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# An analytical approach for the nonlinear modified Thomas–Fermi equation to derive the ground-state and dynamic properties of a spherically and cylindrically trapped Bose–Einstein condensate

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## Abstract

It has been shown previously that the modified Thomas–Fermi (MTF) equation can be solved analytically by using a higher order iteration method (MTF(p)) for a spherically trapped atomic Bose–Einstein condensate (BEC). The ground-state properties, e.g. chemical potential, peak gas parameter and the ground state density of atoms (except in the surface region), thus obtained can successfully reproduce the results obtained by solving the modified Gross–Pitaevskii (MGP) equation numerically. In this paper, we have extended this analytical method for obtaining the ground-state and dynamical properties of a cylindrically trapped atomic BEC. In this analytical approach, the ground-state density of atoms at the surface of the trap fails to reproduce the correct behaviour due to the neglect of kinetic energy in the MTF equation. We have proposed a model function which when fitted with the analytical wavefunction (from the MTF equation) near the boundaries of the trap can reproduce the correct behaviour of the ground-state density of atoms at the surface region. The kinetic energy and the other energy components thus obtained using the modified analytical method (MTF(p)+model function fitting) can successfully reproduce the results obtained by solving the MGP equation numerically for the  $^{85}\text{Rb}$  BEC containing  $10^4$  atoms both for spherical and cylindrical traps. The excitation frequency thus obtained for the compressional mode of both spherically and axially symmetric traps is in good agreement with the numerical results. For these calculations, the virial relation is satisfied within the limit  $\leq 10^{-4}$ .

## 1. Introduction

The Bose–Einstein condensation (BEC) in dense atomic gases confined in magnetic traps has been successfully observed experimentally [1–5]. Various properties of the trapped Bose gases have been investigated recently [1, 2] using the magnetic-field-induced Feshbach resonance technique that varies the s-wave scattering length from large positive to large negative values. Thus, one can manipulate the interaction strength

smoothly over a vast region. For example, the scattering length of  $^{85}\text{Rb}$  atoms can be increased using Feshbach resonances so that peak gas parameter  $x_{\text{pk}} \simeq 10^{-2}$  ( $x_{\text{pk}} = n_{\text{pk}} a^3$ , where  $n_{\text{pk}}$  is the peak density of Bose gas and  $a$  is the s-wave scattering length of interatomic interaction). In this gas parameter region, the new phenomena involving the interaction between atoms in the condensate and those above the condensate will play an important role. For such large values of the gas parameter ( $\simeq 10^{-2}$ ) to determine both the ground-state

(chemical potential, total energy and ground state density of atoms) and dynamic properties (frequencies of collective oscillations) of a BEC correctly one will have to consider the higher order nonlinearity which is described by modified Gross–Pitaevskii (MGP) theory [6–12].

The numerical solutions of the MGP equation for the BEC in spherically symmetric and axially symmetric traps have been presented by several authors [7, 9, 16, 19]. In our earlier work [12], we have proposed an alternative analytical scheme to describe the ground-state and dynamic properties of a spherically symmetric condensate. We adopted a Thomas–Fermi approach to the MGP equation (i.e. modified Thomas–Fermi or MTF approach) where the MGP equation has been solved analytically by neglecting the kinetic energy term. It is known that the MTF equation can be solved by considering the first-order iterative method which will be termed here the MTF(1) method [9, 15]. The results obtained from the MTF(1) approach are significantly different from those obtained by numerically solving the MGP equation. In our earlier work it has been shown that by solving the MTF equation for a spherically trapped atomic BEC by considering the higher order iterative method (MTF(p)) one can derive the expressions for the chemical potential, density of atoms in the ground state and hence the frequency of monopole excitation [12]. The values thus obtained are in very good agreement with the numerical solutions of the MGP equation. Here, we extend the previously mentioned higher order iterative method for solving the MTF equation of an anisotropically trapped Bose gas and hence to find out the chemical potential, column density and the different components of the total energy. The collective excitation frequencies obtained by the sum rule approach are also calculated by using the ground-state wavefunctions (i.e. ground-state density of atoms). It is well known that the Thomas–Fermi method does not reproduce correctly the surface region of the density profile [12, 15] and hence the kinetic energy of the system cannot be obtained in this approach. Therefore, it becomes necessary to get the proper wavefunction or the density profile at the edges of the trap for the calculation of the kinetic energy of the condensate as well as the collective excitation frequencies. In our work, we have made an attempt to achieve the correct asymptotic behaviour of the ground-state density of atoms by fitting a model function with the wave function derived from the MTF(p) approach at the edges of the trap. For comparison, we have also solved the MGP equation by the steepest descent method [17, 18] for calculating the ground-state and dynamic properties of a spherically and cylindrically trapped atomic BEC. Previously [12], to solve the MGP equation we used the Runge–Kutta method which fails in the case of large nonlinearity. In the steepest-descent method this difficulty does not arise in the range of the gas parameter  $10^{-3} < x_{\text{pk}} < 10^{-2}$ .

