

Ground state properties and elementary excitation of ^{85}Rb Bose-Einstein condensate:
analytical method for modified Thomas-Fermi model with large-gas-parameter

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2007 J. Phys.: Conf. Ser. 80 012038

(<http://iopscience.iop.org/1742-6596/80/1/012038>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.174.55.245

The article was downloaded on 08/05/2012 at 10:33

Please note that [terms and conditions apply](#).

Ground state properties and elementary excitation of ^{85}Rb Bose-Einstein condensate : analytical method for modified Thomas-Fermi model with large-gas-parameter

Moumita Gupta¹ and Krishna Rai Dastidar²

Department of Spectroscopy, Indian Association for the Cultivation of Science, Kolkata
700032, India

E-mail: ¹ moumita_81@yahoo.co.in

E-mail: ² krishna_raidastidar@yahoo.co.in

Abstract. Bose-Einstein condensation in trapped gases of ^{85}Rb atoms can now be obtained in the large gas-parameter region in presence of Feshbach resonance and the gas density which is characterized by peak gas parameter x_{pk} can attain the value $\sim 10^{-2}$. For such large gas-parameter, the first correction term to the Bogoliubov energy functional is considered to give modified Gross-Pitaevskii (MGP) equation. In this work analytical expressions for the chemical potential, the density of particles and the excitation frequency of the monopole mode have been derived in Thomas-Fermi (TF) approximated approach to the MGP equation (modified TF approach) following method of higher order iteration for Bose-Einstein condensate (BEC) of atoms in spherically symmetric trap. We have also solved the MGP equation by using Runge-Kutta method for integration of nonlinear differential equation considering spherically symmetric trap. The analytical results for chemical potential and density of particles for BEC of 10^3 and 10^4 ^{85}Rb atoms in a spherically symmetric trap are in very good agreement with the numerical results from MGP equation at low as well as at large scattering length i.e., at large gas-parameter region. The frequency of monopole mode calculated using the density of particles in the ground state (found out in higher order iterative method) are also in very good agreement with the existing numerical results. The difference between the analytical and numerical results decreases as the value of scattering length i.e., gas-parameter is increased.

1. Introduction

Most of the experimental and theoretical studies of the Bose-Einstein condensate (BEC) of the magnetically trapped alkali atoms have been restricted in dilute gas condition $na^3 < 10^{-3}$ (where n is atomic density, a is s-wave scattering length of interatomic potential and the parameter na^3 is called gas parameter). In a dilute atomic gas where the average distance between the Bose atoms is much larger than the range of interatomic interaction which is characterized by the s-wave scattering length a , mean-field Gross-Pitaevskii (GP) theory [1] is quite successful to study the system. However in recent experiments [2,3] the gas-parameter may exceed this value due to the possibility of tuning scattering length over a wide range in the presence of Feshbach resonance and a static condensate with $x_{pk} = n_{pk}a^3 \sim 10^{-2}$ (x_{pk} = peak gas parameter and

n_{pk} =peak density of the condensate) has been created. Previously [4,5] ground state properties of BEC with large values of gas parameter (as achieved in experiment [2]) have been studied theoretically in spherical and cylindrical traps going beyond GP theory by including higher order non-linear terms in the interatomic correlation energy. In ref[4] the results obtained by numerically solving modified Gross-Pitaevskii (MGP) equation for 10^4 ^{85}Rb atoms are compared with those obtained by analytical solution of modified version of Thomas-Fermi equation (which is obtained by disregarding kinetic energy term in MGP equation) at the very first step of an iterative procedure (MTF(1))[6]. A fairly good agreement is obtained at lower scattering length but serious differences occur at large a values. But it is expected that the chemical potential obtained by numerically solving the MGP equation should become closer and closer to the modified Thomas-Fermi values when a increases, since with increasing a the scattering energy part grows with respect to kinetic energy. According to ref[4] modified Thomas-Fermi (MTF) equation which is nonlinear in density loses the property of having analytical solution except at the very first step of iterative procedure [MTF(1)]. We have taken up this work to show that how far the iterative procedure can be extended beyond first order to give the correct analytical solution of MTF equation. We begin by solving the modified TF equation analytically by considering the m th order of iteration to give converged value of chemical potential (μ) and then this value of chemical potential is substituted in the MTF equation to get the value of the density of particles using higher order iterative method until the value of density of particles is converged. Here we have compared the results of our analytical approach with those obtained by solving the modified GP equation numerically (considering spherically symmetric trap) in a case where the number of atoms are kept fixed and scattering length is varied in a range of values so that $10^{-3} \leq x_{pk} \leq 10^{-2}$. MGP equation has been solved by Runge-Kutta method [7] in case of spherical trap with an oscillator angular frequency same as in ref[4]. We find that the analytical results under MTF approach beyond the first step iteration are in very good agreement with the numerical MGP results at low as well as at high scattering lengths. The deviations between analytical MTF and numerical MGP results for peak gas parameter ($10^{-3} < x_{pk} < 10^{-2}$) is within 1% throughout the range of variation in a and for chemical potential this deviation further decreases with increasing a . Analytical expression for the frequency of the monopole mode of spherically trapped bosons including the LHY term in the correlation energy have been derived previously [5] considering the solution of MTF equation in the very first step of iterative process. But their analytical results are systematically higher than their variational results and the difference between the two increases as the value of gas-parameter increased. In our work, the collective oscillation frequencies are obtained by using sum-rule approach [18,19] of many-body response theory as used in Ref.[5]. In the sum-rule approach the knowledge of ground-state wave function (i.e, ground state density of particles) is sufficient to calculate the excitation frequency. Keeping this in mind, our aim is to find out the value of excitation frequency within TF approximation using the analytical values of ground state density (derived in higher order iterative method). Our results are in excellent agreement with the variational results of [5] and the agreement becomes better with increasing values of gas-parameter up to 10^{-2} .

This attempt to get the analytical values of chemical potential, particle density as a function of distance from the centre of a spherically symmetric trap and the excitation frequency of the monopole mode by using higher order iterative method for solving modified Thomas-Fermi equation has been found to be adequate for successfully reproducing the numerical MGP results up to a large value of peak-gas-parameter $\sim 10^{-2}$. This new analytical approach can be useful in finding out the properties of BEC of atoms up to a quite large gas-parameter $\sim 10^{-2}$.

