

On the numerical solution of the Gross–Pitaevskii equation

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Abstract

The Gross–Pitaevskii equation is solved using an approach developed for the solution of the Bogoliubov–de Gennes equations for type II superconductivity. The solution is compared with others in the literature and is shown to be easily adapted to the study of an isolated vortex recently discovered in Bose-Einstein Condensation in trapped gases.

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1.0 Introduction

There has been a recent surge in interest in Bose–Einstein Condensation (BEC) after it was observed in a remarkable series of experiments on vapors of Rubidium and Sodium in which the atoms were confined in magnetic traps and cooled down to extremely low temperatures, of the order of Microkelvins [1]. The interesting feature of BEC in trapped gases is that it shows up in *coordinate* space. This is different from the BEC observed in superfluid Helium that is observed in *momentum* space. Thus a relatively new phenomenon is opened up to experimental and theoretical probes. Also vortex formation has been observed in a stirred Bose–Einstein Condensate [2]. This is analogous to vortex formation in superfluid Helium and type II superconductors [3]. Thus the theoretical understanding of the properties of BEC in trapped gases must necessarily include that of its vortex state.

An important equation used in the study of BEC is the Gross-Pitaevskii (GP) equation ([1] and references therein) which describes the condensate wavefunction. This equation is derived from mean field theory and has the form of a nonlinear Schrödinger equation, the nonlinearity coming from the mean – field term, proportional to the particle density. The nonlinearity also makes it difficult to solve analytically and hence a numerical approach is necessary. This work is motivated by the necessity to modify the GP equation so as to incorporate a vortex and show how it may be solved numerically.

The layout of the paper is as follows. The next section describes the GP equation. Section III develops a method to introduce the vortex into the equation and a numerical scheme to solve it. The case of the ground state is actually solved. The last section discusses the results and conclusion.

2.0 The Gross-Pitaevskii equation

A trapped gas can be described by N interacting bosons, which are trapped by an external potential $V_{\text{ext}}(r)$. The many – body Hamiltonian in second quantized form is written as

$$H = \int dr \Psi^\dagger(r) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) \right] + \frac{1}{2} \int dr dr' \Psi^\dagger(r) \Psi^\dagger(r') V(r-r') \Psi(r') \Psi(r), \quad (2.1)$$

where $\Psi(\mathbf{r})$ and $\Psi^\dagger(r)$ are the boson field operators that annihilate and create a particle at the position \mathbf{r} , respectively and $V(r - r')$ is the two–body interatomic potential. The time evolution of the field operator $\Psi(\mathbf{r}, t)$ can be determined using the Heisenberg equation of motion with the many–body Hamiltonian (2.1):

$$i\hbar \frac{\partial}{\partial t} \Psi(r, t) = [\Psi, H] = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + \int dr' \Psi^\dagger(r', t) V(r' - r) \Psi(r', t) \right] \Psi(r, t) \quad (2.2)$$

For the case in hand the interaction can be represented by the dilute gas approximation

$$V(r - r') = g \delta(r - r'), \quad (2.3)$$

where g is the coupling constant which measures the strength of the interaction. The use of (2.3) reduces

$$(2.2) \text{ to the form } i\hbar \frac{\partial}{\partial t} \Psi(r, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) + g \Psi^\dagger(r, t) \Psi(r, t) \right] \Psi(r, t) \quad (2.4)$$

and also makes possible the use of the mean – field approximation that replaces the operator $\Psi(r,t)$ by its mean– field value $\Phi(r,t) \equiv \langle \Psi(r,t) \rangle$. $\Phi(r,t)$ is a complex function called the wave function of the condensate, its modulus fixes the condensate density through $n(\mathbf{r},t) = |\Phi(r,t)|^2$. Making this replacement (2.4) now becomes

$$i\eta \frac{\partial}{\partial t} \Phi(r,t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(r) + g|\Phi(r,t)|^2 \right] \Phi(r,t), \quad (2.5)$$

known as the Gross -Pitaevskii equation. The wave function can be written as

$$\Phi(r,t) = \varphi(r) e^{-i\varepsilon t / \hbar} \quad (2.6)$$

where ε is the chemical potential and φ is a function and normalized to the total number of particles, $\int dr |\varphi|^2 = N$. Then the GP equation becomes

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(r) + g|\varphi(r)|^2 \right] \varphi(r) = \varepsilon \varphi(r). \quad (2.7)$$

This has the form of a nonlinear Schrödinger equation, the nonlinearity coming from the mean – field term proportional to the particle density $n(r) = |\varphi(r,t)|^2$. In the absence of interactions ($g = 0$) this equation reduces to the normal Schrödinger equation for a single particle. The trapping potential is usually represented by the Harmonic potential:

$$V_{ext}(r) = \frac{1}{2} m \omega_{ho}^2 r^2, \quad (2.8)$$

ω_{ho} is the geometric average of the oscillator frequencies

$$\omega_{ho} = (\omega_x \omega_y \omega_z)^{1/3} \quad (2.9)$$

It also defines the harmonic oscillator length:

$$a_{ho} = \left(\frac{\hbar}{m \omega_{ho}} \right)^{1/2} \quad (2.10)$$

Measuring length in terms of a_{ho} , energy in terms of $\hbar \omega_{ho}$ and density in terms of a_{ho}^{-3} the expression (2.7) becomes