This paper is organized as follows. In section 2.1, we extend the higher order iterative [MTF(p)] approach to solve the modified Thomas–Fermi equation for an anisotropic (cylindrically symmetric) trap. In section 2.2, we provide the model function which is fitted at the edges of the trap with the MTF(p) wavefunction. Section 2.3 describes the

numerical method for solving the modified Gross–Pitaevskii equation. Section 2.4 contains the formulations for the collective excitation frequencies obtained in the sum-rule approach. In section 3, we give the results for the ground-state and dynamic properties of the condensate found in our calculations and compare different analytical and numerical results for both isotropic and anisotropic traps. We conclude our paper in section 4.

## 2. Theory

### 2.1. Modified Thomas–Fermi model for an anisotropic trap

The nonlinear Schrödinger equation which describes the condensate wavefunction within the local-density approximation (LDA) [22] can be written as [8, 12, 19]

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

where  $m$  is the mass of a single atom,  $\mu$  is the chemical potential and  $a$  is the scattering length characterizing the interatomic interaction. The above equation is known as the modified Gross–Pitaevskii (MGP) equation. The first term in the first parentheses of equation (1) corresponds to the energy of the homogeneous Bose gas within the mean field theory calculated by Bogoliubov [13]. The second term in the first parentheses was obtained by Lee, Huang and Yang (LHY) [14] using the hard-sphere model for the interatomic potential.

The trapping potential  $V_t(\mathbf{r})$  is taken to be spherically symmetric characterized by the harmonic oscillator frequency  $\omega_{\text{HO}}$ :

$$V_t(\mathbf{r}) = \frac{1}{2} m \omega_{\text{HO}}^2 r^2 \quad (2)$$

and also cylindrically symmetric characterized by the two angular frequencies  $\omega_{\perp}$  and  $\omega_z$  ( $\omega_x = \omega_y = \omega_{\perp} \neq \omega_z$ ). It is given by

$$V_t(\mathbf{r}) = \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \quad (3)$$

where  $\lambda = \omega_z/\omega_{\perp}$  is the anisotropy parameter.

The condensate wavefunction  $\Psi(\mathbf{r})$  is normalized by the condition

$$\int n(\mathbf{r}) d\mathbf{r} = \int |\Psi(\mathbf{r})|^2 d\mathbf{r} = N \quad (4)$$

where  $n(\mathbf{r})$  is the density of atoms and  $N$  is the total number of atoms in the condensate.

For very large positive values of scattering length  $a$ , the repulsive interaction between atoms becomes much stronger than the kinetic energy and hence the kinetic energy can be neglected from the MGP equation. Under this condition, the Thomas–Fermi (TF) approximation (which neglects kinetic energy) will be valid. This TF limit has already been discussed in [9, 12, 15, 23]. By using the TF approximation to the MGP equation (equation (1)), the MTF equation can be written as follows:

$$g \times n(\mathbf{r}) + g \times \frac{32}{3\sqrt{\pi}} n(\mathbf{r})^{3/2} a^{3/2} = \mu - V_t(\mathbf{r}) \quad (5)$$

where  $g = 4\pi\hbar^2 a/m$  is the coupling constant.

In the case of a cylindrical trap equation (5) can be rewritten as

$$n(r_{\perp}, z) = g^{-1} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right] - \frac{32}{3\sqrt{\pi}} n(r_{\perp}, z)^{3/2} a^{3/2} \quad (6)$$

where  $n(r_{\perp}, z)$  is the density of atoms in the ground state.