2. Theory

A system of N bosons at $T=0$ temperature is described by the Hamiltonian,

$$H = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_i V_{trap}(\mathbf{r}_i) + \sum_{i<j} V(\mathbf{r}_{ij}) \quad (1)$$

where, $V_{trap}(\mathbf{r}_i)$ is the external confining trap potential, $V(\mathbf{r}_{ij})$ is the interatomic potential and m is the mass of the atom. The energy functional as a function of density of particles n is given by,

$$E[n] = \int d\mathbf{r} \left[\frac{\hbar^2}{2m} \sqrt{n(\mathbf{r})} \nabla^2 \sqrt{n(\mathbf{r})} + V_{trap}(\mathbf{r})n(\mathbf{r}) + \epsilon(n)n(\mathbf{r}) \right] \quad (2)$$

where first, second and third term represent the kinetic energy of the bosons, the energy due to the trapping potential and the energy due to the interatomic correlation, respectively. In the case of a uniform hard sphere bose gas the perturbation expansion of correlation energy density $\epsilon(n)$ in terms of na^3 by means of low density expansion [8] is,

$$\epsilon(n) = \frac{E}{N} = \frac{2\pi\hbar^2 a n}{m} \left[1 + \frac{128}{15\sqrt{\pi}} (na^3)^{1/2} \right] \quad (3)$$

Here the atom is treated as a hard sphere and a is the diameter of the hard sphere which coincides with the scattering length. The first term in the above expansion corresponds to the energy of the homogeneous Bose gas within mean field theory as considered in GP theory, was calculated by Bogoliubov [9]. The second term was obtained by Lee, Huang, Yang (LHY) [10] using hard sphere model for interatomic potential. From equation (3) one can get energy density as

$$\frac{E}{V} = \frac{2\pi\hbar^2 a n^2}{m} \left[1 + \frac{128}{15\sqrt{\pi}} (na^3)^{1/2} \right] \quad (4)$$

where $n = \frac{N}{V}$, N is the total number of particles in the volume V .

The energy functional associated with the GP theory is obtained in the local-density-approximation (LDA) by keeping only first term of equation(4)

$$E_{GP}[\psi] = \int d\mathbf{r} \left[\frac{\hbar^2}{2m} |\nabla\psi(\mathbf{r})|^2 + V_{trap}(\mathbf{r})|\psi(\mathbf{r})|^2 + \frac{2\pi\hbar^2 a}{m} |\psi(\mathbf{r})|^4 \right] \quad (5)$$

where the wave function $\psi(\mathbf{r})$ is normalized to the total number of atoms

$$N = \int d\mathbf{r} |\psi(\mathbf{r})|^2 = \text{constant} \quad (6)$$

By performing functional variation of $E_{GP}[\psi]$ one finds the Euler-Lagrange equation

$$\delta E - \mu dN = 0$$

$[\mu$ ensures the constancy of particle number] which is known as the Gross-Pitaevskii (GP) equation:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m} |\psi|^2 \right] \psi(\mathbf{r}) = \mu \psi(\mathbf{r}) \quad (7)$$

where μ is the chemical potential.

Within LDA theory, including the next term of equation(4) into the energy functional, we obtain modified Gross-Pitaevskii (MGP) energy functional,

$$E_{MGP}[\psi] = \int \mathbf{dr} \left[\frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r})|^2 + V_{trap}(\mathbf{r}) |\psi(\mathbf{r})|^2 + \frac{2\pi\hbar^2 a}{m} |\psi(\mathbf{r})|^4 \right. \\ \left. \times \left(1 + \frac{128}{15\sqrt{\pi}} (|\psi(\mathbf{r})|^2 a^3)^{1/2} \right) \right] \quad (8)$$

The functional variation gives rise to the so called MGP equation [4,11,17] as:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m} |\psi|^2 \left(1 + \frac{32a^{3/2}}{3\sqrt{\pi}} |\psi| \right) \right] \psi(\mathbf{r}) = \mu \psi(\mathbf{r}) \quad (9)$$

Here $\psi(\mathbf{r})$ is normalized to total number of particles N, hence $\psi(r)$ can be written as,

$\psi(\mathbf{r}) = \sqrt{N} \psi_1(\mathbf{r})$, where $\psi_1(\mathbf{r})$ is normalized to unity i.e. $\int \mathbf{dr} |\psi_1(\mathbf{r})|^2 = 1$

In terms of $\psi_1(\mathbf{r})$, the GP and MGP equations take the form as follows:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) + \frac{4\pi\hbar^2 Na}{m} |\psi_1|^2 \right] \psi_1(\mathbf{r}) = \mu \psi_1(\mathbf{r}) \quad (10)$$

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) + \frac{4\pi\hbar^2 Na}{m} |\psi_1|^2 \left(1 + \frac{32N^{1/2}a^{3/2}}{3\sqrt{\pi}} |\psi_1| \right) \right] \psi_1(\mathbf{r}) = \mu \psi_1(\mathbf{r}) \quad (11)$$

We have solved eqs (10) and (11) numerically by using Runge-Kutta method for chemical potential and density of particles. We have also derived analytical expressions for chemical potential and density of particles from TF and MTF equations obtained by neglecting K.E. term from eqs (10) and (11).

2.1. Iterative analysis within Thomas-Fermi Approximation

A Thomas-Fermi (TF) approach to the GP and MGP equation was proposed earlier in ref[6], by neglecting the kinetic energy term of equations (7) and (9). Equation (7) takes the form in TF limit as,

$$V_{trap}(\mathbf{r}) \psi(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m} |\psi(\mathbf{r})|^2 \psi(\mathbf{r}) = \mu \psi(\mathbf{r}) \quad (12)$$

Writing $|\psi(\mathbf{r})|^2$ as particle density, we get,

$$n(\mathbf{r}) = \frac{\mu - V_{trap}(\mathbf{r})}{\frac{4\pi\hbar^2 a}{m}} = n_{TF}(\mathbf{r}) \quad (13)$$

