



Numerical solution to the time-independent gross-Pitaevskii Equation

Tsogbayar Tsednee[†], Banzragch Tsednee, and Tsookhuu Khinayat

Institute of Physics and Technology, Mongolian Academy of Sciences, Ulaanbaatar, Mongolia

ABSTRACT. We solve the time-independent Gross-Pitaevskii equation modeling the Bose-Einstein condensate trapped in an anisotropic harmonic potential using a pseudospectral method. Numerically obtained values for an energy and a chemical potential for the condensate with positive and negative scattering length have been compared with those from the literature. The results show that they are in good agreement when an atomic interaction is not too strong.

KEYWORDS. Bose-Einstein condensate, nonlinear Schroedinger equation, chemical potential, rubidium, lithium

1. INTRODUCTION

When the thermal de Broglie wavelength exceeds the mean spacing between identical boson-particles, bosons are stimulated by presence of other bosons in the lowest energy state to occupy that state as well, resulting in macroscopic occupation of a single quantum state [1, 2]. This phenomenon is named the Bose-Einstein condensation and the condensate that forms constitutes a macroscopic quantum mechanical object. This theoretical prediction had been confirmed experimentally 70 years later, particularly for ^{87}Rb [3], ^7Li [4] and ^{23}Na [5]. The vapors of alkali atoms employed in the experiments are very dilute, so one can expect that the two-body collision accounting for by the knowledge of the s -wave scattering length might be dominate. This also implies that the Gross-Pitaevskii theory [6, 7] for weakly interacting bosons can be suitable for the system which can be simulated to be confined in an isotropic [8, 9] and an anisotropic [10, 11] traps.

In this work we solve the time-independent Gross-Pitaevskii equation (GPE) for N alkali atoms in an anisotropic trap. We compute the condensate wave function at $T = 0$ for bosons interacting through positive and negative scattering lengths and obtain the chemical potential and

Received: 04 November 2021 / Revised: 22 November 2021 / Accepted: 30 November 2021

[†] Corresponding author's email. tsog215@gmail.com, tsogbayar.ts@mac.ac.mn

energy as a function of N . Numerical method we choose to solve the GPE is a pseudospectral method, which we had applied successfully in the past [12].

The paper is organized as follows. In Section 2, we show the formalism of the Gross-Pitaevskii theory for the anisotropic trap. In Section 3 we give a brief discussion of a pseudospectral approach for the 3D problem. In Section 4 we present the numerical results for the two cases of positive ^{87}Rb and negative ^7Li scattering lengths. Then a conclusion follows.

2. GROSS-PITAEVSKII THEORY FOR TRAPPED BOSONS

The mean field theory for a dilute assembly of bosons at $T = 0$ results in an effective nonlinear Schrödinger equation for the condensate's wave function. This equation, the Gross-Pitaevskii, nonlinear Schrödinger equation for condensed bosons has a form:

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{ext} + \frac{4\pi\hbar^2 a N}{m} |\Psi(\mathbf{r}, t)|^2 \right) \Psi(\mathbf{r}, t). \quad (1)$$

Here $\Psi(\mathbf{r}, t)$ is the Bose-Einstein condensate (BEC) wave function, (also called the order parameter), m is the mass of boson, V_{ext} is an external confining potential (trap), a is the s -wave scattering length and N is the number of bosons in the condensate.

A stationary solution $\Psi(\mathbf{r}, t) = e^{i\mu t/\hbar} \psi(\mathbf{r})$ obeys

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\mathbf{r}) + V_{mf}(\mathbf{r}) \right] \psi(\mathbf{r}) = \mu \psi(\mathbf{r}), \quad (2)$$

where the mean-field (mf) potential is $V_{mf} = \frac{4\pi\hbar^2 a N}{m} |\psi(\mathbf{r})|^2$. Once this equation is solved the chemical potential μ is known and the free energy can be calculated using

$$E = \mu - \frac{1}{2} \langle V_{mf} \rangle = \int \psi(\mathbf{r})^* \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\mathbf{r}) + \langle V_{mf} \rangle \right) \psi(\mathbf{r}) d\mathbf{r}. \quad (3)$$

Since ψ and V_{mf} in equation (2) depend on each other, the GP equation must be solved self-consistently. One first uses an initial guess for the wave function ψ to calculate V_{mf} using equation (4). This value is then employed in equation (2) to obtain a new ψ , which is then used to calculate V_{mf} again. This process is repeated until self-consistency is reached.

