (LHY) correction or the Lieb-Liniger model.
3. As we increase the number of atoms in the system the Crank- Nicholson algorithm takes more and more time for execution. Hence it is not suitable for a large system.

Relevance of the Study:

1. A rather massive amount of work has been done in the last couple of years, both to interpret the initial observations and to predict new phenomena. The Gross Pitaevskii equation where we consider weak interactions between bosons in inhomogeneous state presents a simple equation which helps us understand relevant properties like propagation of collective excitations and the interference effects originating from the phase of the order parameter.
2. We can modify this equation for many different situations, for example we can consider different potential traps like toroidal trap, ring traps etc or we can consider systems with rotations.
3. BEC has various applications in different fields of physics such as Quantum information processing in quantum computers, precision measurement with sensitive detectors using BEC, development of optical lattices which could be easily modifiable by varying the interplanar spacing, development of atomic lasers, etc.

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Python Programme:

CODE Link