The normalization condition implies that,

$$\mu_{TF} = \frac{\hbar\omega}{2} (15N\bar{a})^{2/5} \quad (14)$$

where $\bar{a} = a/\sqrt{\frac{\hbar}{m\omega}}$

In TF limit MGP equation takes the following form:

$$g \times n(\mathbf{r}) + g \times \frac{32}{3\sqrt{\pi}} n(\mathbf{r})^{3/2} a^{3/2} = \mu - V_{trap}(\mathbf{r}) \quad (15)$$

where $g = 4\pi\hbar^2 a/m$

In ref[6], equation(15) was solved by first order iteration method [MTF(1)] to give,

$$n(\mathbf{r}) = g^{-1}[\mu - V_{trap}(\mathbf{r})] - \frac{4m^{3/2}}{3\pi^2\hbar^3}[\mu - V_{trap}(\mathbf{r})]^{3/2}$$

and imposing normalization condition (for a spherical trap with angular frequency ω i.e., $V_{trap}(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2$) they obtained

$$\mu_{MTF(1)} = \mu_{TF}[1 + \sqrt{\pi a^3 n(0)}] \quad (16)$$

where, $a^3 n(0) = \frac{15^{2/5}}{8\pi}(N^{1/6}\bar{a})^{2/5}$

We solve equation (15) following an iteration method going beyond the first step and extended it to the mth order to obtain the analytical expression for $n(r)$ given as follows :

$$n(\mathbf{r}) = g^{-1}[\mu - V_{trap}(\mathbf{r})] - \frac{4m^{3/2}}{3\pi^2\hbar^3}[\mu - V_{trap}(\mathbf{r})]^{3/2} \times (1 - x \times (1 - x \times (1 - x \times \dots x \times (1 - x \times \dots \times ((m-1)^{th} term)^{3/2})^{3/2})^{3/2} \dots)^{3/2} \dots up \quad to \quad (m-1)th)^{3/2} \quad (17)$$

where $x = \frac{16m^{1/2}a}{3\pi\hbar}(\mu - V_{trap}(\mathbf{r}))^{1/2}$

Hence from eq.(17) using the normalization condition [eq.(6)] the equation for μ is obtained as (for mth order iteration) :

$$\begin{aligned} & C_1 \times F(k=-1)\mu^{\frac{5}{2}} + C_2 \times [F(k=0)\mu^3 - \sum_{k_1=1}^{n_1} C_{k_1, \frac{3}{2}} b^{k_1} \times [(\hbar\omega)^{\frac{k_1}{2}} F(k_1)\mu^{(\frac{k_1}{2}+3)} + \\ & \sum_{k_2=1}^{n_2} C_{k_2, \frac{3}{2}} b^{k_2} \times [(\hbar\omega)^{\frac{k_1+k_2}{2}} F(k_1+k_2)\mu^{(\frac{k_1+k_2}{2}+3)} + \sum_{k_3=1}^{n_3} C_{k_3, \frac{3}{2}} b^{k_3} \times [(\hbar\omega)^{\frac{k_1+k_2+k_3}{2}} F(k_1+k_2+k_3) \times \\ & \mu^{(\frac{k_1+k_2+k_3}{2}+3)} + \dots + \sum_{k_{m-2}=1}^{n_{m-2}} C_{k_{m-2}, \frac{3}{2}} b^{k_{m-2}} \times [(\hbar\omega)^{\frac{k_1+k_2+\dots+k_{m-2}}{2}} F(k_1+k_2+\dots+k_{m-2}) \times \\ & \mu^{(\frac{k_1+k_2+\dots+k_{m-2}}{2}+3)} + \sum_{k_{m-1}=1}^{n_{m-1}} C_{k_{m-1}, \frac{3}{2}} b^{k_{m-1}} (\hbar\omega)^{\frac{k_1+k_2+\dots+k_{m-1}}{2}} F(k_1+k_2+\dots+k_{m-1}) \times \\ & \mu^{(\frac{k_1+k_2+\dots+k_{m-1}}{2}+3)}] \dots] \dots up \quad to \quad (m-1)th] = N \end{aligned} \quad (18)$$

where,

$$C_1 = \frac{2\sqrt{2}\hbar^{1/2}}{am^{1/2}\omega^{1/2}}$$

$$C_2 = -\frac{32\sqrt{2}}{3\pi}$$

$$and \quad b = -\frac{16m^{1/2}a}{3\pi\hbar},$$

and $C_{k_1, \frac{3}{2}}, C_{k_2, \frac{3}{2}}, C_{k_3, \frac{3}{2}}, \dots, C_{k_{m-1}, \frac{3}{2}}$ etc. are binomial coefficients for general expansion given as

$$(1-y)^{\frac{3}{2}l} = \sum_{l_1=0}^{\infty} \frac{(\frac{3}{2}l)!}{(\frac{3}{2}l-l_1)!l_1!} y^{l_1} = \sum_{l_1=0}^{\infty} C_{l_1, \frac{3}{2}l} y^{l_1}$$

$$F(k) = \left[\frac{2^{(k+3)} \left\{ \left(\frac{k+3}{2} \right)! \right\}^2}{(k+4)!} - \frac{2^{(k+5)} \left\{ \left(\frac{k+5}{2} \right)! \right\}^2}{(k+6)!} \right]$$

(for $k=-1,1,3,5,7,\dots$)

and

$$F(k) = \frac{\pi}{2} \left[\frac{(k+4)!}{2^{(k+4)} \left\{ \left(\frac{k+4}{2} \right)! \right\}^2} - \frac{(k+6)!}{2^{(k+6)} \left\{ \left(\frac{k+6}{2} \right)! \right\}^2} \right]$$

(for $k=0,2,4,6,8,\dots$)

The derivation of eq.(18) from eq.(17) requires binomial series expansion in the form of $(1-y)^{\frac{3}{2}l}$ where 'y' takes the form $x, x(1-x)^{3/2}, x(1-x(1-x)^{3/2})^{3/2}, \dots$ etc. Thus the validity of eq.(18) is based on the criterion $-1 < y < 1$ which implies $-1 < x < 1$.

From eq.(18) summing the coefficients of the same power of μ we get,

$$\sum_{j=1}^{j_{max}} C'_j \mu^{2+\frac{j}{2}} = N \quad (19)$$

where C'_j 's are the sum of the coefficients of $\mu^{(2+\frac{j}{2})}$ and are functions of a , m and ω . μ 's are in the unit of $\hbar\omega$.

Here the value of j_{max} depends on the chosen values of $n_1, n_2, n_3, \dots, n_{m-1}$ in eq.(18). Equation (19) can be solved by the method of successive iteration with the initial value of $\mu = \mu_{TF}$ and continue the process until one gets the convergence in the final value of μ , which is denoted by $\mu_{MTF(m)}$. The expression for $\mu_{MTF(1)}$ (as in eq.(16)) can also be obtained by considering only the first two terms of eq.(19) and then adopting a first order iterative process. Similarly by extending eq.(17) to p th order one can calculate the value of particle density such that the value of $n(r)$ is converged. We have used the value of $\mu = \mu_{MTF(m)}$ to calculate $n(r)$. The peak values of gas parameter (x_{pk}) can also be computed analytically. The expression for peak values of gas parameter are given as follows:

$$x_{pk,MTF(1)} = [n_{MTF(1)}(0)]a^3, \quad x_{pk,MTF(p)} = [n_{MTF(p)}(0)]a^3$$

In principle the value x may lie between -1 to +1, but as $x \rightarrow 1 (> 0.7)$ a large number of iterations is required to get convergence in the value of $\mu_{MTF(m)}$ and $n_{MTF(r)}$.