In our calculation we use a following anisotropic harmonic oscillator potential:

$$V_{ext}(x, y, z) = \frac{m}{2} \omega_x^2 x^2 + \frac{m}{2} \omega_y^2 y^2 + \frac{m}{2} \omega_z^2 z^2. \quad (4)$$

By introducing the standard lengths $a_{\perp} = (\hbar/m\omega_{\perp})^{1/2}$ and $a_z = (\hbar/m\omega_z)^{1/2}$, we can rescale the spatial coordinate, the energy, and the wave function as $\mathbf{r} = a_{\perp} \mathbf{r}_1$, $E = \hbar\omega_{\perp} E_1$ and $\psi(\mathbf{r}) = \sqrt{N/a_{\perp}^3} \psi_1(\mathbf{r}_1)$, with $\omega_x = \omega_y = \omega_{\perp}$. Here the wave function ψ_1 is normalized to 1. With help of the introduced asymmetry parameter $\lambda = \omega_z/\omega_{\perp}$ and the quantity $g = 4\pi a N/a_{\perp}$, the time-independent GP equation (2) can be written as:

$$\left[-\frac{1}{2} \nabla_1^2 + \frac{(x_1^2 + y_1^2)}{2} + \frac{\lambda^2 z_1^2}{2} + g |\psi(\mathbf{r}_1)|^2 \right] \psi(\mathbf{r}_1) = \mu \psi(\mathbf{r}_1), \quad (5)$$

3. NUMERICAL PRODECURE

In our calculation we use the Legendre-pseudospectral method [12]. In terms of this approach, function $\psi(r)$ can be expressed as:

$$\psi(r) \approx \psi_{N_r}(r) = \sum_{i=0}^{N_r} \psi(r_i) g_i[x(r)], \quad (6)$$

where $g_i[x(r)]$ is a cardinal function given with

$$g_i[x(r)] = -\frac{1}{N_r(N_r+1)P'_{N_r}(x_i)} \frac{(1-x^2)P'_{N_r}(x)}{x-x_i} \quad (7)$$

and $g_i(x_j) = \delta_{ij}$. Here N_r is a number of grid point along $r(x) = a + (1+x)(b-a)/2$, $x \in [-1, 1]$ and $r \in [a, b]$ with a length parameters (a, b) . Here the Legendre-Gauss-Lobatto grid points x_i are determined as the roots of the first derivative of the Legendre polynomial $P_N(x)$ with respect to x , $P'_{N_r}(x_i) = 0$, $i = 0, \dots, N_r$. In the approach, the Laplace operator ∇^2 can be approximated with a differentiation matrix d_{ij} [12]. So, for the 3D calculation, we can approximate $\nabla_x^2 + \nabla_y^2 + \nabla_z^2 \approx I_{zz} \otimes (d_{xx}^2 \otimes I_{yy}) + I_{zz} \otimes (I_{xx} \otimes d_{yy}^2) + (I_{xx} \otimes I_{yy}) \otimes d_{zz}^2$. Here I is the unit matrix, and \otimes expresses the Kroneckor (tensor) product [12]. In our numerical calculation we use $a_x = a_y = a_z = a = -5$, $b_x = b_y = b_z = b = 5$ in units of a_\perp , and $N_x = N_y = N_z = 32$.