Following [9, 15], the density ( $n(\mathbf{r})$ ), chemical potential ( $\mu$ ), peak gas parameter ( $x_{pk}$ ) and the total energy ( $E$ ) of the condensate can be evaluated in the first-order iterative method (MTF(1)). In the first order iteration (MTF(1)) the expression for  $n(r_{\perp}, z)$  is obtained by substituting the the ground-state density in the TF limit ( $n(r_{\perp}, z) = g^{-1} [\mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2)]$ ) on the right-hand side of equation (6) as

$$n(r_{\perp}, z) = g^{-1} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right] - \frac{4m^{3/2}}{3\pi^2 \hbar^3} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right]^{3/2} \quad (7)$$

We have extended this iterative method for higher orders as follows. Substituting equation (7) in place of  $n(r_{\perp}, z)$  on the right-hand side of equation (6), the expression of  $n(r_{\perp}, z)$  in the second-order iteration can be written as

$$n(r_{\perp}, z) = g^{-1} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right] - \frac{4m^{3/2}}{3\pi^2 \hbar^3} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right]^{3/2} \times \left( 1 - \frac{16m^{1/2}a}{3\pi\hbar} \left( \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right) \right)^{3/2}. \quad (8)$$

Hence the expression of  $n(r_{\perp}, z)$  in the third-order iteration can be obtained by substituting equation (8) in place of  $n(r_{\perp}, z)$  on the right-hand side of equation (6) as

$$n(r_{\perp}, z) = g^{-1} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right] - \frac{4m^{3/2}}{3\pi^2 \hbar^3} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right]^{3/2} \times \left( 1 - \frac{16m^{1/2}a}{3\pi\hbar} \left( \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right) \right) \times \left( 1 - \frac{16m^{1/2}a}{3\pi\hbar} \left( \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right) \right)^{3/2}. \quad (9)$$

Equations (8) and (9) can be rewritten by substituting  $x = \frac{16m^{1/2}a}{3\pi\hbar} \left( \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right)$  as follows:

$$n(r_{\perp}, z) = g^{-1} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right] - \frac{4m^{3/2}}{3\pi^2 \hbar^3} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right]^{3/2} (1-x)^{3/2} \quad (10)$$

and

$$n(r_{\perp}, z) = g^{-1} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right] - \frac{4m^{3/2}}{3\pi^2 \hbar^3} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right]^{3/2} \times (1-x \times (1-x)^{3/2})^{3/2}. \quad (11)$$

Similarly, one can derive expressions for  $n(r_{\perp}, z)$  in subsequent iterations, e.g., the expression of  $n(r_{\perp}, z)$  for the  $p$ th order iteration can be written as

$$n(r_{\perp}, z) = g^{-1} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right] - \frac{4m^{3/2}}{3\pi^2 \hbar^3} \left[ \mu - \frac{1}{2} m \omega_{\perp}^2 (r_{\perp}^2 + \lambda^2 z^2) \right]^{3/2} \times (1-x \times (1-x \times (1-x \times \dots \times (1-x \times \dots \times ((p-1)^{\text{th}} \text{ term})^{3/2})^{3/2} \dots)^{3/2} \dots) \text{ up to } (p-1)^{\text{th}})^{3/2} \quad (12)$$

We note that  $n(\mathbf{r})$  is normalized to  $N$  and from equation (4) the equation for chemical potential looks like

$$\sum_{j=1}^{I_{\max}} A_j \mu^{2+\frac{j}{2}} = N \quad (13)$$

where the  $A_j$ 's are the sum of the coefficients of  $\mu^{(2+\frac{j}{2})}$  and are functions of  $a, m, \omega_{\perp}$  and  $\lambda$ . The  $A_j$ 's are coefficients  $C_j$ 's of equation (19) of [12] divided by the number  $\lambda$  and  $\omega$  replaced by  $\omega_{\perp}$ . The  $\mu$ 's are in units of  $\hbar\omega_{\perp}$ . The method of successive iteration is used for solving equation (13) to give the final and converged value of  $\mu$  ( $\mu_{\text{MTF}(q)}$ ) after the  $q$ th iteration. This value of  $\mu_{\text{MTF}(q)}$  is substituted into equation (12) and the high order of iteration (say  $p$ th order which is higher than  $q$ ) has been used to get the converged value of  $n(\mathbf{r})$ . The peak gas parameter is given as

$$x_{pk, \text{MTF}(p)} = n_{\text{MTF}(p)}(r_{\perp} = z = 0) a^3. \quad (14)$$

The column density of the condensate is defined as

$$n_c(z) = \int dr_{\perp} n(r_{\perp}, z). \quad (15)$$

We consider the wavefunctions of the condensate as

$$\Psi_{\text{MTF}(p)}(r_{\perp}, z) = |\sqrt{n_{\text{MTF}(p)}(r_{\perp}, z)}|. \quad (16)$$

The wavefunctions obtained from numerically solving the MGP equation are positive for all values of  $r_{\perp}$  and  $z$  and are in good agreement with the analytical wavefunctions except in the surface region.