We have compared our analytical results of MTF equation (using higher order iteration) with the numerical results of MGP equation which is solved by Runge-Kutta method as was used previously for solving the GP equation [12].

2.2. Numerical Analysis

The BEC ground state wave function is spherically symmetric for an isotropic trap, so we need to consider only the radial part of the wave function, which can be written in the form

$$\psi_1(r) = A \frac{\phi(r)}{r} \quad (20)$$

where A is a constant used to ensure proper normalization. Inserting eq (20) into eq.(10) and eq.(11) give,

$$\begin{aligned} & -\frac{\hbar^2}{2m} \frac{d^2\phi}{dr^2} + \frac{1}{2}m\omega^2 r^2 \phi(r) + \frac{4\pi\hbar^2 a}{m} N A^2 \frac{\phi^2(r)}{r^2} \phi(r) = \mu \phi(r) \\ & -\frac{\hbar^2}{2m} \frac{d^2\phi}{dr^2} + \frac{1}{2}m\omega^2 r^2 \phi(r) + \frac{4\pi\hbar^2 a}{m} N A^2 \frac{\phi^2(r)}{r^2} \phi(r) + \frac{128}{3} \sqrt{\pi a^5} \frac{\hbar^2}{m} N^{3/2} A^3 \frac{|\phi(r)|^3}{r^3} \phi(r) \end{aligned} \quad (21)$$

$$= \mu\phi(r) \quad (22)$$

GP equation i.e., eq(21) is solved by Runge-Kutta method [7] for the isotropic trap previously described in ref[12]. The MGP equation i.e., eq (22) has been solved using the similar method described below. It is convenient to use dimensionless variables defined by,

$r = x \times a_{ho}$ and $\beta = \frac{\mu}{\hbar\omega}$ where $a_{ho} = \sqrt{\frac{\hbar}{2m\omega}}$. In terms of these variables eq (22) becomes

$$\frac{d^2\phi}{dx^2} + [\beta - \frac{1}{4}x^2 - NA^2\gamma\frac{\phi^2(x)}{x^2} - \alpha A^3N^{3/2}\frac{\phi^3(x)}{x^3}]\phi(x) = 0 \quad (23)$$

where $\gamma = 8\pi a$, $\alpha = 256\frac{\sqrt{2\pi}}{3}\sqrt{\frac{m\omega}{\hbar}}a^{5/2}$. From the normalization of $\psi_1(\mathbf{r})$ one gets

$$4\pi(\frac{\hbar}{2m\omega})^{1/2}A^2\int_0^\infty |\phi(x)|^2dx = 1 \quad (24)$$

Boundary condition

For a confined condensate, at a sufficiently large r , the full wave function $\psi_1(r)$ must vanish asymptotically. Hence nonlinear terms proportional to $|\phi(x)|^3$ and $|\phi(x)|^4$ can be neglected and eq (23) takes the form as $x \rightarrow \infty$

$$\frac{d^2\phi}{dx^2} + [\beta - \frac{1}{4}x^2]\phi(x) = 0 \quad (25)$$

The asymptotic form of the physically acceptable solution (which goes to zero as $x \rightarrow \infty$) of eq (25) has the form

$$\phi(x) \sim C \exp[-\frac{x^2}{4} + (\beta - \frac{1}{2})\ln(x)] \quad (26)$$

C is a normalization constant.

As $x \rightarrow 0$, the nonlinear terms approach constant values in the limit due to regularity of the wave function at $x=0$. Thus, $\phi(x) \approx \phi'(0)x$ (as $x \rightarrow 0$) and $\phi(x)$ must vanish at $x=0$. Hence eq (23) is approximated (in the limit $x \rightarrow 0$) as

$$\frac{d^2\phi}{dx^2} + [\beta - NA^2\gamma\phi'(0)^2 - \alpha A^3N^{3/2}\phi'(0)^3]\phi(x) = 0 \quad (27)$$

The solution of eq (27) is

$$\phi(x) = A_1 \cos(m_1 x) + A_2 \sin(m_1 x)$$

where $m_1 = [\beta - NA^2\gamma\phi'(0)^2 - \alpha A^3N^{3/2}\phi'(0)^3]^{\frac{1}{2}}$,

The boundary condition at $x = 0$, $\phi(0) = 0$ gives $A_1 = 0$

Therefore $\phi(x)$ can be obtained as

$$\phi(x) = A_2 \sin(m_1 x)$$

and hence

$$\phi'(x) = m_1 A_2 \cos(m_1 x)$$

Therefore as $x \rightarrow 0$,

$$\phi'(0)^2 \approx [\beta - NA^2\gamma\phi'(0)^2 - \alpha A^3N^{\frac{3}{2}}\phi'(0)^3]$$

or

$$\phi'(0)^3 + \frac{NA^2\gamma + 1}{N^{\frac{3}{2}}A^3\alpha}\phi'(0)^2 - \frac{\beta}{N^{\frac{3}{2}}A^3\alpha} \approx 0 \quad (28)$$

To solve eq (28) let us consider

$$\begin{aligned} R &= \frac{(NA^2\gamma + 1)^3}{27N^{9/2}A^9\alpha^3} - \frac{\beta}{2N^{3/2}A^3\alpha} \\ Q &= \frac{(NA^2\gamma + 1)^2}{9N^3A^6\alpha^2} \\ s &= \frac{(NA^2\gamma + 1)}{N^{3/2}A^3\alpha} \\ \theta &= \cos^{-1} \frac{R}{\sqrt{Q^3}} \end{aligned}$$

For $R^2 < Q^3$ there are three possible values of $\phi'(0)$:

$$\begin{aligned} -2\sqrt{Q}\cos\left(\frac{\theta}{3}\right) - \frac{s}{3} \\ -2\sqrt{Q}\cos\left(\frac{\theta + 2\pi}{3}\right) - \frac{s}{3} \end{aligned}$$

and

$$-2\sqrt{Q}\cos\left(\frac{\theta - 2\pi}{3}\right) - \frac{s}{3}$$

and for $R^2 > Q^3$, $\phi'(0) = s_1 + s_2 - \frac{s}{3}$

where $s_1 = [-R + (-Q^3 + R^2)^{1/2}]^{1/3}$ and $s_2 = [-R - (-Q^3 + R^2)^{1/2}]^{1/3}$

Out of these solutions we have chosen the one which gives $\phi'(0) > 0$ and leads to the correct nature of variation of the wave function with r. The other boundary conditions satisfied by $\phi(x)$ are:

$\phi(x) = 0$ as $x \rightarrow 0$ and for $x \rightarrow \infty$,

$$\phi(x) \sim \exp\left[-\frac{x^2}{4} + \left(\beta - \frac{1}{2}\right)\ln(x)\right] = \phi_{asym}(x)$$

$$\phi'(x) \sim \left[-\frac{x}{2} + \left(\beta - \frac{1}{2}\right)\frac{1}{x}\right] \times \phi_{asym}(x) = \phi'_{asym}(x)$$

The boundary conditions said above together with the normalization condition form the basis of the numerical integration technique.