4. RESULTS AND DISCUSSION

As an example of atoms with repulsive interaction, we choose ^{87}Rb , as in the experiment of Ref. [3]. In our calculation, all values of the physical parameters are taken from Ref. [10]: the s -wave triplet-spin scattering length, $a_s = 100a_0$ where a_0 is the Bohr radius; the asymmetry parameter of the experimental trap is $\lambda = \omega_z/\omega_\perp = \sqrt{8}$; the axial frequency $\omega_z/2\pi = 220 \text{ Hz}$; the corresponding characteristic length is $a_\perp = 1.222 \times 10^{-12} \text{ cm}$ and the ratio between the scattering and the oscillator lengths is $a/a_\perp = 4.33 \times 10^{-3}$. In our calculation number of grid points is $N_x = N_y = N_z = 24$, and results are independent on this number. Table 1 shows the excess chemical potential and energy per particle for three values of $N = 100, 1000$ and 1000 , and our calculated values are close to those in Ref. [10], which had been obtained with a direct minimization approach combined with an imaginary time technique. Both quantities are expressed in units of $\hbar\omega_\perp$. In Figure 1 we show plots of the wave function along the x (panel

TABLE 1. Results for the ground state of ^{87}Rb atoms in a trap with $\lambda = \sqrt{8}$. Chemical potential and energy are in unit of $\hbar\omega_\perp$. A number of grid point is $N_x = N_y = N_z = 24$.

	$N = 100$		$N = 1000$		$N = 5000$	
	μ	E	μ	E	μ	E
This work	2.88	2.67	4.77	3.84	8.15	6.13
[10]	2.88	2.66	4.77	3.84	8.14	6.12

a) and the z axis (panel b) for four values of N . When N increases the repulsion among the atoms tends to lower the central density, and expands the cloud of the atoms towards region where the trapping potential is higher. This results in increase of an energy per particle.

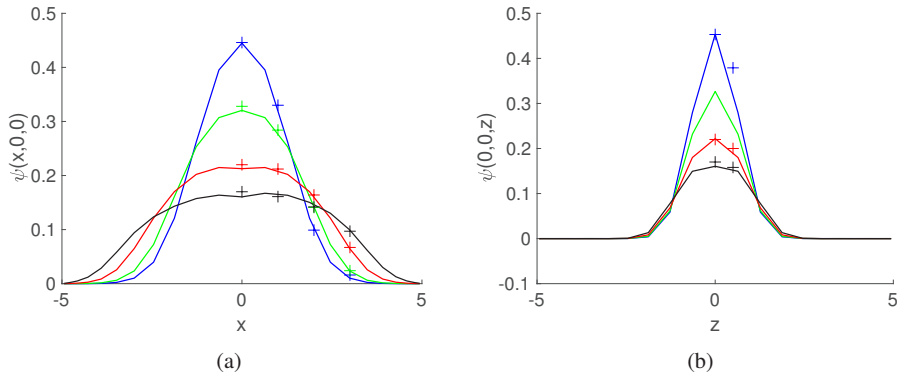


FIGURE 1. The ground-state wave function for ^{87}Rb along the x axis (a) and along the z -axis (b). Distances are in units of a_{\perp} . Blue, green, red and black lines corresponds to $N = 100, 500, 2000$ and 5000 , in descending order of central density. Cross are taken from Ref. [10].

As an example of atoms with an attractive interaction we choose ^7Li , as in the experiment of Ref. [4]. In the calculation, we use $a_s = -27 a_0$; $\omega_z = 2\pi \times 117 \text{ Hz}$; $a_{\perp} = 2.972 \times 10^{-4} \text{ cm}$; $|a|/a_{\perp} = 0.48 \times 10^{-3}$; $\omega_{\perp} = 2\pi \times 163 \text{ Hz}$, and $\lambda = \omega_z/\omega_{\perp} = 0.72$. Table 2 shows numerical values of chemical potential and energy for the ^7Li ground state in unit of $\hbar\omega_{\perp}$ for three values of N . Figure 2a presents the ground state wave function for the ^7Li atom for three values of

TABLE 2. Same results as shown in Table 1, but for ^7Li atoms in a trap with $\lambda = 0.72$.

	$N = 100$		$N = 500$		$N = 1000$	
	μ	E	μ	E	μ	E
This work	1.33	1.34	1.17	1.27	0.86	1.16

N . In this plot, the central density of cloud increases rapidly with N since more attractive potential energy is added. Fig. 2b shows two-dimensional description of ground state wave function $\psi(x, y, 0)$ for $N = 1000$.