$$\left[-\nabla^2 + r^2 + g|\varphi(r)|^2 \right] \varphi(r) = 2\varepsilon \varphi(r) \quad (2.11)$$

with all quantities in the equation now dimensionless and the normalization condition now satisfying $\int dr |\varphi|^2 = 1$. It now remains to describe a vortex structure. This can be done using the description of de Gennes [4,5] by writing the wave function as

$$\varphi(r) = \varphi(r) e^{i\mu\theta} e^{ik_z z} \quad (2.12)$$

describing a cylindrical vortex structure with μ the orbital angular momentum quantum number, taking on integral values $0, \pm 1, \pm 2, \pm 3, \dots$ and k_z the z -component of momentum. Equation (2.11) is now written as

$$\left[-\frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \frac{\mu^2}{r^2} + k_z^2 + r^2 + g\varphi^2(r) \right] \varphi(r) = 2\varepsilon \varphi(r) \quad (2.13)$$

The equation depends on the square of μ and hence we can confine ourselves to zero and positive values of μ . The equation with $\mu = 0$ is interpreted as the equation of the ground state (in the absence of a vortex). The solution with $\mu > 0$ now describes the vortex structure.

3.0 Numerical scheme

We follow closely a scheme already developed [6]. Equation (2.13) will be solved for $\mu = 0$ and $k_z^2 - 2\varepsilon \approx 0$:

$$\left[-\frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + r^2 + g\varphi^2(r) \right] \varphi(r) = 0 \quad (3.1)$$

This equation is a second order nonlinear ordinary differential equation (ODE). To solve it, an initial assumption for the wave function is required. It has already been mentioned that in the absence of interactions the GP equation reduces to the ordinary Schrödinger equation. Since the external potential is harmonic, the initial assumption for the wave function is the ground–state wave function of the harmonic

oscillator which is Gaussian:

$$\varphi_{\text{ass}}(r) = Ae^{-r^2/2} \quad (3.2)$$

A is a constant. The equation is then solved by iteration until the solution converges. The term first order in derivative can be removed via a change in variable

$$\varphi(r) = \frac{f(r)}{\sqrt{r}} \quad (3.3)$$

equation. (3.1) becomes

$$\frac{d^2 f}{dr^2} = \left[\frac{1}{4r^2} + r^2 + g \frac{f^2(r)}{r} \right] f(r), \quad (3.4)$$

which can be solved using known techniques [7].

4.0 Results, discussion and conclusion

Calculations were carried out for $g = -0.1, -0.3, -0.5$ (attractive interaction) and $g = 1, 10, 100$ (repulsive interaction). In general the solutions converged after approximately ten iterations. The results are shown in Figures 1 and 2. Figure 1 shows how the density of the particles peak as the strength of the attractive interaction increases while Figure 2 shows how they spread out as the strength of the repulsion increases, similar to what has already been obtained ([1] and references therein). What is interesting about this approach is that a vortex structure can now be introduced by using a non – zero value for μ and the corresponding harmonic oscillator wave function as the initial assumption. Work is in progress on this and shall be reported elsewhere.

In conclusion, a numerical scheme has been developed to solve the Gross–Pitaevskii equation. Also a method, which allows the study of vortex formation, has been shown.

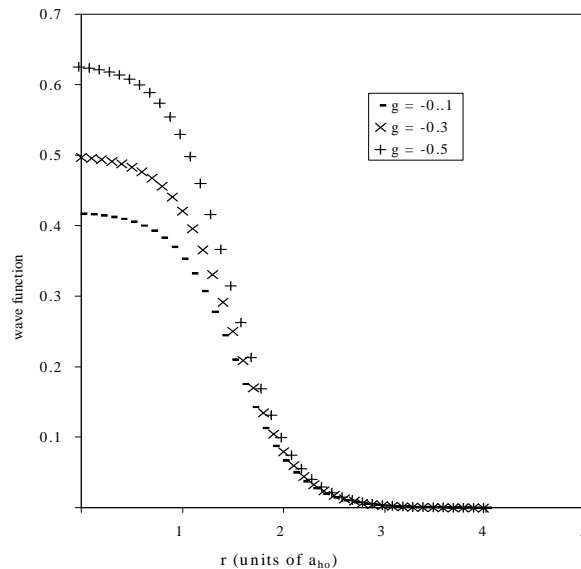


Figure 1. Condensate wave function for attractive interaction

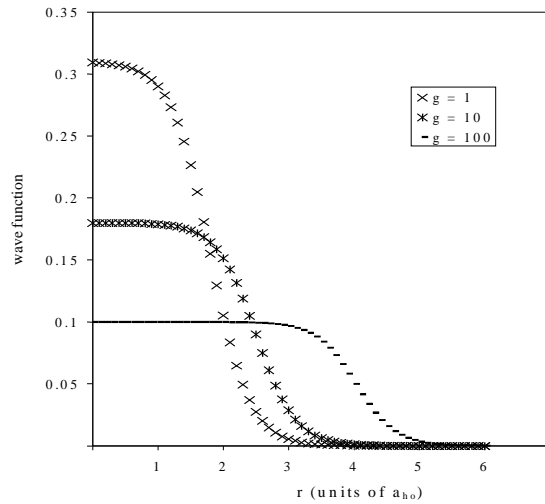


Figure 2. Condensate wave function for repulsive interaction.

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