Numerical Integration Technique

When N , γ , β , α and A are assigned numerical values, both $\phi(0)$ and $\phi'(0)$ can be determined. Numerical integration of eq. (23) can be performed using Fourth order Runge-Kutta method up to large values of $x = x_m$. We held the values of N, γ and β constant and vary A to get the solution which satisfies the boundary conditions both at $x=0$ and at large x . For a given A , wronskian $W = (\phi_{num}(x) \times \phi'_{asym}(x) - \phi_{asym}(x) \times \phi'_{num}(x))$ is computed at $x = x_m$. The value of A is varied until W changes its sign. Let the value of A be A_0 when $W=0$ and the corresponding solution $\phi_{num}(A_0, N_0; x)$ satisfies all the boundary conditions except the normalization criterion. Let the wave functions $\phi_{num}(A_0, N_0; x)$ and $\phi_{num}(A_1, N_1; x)$ are the solutions of the equations:

$$\frac{d^2\phi_{num}(A_0, N_0; x)}{dx^2} + \left[\beta - \frac{x^2}{4} - N_0A_0^2\gamma\frac{\phi_{num}^2(A_0, N_0; x)}{x^2}\right]$$

$$-\frac{\alpha A_0^3 N_0^{3/2} \phi_{num}^3(A_0, N_0; x)}{x^3}] \phi_{num}(A_0, N_0; x) = 0$$

and

$$\begin{aligned} \frac{d^2 \phi_1(A_1, N_1; x)}{dx^2} + [\beta - \frac{x^2}{4} - N_1 A_1^2 \gamma \frac{\phi_1^2(A_1, N_1; x)}{x^2} \\ - \frac{\alpha A_1^3 N_1^{3/2} \phi_1^3(A_1, N_1; x)}{x^3}] \phi_1(A_1, N_1; x) = 0 \end{aligned}$$

The two solutions will be the same if $N_0 A_0^2 = N_1 A_1^2$ i.e., $\phi_1(A_1, N_1; x) = \phi_{num}(A_0, N_0; x)$ But the full wave functions will be different,

$$\psi_0(A_0, N_0; r) = \frac{A_0}{r} \phi_{num}(A_0, N_0; r)$$

$$\psi_1(A_1, N_1; r) = \frac{A_1}{r} \phi_{num}(A_1, N_1; r) = \frac{A_1}{r} \phi_{num}(A_0, N; r) \quad (29)$$

where A_1 is determined from the normalization condition,

$$A_1 = [4\pi \times (\frac{\hbar}{2m\omega})^{1/2} \int_0^\infty |\phi_{num}(A_0, N_0; x)|^2 dx]^{-1/2} \quad (30)$$

and

$$N_1 = (\frac{A_0}{A_1})^2 N_0 \quad (31)$$

and the final solution of the MGP equation is given by,

$$\psi_1(A_1, N_1; r) = \frac{A_1}{r} \phi_{num}(A_0, N_0; r)$$

where $\phi_{num}(A_0, N_0; r)$ and A_0 are obtained numerically from Runge-Kutta integration, A_1 is determined later from eq.(30) and N_1 from eq.(31). It is to be mentioned here that for a particular scattering length, starting with any value of N_0 ; one can get a fixed value of N_1 , total number of particles by varying the value of μ in the MGP equation.

In the Runge-Kutta method, larger nonlinearity leads to an exponentially divergent solution in the asymptotic region which was mentioned earlier [13]. Thus the numerical instability restricts us to find the ground state solutions for GP and MGP equation up to the value of the gas parameter $\sim 10^{-2}$.

3. Calculation of frequency of the monopole mode of a condensate in a spherically symmetric trap using analytical ground state wave functions

According to ref.[5] lowest excitation frequency of the monopole mode of bosons in a spherical trap within Thomas-Fermi (TF) approximation can be written as :

$$\frac{\Omega^2}{(\omega)^2} = 2 \times [\frac{U + \frac{9}{4} E_{int}^1 + \frac{81}{16} E_{int}^2}{U}] \quad (32)$$

where E_{int}^1 and E_{int}^2 give interaction energy per particle in the mean-field approximation as considered in the GP theory and the correction in the interaction energy due to LHY term in the expansion (3) respectively. Sum-rule approach [18,19] of many-body system has been used to derive the frequency of collective oscillation. Using virial relation [5,20]

$$2T - 2U + 3E_{int}^1 + \frac{9}{2} E_{int}^2 = 0 \quad (33)$$

U can be eliminated from eq.(32) to give :

$$\frac{\Omega^2}{(\omega)^2} = 2 \times \left[\frac{\frac{15}{4}E_{int}^1 + \frac{117}{16}E_{int}^2}{\frac{3}{2}E_{int}^1 + \frac{9}{4}E_{int}^2} \right] \quad (34)$$

The interaction energy E_{int}^1 and E_{int}^2 are given by

$$E_{int}^1 = \frac{2\pi\hbar^2 a}{m} \int d\mathbf{r} |\psi(\mathbf{r})|^4 \quad (35)$$

and

$$E_{int}^2 = \frac{2\pi\hbar^2 a}{m} \frac{128}{15} \left(\frac{a^3}{\pi}\right)^{1/2} \int d\mathbf{r} |\psi(\mathbf{r})|^5 \quad (36)$$

The ground state wave function [$\psi(\mathbf{r}) = \sqrt{n(\mathbf{r})}$] derived analytically as in the section (2.1) are substituted in the eqs (35) and (36) to get the values of E_{int}^1 and E_{int}^2 and then the value of the frequency of the monopole mode of bosons is obtained from eq (34). Our results have been compared with the results obtained from MTF(1) (eq (21) of Ref.[5]) and the variational beyond GP (BGP) results of Ref.[5] in section 4.