## 2.2. Model function fitting

The analytical higher order MTF method described above fails to reproduce the correct behaviour of the density of atoms in the ground state in the surface region of the trap. In the surface region, the interaction energy decreases and hence the kinetic energy can no longer be ignored. Previously [24, 25], to obtain the correct behaviour of the wavefunction of the ground state at the boundary, the asymptotic form of the Airy function was used. We have proposed here a model function which is fitted with the analytical MTF( $p$ ) wave function ( $\Psi_{\text{MTF}(p)}$ ) at the surface region to give the correct asymptotic behaviour of the density of atoms in the ground state. This model function is given as (in terms of the dimensionless variables)

$$\Psi(r_1) = \alpha \exp \left[ -\frac{r_1^2}{2} + (\mu_1 - 1) \ln(r_1 - \beta) \right] \quad (17)$$

and

$$\Psi(r_{\perp,1}, z_1) = \alpha \exp \left[ -\frac{(r_{\perp,1}^2 + z_1^2)}{2} + (\mu_1 - 1) \ln \left( \sqrt{r_{\perp,1}^2 + z_1^2} - \beta \right) \right] \quad (18)$$

for spherically and cylindrically trapped condensates respectively. Here,  $r_1 = r/a_{\text{HO}}$ ,  $a_{\text{HO}} = (\frac{\hbar}{m\omega_{\text{HO}}})^{1/2}$  and  $\mu_1 = \mu/\hbar\omega_{\text{HO}}$  in equation (17) and  $r_{\perp,1} = r_{\perp}/a_{\perp}$ ,  $z_1 = z/a_{\perp}$ ,  $a_{\perp} = (\frac{\hbar}{m\omega_{\perp}})^{1/2}$  and  $\mu_1 = \mu/\hbar\omega_{\perp}$  in equation (18). The value of  $\mu = \mu_{\text{MTF}(q)}$  is used in equations (17) and (18). We have fitted the slope and the magnitude of these model functions with those of  $\Psi_{\text{MTF}(p)}$  wavefunctions at a distance  $r = r_{\text{fit}}$  from the centre of the trap by adjusting the values of the fitting parameters  $\alpha$  and  $\beta$ . For a cylindrical trap, at each value of  $z$  the fitting of the model function (18) with the  $\Psi_{\text{MTF}(p)}$  wavefunction at  $r = r_{\text{fit}}$  has been performed. Here, the distance  $r_{\text{fit}}$  is chosen such that after this value of  $r$  the density of the condensate (obtained from  $\Psi_{\text{MTF}(p)}$ ) falls sharply and hence the derivative of wavefunction  $\Psi_{\text{MTF}(p)}$  rises sharply. Thus, for the calculation of different energy components we have used the analytical wavefunctions ( $\Psi_{\text{MTF}(p)}$ ) up to  $r = r_{\text{fit}}$  and the model function for  $r > r_{\text{fit}}$ . For each set of the values of parameters  $\alpha$  and  $\beta$ , the virial relation has been found to be within the limit  $\leq 10^{-4}$ .

The kinetic energy of the system can be calculated by using this modified analytical ( $\Psi_{\text{MTF}(p)}$ +fitted model function) wavefunction as follows:

$$T = \frac{\hbar^2}{2m} \int d\mathbf{r} |\nabla \Psi(\mathbf{r})|^2. \quad (19)$$

Similarly, the harmonic oscillator energy due to the spherically symmetric potential is given as

$$U = \frac{1}{2} m \omega_{\text{HO}}^2 \int d\mathbf{r} r^2 |\Psi(\mathbf{r})|^2, \quad (20)$$

and that for a cylindrical trap is given as

$$U = \frac{1}{2} m \omega_{\perp}^2 \int d\mathbf{r} (r_{\perp}^2 + \lambda^2 z^2) |\Psi(\mathbf{r})|^2. \quad (21)$$

The interaction energies are given as

$$E_{\text{int}}^{(1)} = \frac{2\pi\hbar^2 a}{m} \int d\mathbf{r} |\Psi(\mathbf{r})|^4. \quad (22)$$

and

$$E_{\text{int}}^{(2)} = \frac{2\pi\hbar^2 a}{m} \left( \frac{128}{15} \right) \left( \frac{a^3}{\pi} \right)^{1/2} \int d\mathbf{r} |\Psi(\mathbf{r})|^5 \quad (23)$$

The virial relation among the different energy components provides a method of checking the accuracy of the analytical and numerical solutions. The virial relation is given as

$$2T - 2U + 3E_{\text{int}}^{(1)} + \frac{9}{2} E_{\text{int}}^{(2)} = 0. \quad (24)$$