5. CONCLUSION

In this paper we have solved the time-independent Gross-Pitaevskii equation, non-linear eigenvalue problem, for a dilute gas of alkali atoms in an anisotropic traps using the pseudospectral method. The ground state wave function for the condensate with repulsive (^{87}Rb)

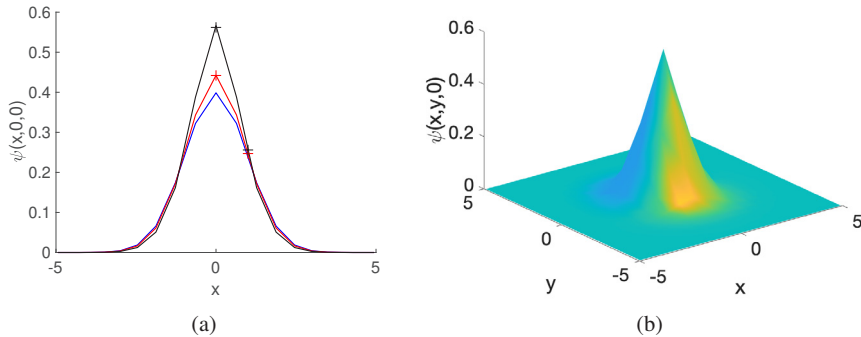


FIGURE 2. Same plots as shown in Figure 1, but for the ${}^7\text{Li}$ ground state along the x axis (a), and blue, red and black lines correspond to $N = 100, 500$ and 1000 , in ascending order of central density (a). Panel (b) shows an interpolated two-dimensional plot for $N = 1000$. Crosses are taken from Ref. [10].

and attractive (${}^7\text{Li}$) behaviors at $T = 0$ has been obtained and natures of these wave function depending on number of particle have been discussed. Chemical potential and energy per particle for the (${}^{87}\text{Rb}$) and (${}^7\text{Li}$) condensates for different values of N have been presented as well.

REFERENCES

- [1] S.N. Bose, *Planck's Law and Light Quantum Hypothesis*, Z. Phys., **26** (2004), 178-181.
- [2] A. Einstein, *Quantentheorie des einatomigen idealen Gases*, Sitzber. Kgl. Preuss. Akad. Wiss. **1925** (1925), 3-14.
- [3] M.H. Anderson, J. R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor*, Science **269**, (1995), 198-201.
- [4] C.C. Bradley, C.A. Sackett, J.J. Tollett, and R.G. Hulet, *Evidence of Bose-Einstein Condensation in an Atomic Gas with Attractive Interactions*, Phys. Rev. Lett. **75**, (1995), 1687-1690.
- [5] K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, and W. Ketterle, *Bose-Einstein Condensation in a Gas of Sodium Atoms*, Phys. Rev. Lett. **75**, (1995), 3969-3973.
- [6] L.P. Pitaevskii, *Vortex lines in the imperfect Bose-gas*, Zh. Eksp. Teor. Fiz. **40**, (1961), 646-649.
- [7] E.P. Gross, *Structure of a quantized vortex in boson systems*, Nuovo Cimento **20**, (1961), 454-477.
- [8] M. Edwards and K. Burnett, *Numerical solution of the nonlinear Schrödinger equation for small samples of trapped neutral atoms*, Phys. Rev. A **51**, (1995), 1382-1386.
- [9] P.A. Ruprecht, M.J. Holland, K. Burnett, and M. Edwards, *Time-dependent solution of the nonlinear Schrödinger equation for Bose-condensed trapped neutral atoms*, Phys. Rev. A **51**, (1995), 4704-4711.
- [10] F. Dalfovo and S. Stringari, *Bosons in anisotropic traps: Ground state and vortices*, Phys. Rev. A **53**, (1996), 2477-2485.
- [11] G. Baym and C. Pethick, *Ground-State Properties of Magnetically Trapped Bose-Condensed Rubidium Gas*, Phys. Rev. Lett. **76**, (1996), 6-9.
- [12] Ts. Tsogbayar, M Horbatsch, *Calculation of Stark resonance parameters for the hydrogen molecular ion in a static electric field*, J. Phys. B **46**, (2013), 085004 (8pp).



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