4. Results and Discussion

For numerical and analytical calculations we consider the spherical trap with oscillation angular frequency $\frac{\omega}{2\pi} = \frac{(w_z^2 \omega_z)^{1/3}}{2\pi} = 12.83\text{Hz}$ where, $\frac{\omega_r}{2\pi} = 17.5\text{Hz}$ and $\frac{\omega_z}{2\pi} = 6.9\text{Hz}$ are the radial and axial frequencies associated with the cylindrical trap as used in ref [4]. The scattering length is varied from $3000 a_0$ to $7000 a_0$, a_0 being the Bohr radius of hydrogen atom and the number of confining atoms $N = 10^3$ [14-16] in order to avoid numerical instability in the Runge-Kutta method that arises from sufficiently large nonlinearity in the GP and MGP equation [13]. However to get a feeling of direct comparison of our results (numerical and analytical) with ref.[4] we list here also the MGP and analytical MTF results for $a=1400$ and $3000 a_0$ for $N=10^4$ ^{85}Rb atoms. For $a=4000 a_0$ we have tabulated the values of MTF(1) and MTF(m) only since the results for MGP is not available. The largest value of x used in our calculation is 0.65 and the largest number of iterations required for getting convergence in the value of μ is 13 and that in $n(\mathbf{r})$ is 62. However as $x \rightarrow 1$, further higher order of iterations are required to get convergence in μ .

In TABLE-1, dependence of chemical potential(μ) and peak gas parameter (x_{pk}) (found in MTF(1), higher order MTF and numerical MGP approaches) on scattering length a are shown keeping N fixed at 10^3 . GP and TF results are also tabulated. Comparative study yields the following results.

- (1) As expected GP and TF results are much closer to each other as a increases.
- (2) A good agreement between MTF(1) and MGP values at lower scattering length. At $a=3000 a_0$ deviations of $\mu_{MTF(1)}$ from μ_{MGP} is 1.6% and that for the value of x_{pk} is 8.2%. But with increase in the value of a , deviations in the values of μ and x_{pk} increase. At $a=7000 a_0$ $\mu_{MTF(1)}$ becomes greater than μ_{MGP} by 2.38% and the value of x_{pk} for MTF(1) is even worse, the disagreement is 54.3%.
- (3) The analytical values of chemical potential obtained from MTF equation using high order(m) of iterations become closer to μ_{MGP} with increasing values of a , since kinetic energy becomes much smaller than the interaction energy for large a . The value of $\mu_{MTF(m)}$ deviate from that of μ_{MGP} by 2.3% at $a=3000 a_0$ and by 0.87% at $a=7000 a_0$, whereas this deviation in the values of x_{pk} is 1% at $a=3000 a_0$ and 0.09 % at $a=7000 a_0$. In notations $\mu_{MTF(m)}$ and $x_{pk,MTF(p)}$ 'm' and 'p' indicate the separate order of iterations. Higher order of iterations is

Table 1. Ground State properties of $N=10^3$ ^{85}Rb atoms confined in a spherical trap ($\frac{\omega}{2\pi}=12.83$ Hz) in GP, TF, MGP, MTF(1) and higher order MTF approaches. μ =chemical potential, x_{pk} =peak gas-parameter, μ 's are in $\hbar\omega$ unit

a (a_0)	3000	5000	6000	7000
μ_{GP}	7.370	8.9710	9.630	10.225
μ_{TF}	7.1825	8.8109	9.4774	10.080
μ_{MGP}	7.8140	9.9150	10.8550	11.7464
$\mu_{MTF(m)}$	7.6351	9.7654	10.7113	11.6434
$\mu_{MTF(1)}$	7.6844	9.9470	10.990	12.0270
$x_{pk,GP}$	1.571×10^{-3}	5.3378×10^{-3}	8.2609×10^{-3}	1.1951×10^{-2}
$x_{pk,TF}$	1.5539×10^{-3}	5.2951×10^{-3}	8.2018×10^{-3}	1.1873×10^{-2}
$x_{pk,MGP}$	1.3668×10^{-3}	4.2505×10^{-3}	6.3189×10^{-3}	8.8018×10^{-3}
$x_{pk,MTF(p)}$	1.3525×10^{-3}	4.2194×10^{-3}	6.2769×10^{-3}	8.7932×10^{-3}
$x_{pk,MTF(1)}$	1.2545×10^{-3}	3.1964×10^{-3}	3.9289×10^{-3}	4.0192×10^{-3}

Table 2. Ground State properties of $N=10^4$ ^{85}Rb atoms confined in a spherical trap ($\frac{\omega}{2\pi}=12.83$ Hz) in GP, TF, MGP, MTF(1) and higher order MTF approaches. μ =chemical potential, x_{pk} =peak gas-parameter, μ 's are in $\hbar\omega$ unit

a (a_0)	1400	3000	4000
μ_{GP}	13.4170 (13.42)*	- (18.13)*	-
μ_{TF}	13.30	18.04	20.242
μ_{MGP}	13.962 (13.97)*	- (19.84)*	-
$\mu_{MTF(m)}$	13.852	19.768	22.832
$\mu_{MTF(1)}$	13.89	20.039	23.408
$x_{pk,GP}$	6.293×10^{-4} (6.30×10^{-4})*	- (3.91×10^{-3})*	-
$x_{pk,TF}$	6.266×10^{-4}	3.91×10^{-3}	7.785×10^{-3}
$x_{pk,MGP}$	5.729×10^{-4} (5.73×10^{-4})*	- (3.20×10^{-3})*	-
$x_{pk,MTF(p)}$	5.705×10^{-4}	3.192×10^{-3}	5.991×10^{-3}
$x_{pk,MTF(1)}$	5.537×10^{-4}	2.617×10^{-3}	3.862×10^{-3}

()* = results from ref.[4]

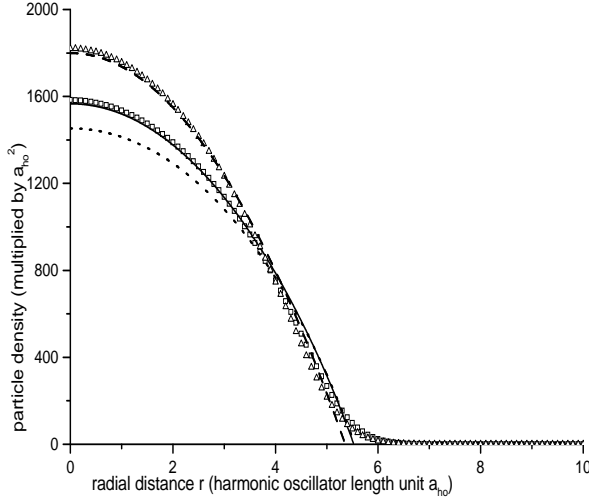


Figure 1. Condensate particle densities of ^{85}Rb atoms ($n_1(r)$) multiplied by a_{ho}^2 as a function of radial distance at $a=3000 a_0$ and $N=10^3$ for spherically symmetric trap $\frac{\omega}{2\pi}=12.83$ Hz ($\frac{\omega_\perp}{2\pi}=17.5$ Hz, $\frac{\omega_z}{2\pi}=6.9$ Hz). \triangle = GP, - - - = TF, \square = MGP, \cdots = MTF(1), —=MTF(p) (see text). Horizontal axis is scaled in harmonic oscillator length units whose value is given by, $a_{ho} = (\frac{\hbar}{2m\omega})^{1/2}$.

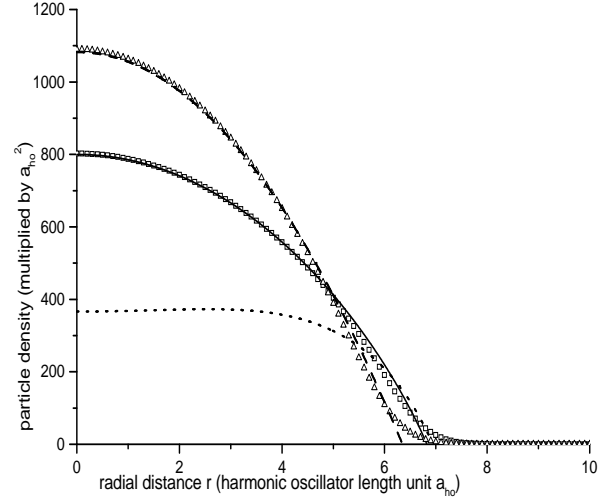


Figure 2. Condensate particle densities of ^{85}Rb atoms ($n_1(r)$) multiplied by a_{ho}^2 as a function of radial distance at $a=7000 a_0$. The other parameters are same as in Figure 1.

required to give convergence in the value of $n_{MTF(p)}(0)$ than that in $\mu_{MTF(m)}$ i.e. $p > m$. Unlike $\mu_{MTF(1)}$, the values of $\mu_{MTF(m)}$ is always less than those of μ_{MGP} with increase in a .

We have calculated the convergence parameter (for μ in the m th order iterative method) defined as $\epsilon = |\frac{\mu(m)-\mu(m-1)}{\mu(m)}| \times 100\%$. For $a=3000 a_0$ $m=8$ and $\epsilon = 0.001\%$ and The value of ϵ is of the same order up to $a=6000 a_0$. However for $a=7000 a_0$, $\epsilon = 0.27\%$ and $m=13$. TABLE-2 summarizes the results for $N=10^4$ Rb^{85} atoms which shows that our results are in good agreement with those of ref[4] (presented in parenthesis in Table-2) for $a=1400 a_0$ and $3000 a_0$.

In Fig 1 and Fig 2, the variation of particle density $n_1(r) = |\psi_1(r)|^2 = \frac{|\psi(r)|^2}{N} = \frac{n(r)}{N}$ with radial distance from the centre of the spherical trap has been shown for $a=3000 a_0$ and $7000 a_0$ respectively. Different results obtained from numerical and different analytical calculations as mentioned above for $N=10^3$ atoms have been plotted. Squares, dotted and solid lines correspond to MGP, MTF(1) and MTF(p) results, respectively. Triangles and dashed lines are GP and TF densities.

For a fixed value of a ($= 7000a_0$) and $N = 10^3$, at higher values of 'r' ($> 5a_{ho}$) to get convergence in $n_1(r)$ up to sixth decimal place 62 order of iterations are required. However at smaller 'r', convergence in $n_1(r)$ up to second decimal place is sufficient. To achieve the convergence up to second decimal place in $n_1(r=0)$ at $a = 7000a_0$ and $N = 10^3$ the iterative process needs to be extended up to $p = 40$ and the value of $n_1(r=0)$ obtained for 40 iterations differs from previous value (for 62 iterations) by 0.003%. This difference increases with increasing 'r' and becomes 0.08% at $r = 6.8a_{ho}$. The deviations between GP and TF particle densities are prominent in surface region where the kinetic energy becomes important. The particle densities

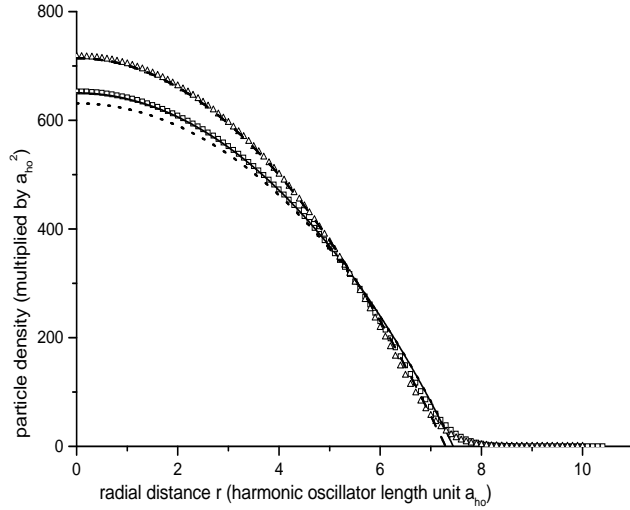


Figure 3. Condensate particle densities of ^{85}Rb atoms ($n_1(r)$) multiplied by a_{ho}^2 as a function of radial distance at $a=1400 a_0$ and $N=10^4$ for spherically symmetric trap $\frac{\omega}{2\pi}=12.83$ Hz ($\frac{\omega_{\perp}}{2\pi}=17.5$ Hz, $\frac{\omega_z}{2\pi}=6.9$ Hz). \triangle = GP, - - - = TF, \square = MGP, \cdots = MTF(1), —=MTF(p) (see text). Horizontal axis is scaled in harmonic oscillator length units whose value is given by, $a_{ho} = (\frac{\hbar}{2m\omega})^{1/2}$.

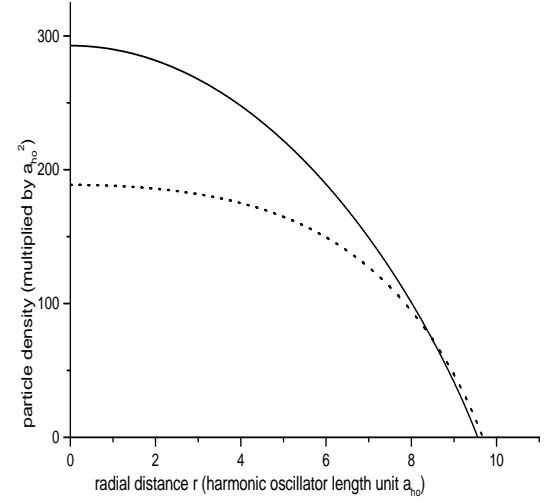


Figure 4. Condensate particle densities of ^{85}Rb atoms ($n_1(r)$) multiplied by a_{ho}^2 as a function of radial distance at $a=4000 a_0$. The other parameters are same as in Figure 2. \cdots =MTF(1), —=MTF(p) (see text).

obtained from analytical MTF(p) approach and numerical MGP calculations are almost identical (disagreement is at most $< 5\%$) up to $r=4a_{ho}$ for $a=3000 a_0$ and up to $r=5.4 a_{ho}$ for $a=7000 a_0$ for $N=10^3$. This shows that the agreement between particle density curves for MTF(p) and MGP are getting better with increasing a . Whereas the disagreement between curves from MTF(1) and MGP calculations is prominent even for small value of $a=3000 a_0$ and it increases with increase in the value of a . In Fig 3 and Fig 4, the particle density profiles are plotted for $N=10^4$ at $a=1400$ and $4000 a_0$ respectively and both the curves (MGP and MTF(p)) show similar trends for $a=1400 a_0$. At $a=4000 a_0$ the numerical MGP result is absent, but the deviation of particle density curves for MTF(1) and MTF(p) is prominent. Therefore this analytical method can be useful for the study of ground-state properties of atomic BEC even at large gas parameter $\sim 10^{-2}$.

In Fig 5, variation of the lowest excitation frequency of monopole mode of ^{85}Rb of $N=10^4$ atoms as a function of scattering length (a) has been shown. Solid line gives results obtained from eq (34) by using analytical ground state wave functions. Dashed line gives MTF(1) results (eq(21) of Ref.[5]) and the dotted line gives variational results of [5]. By comparing these three curves it is clear that our results are in very good agreement with variational BGP results and the agreement is getting better as $x_{pk} \rightarrow 10^{-2}$, whereas the deviations from MTF(1) results grows with increasing x_{pk} . It is to be mentioned here that the interpolated values of variational results are taken from Fig 4 of [5]. We have shown here that analytical density of particles obtained in MTF(p) approximations can successfully reproduce the lowest order excitation frequency for ^{85}Rb BEC of $N=10^4$ atoms obtained previously [5] by numerical method even at large values of gas-parameter $\sim 10^{-2}$.

In conclusion, we have shown here that the modified TF equation for BEC of 10^3 and 10^4 ^{85}Rb

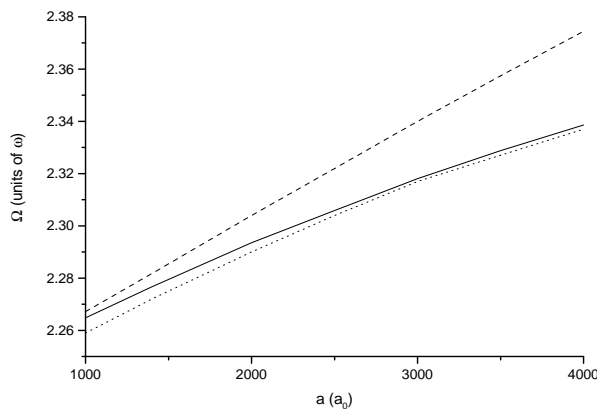


Figure 5. The lowest excitation frequencies (in units of ω) of the monopole mode of 10^4 ^{85}Rb atoms confined in a spherically symmetric trap with $\omega = 2\pi \times 12.83$ Hz. The — corresponds to the results of eq (34) (using ground-state density of particles derived in our higher order iterative method to MTF equation), - - - corresponds to the analytical results (eq.(21) from Ref.[5]) and the represents variational BGP results of Ref.[5]

atoms in an isotropic trap can be solved analytically (using higher order iteration method) for gas-parameters as high as $\sim 10^{-2}$. The ground state properties of BEC can be correctly described and are in very good agreement with those obtained by solving MGP equations numerically. The variation of particle density with distance from the centre of the trap can be correctly reproduced for large gas-parameter $\sim 10^{-2}$. We have also calculated the lowest excitation frequency of the monopole mode of a spherically trapped condensate of 10^4 ^{85}Rb atoms using analytically derived ground-state density of particles and have shown that this analytical method can successfully reproduce the existing numerical results [5] even for large values of $x_{pk} \sim 10^{-2}$.

References

- [1] Pitaevskii L P 1961 *Zh. Eksp. Teor. Fiz* **40** 646 [*Sov. Phys. JETP* **13** 451]
Gross E P 1961 *Nuovo Cimento* **20** 454
- [2] Cornish S L, Claussen N R, Roberts J L, Cornell E A and Wieman C E 2000 *Phys. Rev. Lett.* **85** 1795
- [3] Levi B G 2000 *Phys. Today* **53** 17
- [4] Fabrocini A, Polls A 2001 *Phys. Rev. A* **64** 0636101-5
- [5] Banerjee A, Singh M P 2002 *Phys. Rev. A* **66** 0436091-8
- [6] Dalfovo F, Giorgini S, Pitaevskii L and Stringari S 1999 *Rev. Mod. Phys.* **71**, 463-512
- [7] Press W H, Flannery W H, Teukolsky S A and Vetterling W T 1986 *Numerical Recipes: The art of Scientific Computing* Cambridge (Cambridge : University Press)
- [8] Fetter A L, Walecka J D 1971 *Quantum Theory of Many Particle Systems* (New York : McGraw-Hill)
- [9] Bogoliubov N 1947 *J. Phys. (Moscow)* **11** 23
- [10] Lee T D, Huang K and Yang C N 1957 *Phys. Rev. A* **106** 1135-45
- [11] Fabrocini A, Polls A 1999 *Phys. Rev. A* **60** 2319-23
- [12] Edwards M, Burnett K 1995 *Phys. Rev. A* **51**, 1382-86
- [13] Adhikari S K 2000 *Phys. Rev. E* **62** 2937-44
- [14] Burdley C C, Sackett C A and Hulet R G 1997 *Phys. Rev. Lett.* **78** 985-9
- [15] Kokkelmans S J J M F, Verhaar B J and Gibble K 1998 *Phys. Rev. Lett.* **81** 951-4
- [16] Sakhel A R, DuBois J L and Glyde H R 2002 *Phys. Rev. A* **66** 063610
- [17] Nilsen J K et al. 2005 *Phys. Rev. A* **71** 0536101-7
- [18] Bohigas O, Lane A M and Martorell J 1971 *Phys. Rep.* **51**, 267
- [19] Lipparini E and Stringari S 1989 *Phys. Rep.* **175** 103
- [20] Banerjee A and Singh M P 2001 *Phys. Rev. A* **64** 063604