### 2.3. Numerical procedure

The MGP equation for  $\Psi(\mathbf{r})$  has been solved by the steepest-descent method [17, 18] for the isotropic and anisotropic traps previously described in equations (2) and (3). By discretizing time and introducing a time step  $\Delta t$  and then replacing the time step  $\Delta t$  by the imaginary quantity  $-i\Delta t$ , the MGP equation can be iterated as

$$\Psi(\mathbf{r}, t + \Delta t) \simeq \Psi(\mathbf{r}, t) - \Delta t H \Psi(\mathbf{r}, t). \quad (25)$$

First, we choose an initial trial wavefunction. We start from the ground-state isotropic and anisotropic harmonic oscillator functions

$$\Psi(r) = A\pi^{-3/4} \exp\left[-\frac{1}{2}r^2\right] \quad (26)$$

and

$$\Psi(r_{\perp,1}, z_1) = A\pi^{-3/4} \exp\left[-\frac{1}{2}(r_{\perp,1}^2 + z_1^2)\right] \quad (27)$$

for spherical and cylindrical traps, respectively. Here  $A$  is the normalization constant.

Then we iterate equation (25) and generate a set of wavefunctions  $\Psi(\mathbf{r}, t)$  by normalizing  $\Psi$  to  $N$  at each iteration. The number of iterations in imaginary time depends on the required degree of convergence in the values of wave functions and the goodness of the initial trial wavefunction. When the gas parameter becomes large, the time step ( $\Delta t$ ) which governs the rate of convergence should be taken correspondingly small. The imaginary time-propagation method results in a monotonic decrease in the total energy from iteration to iteration, until it converges to the minimum value. Typically, we use 60 000–200 000 iterations and the degree of convergence achieved is

$$\left| \frac{E(t_n) - E(t_{n-1})}{E(t_n)} \right| \leq 10^{-12}.$$

It has been found that the convergence of the wavefunctions ( $\Psi(\mathbf{r}, t)$ ) corresponding to the converged total energy is  $\leq 10^{-6}$  at each value of  $\mathbf{r}$ . The converged value of the wavefunction  $\Psi$  is substituted into the MGP equation to give the chemical potential ( $\mu$ ) which becomes a constant independent of the position. The values of  $\mu$  (in units of  $\hbar\omega_{\text{HO}}$  or  $\hbar\omega_{\perp}$ ) are constant up to the third decimal place.

In our calculations we use the harmonic oscillator units. In the case of the spherical trap, we write the scattering length in units of  $a_{\text{HO}} = (\frac{\hbar}{m\omega_{\text{HO}}})^{1/2} = 3.04 \mu\text{m}$  and the energy in units of  $\hbar\omega_{\text{HO}} = 0.053 \text{ peV}$  for  $^{85}\text{Rb}$ . For the cylindrical trap,  $a_{\perp} = 2.61 \mu\text{m}$  and  $\hbar\omega_{\perp} = 0.072 \text{ peV}$ .

### 2.4. Excitation frequencies of collective oscillations

The analytical results for the low-energy excitations of a Bose-condensed gas in spherical and cylindrical traps have been obtained by solving the hydrodynamic equations in the TF limit [26, 27] and also using the sum-rule approach [26]. The analytical solution of the Bogolyubov–de Gennes equation for the excitation spectrum of the condensate in the Thomas–Fermi regime was given earlier [28].

In the present work having described the analytical method for obtaining the ground-state wavefunctions and



**Table 1.** Results for the ground-state properties of  $10^4$   $^{85}\text{Rb}$  atoms trapped in a spherical trap in different approaches with  $\frac{\omega_{\text{HO}}}{2\pi} = 12.83$  Hz. Energies are in units of  $\hbar\omega_{\text{HO}}$ .

| $a$ ( $a_0$ ) |        | $\mu$ | $x_{\text{pk}}$ | $E_{\text{int}}^{(1)}/N$ | $E_{\text{int}}^{(2)}/N$ | $U/N$     | $T/N$    | $E/N$  |
|---------------|--------|-------|-----------------|--------------------------|--------------------------|-----------|----------|--------|
| 1400          | MGP    | 13.97 | 5.73(−4)        | 3.469 46                 | 0.324 17                 | 6.076 88  | 0.142 98 | 10.013 |
|               | MTF(p) | 13.85 | 5.71(−4)        | 3.466 87                 | 0.322 492                | 6.073 18  | 0.147 27 | 10.009 |
|               | MTF(1) | 13.89 | 5.54(−4)        | —                        | —                        | —         | —        | 9.868  |
| 3000          | MGP    | 19.84 | 3.20(−3)        | 4.310 16                 | 0.955 83                 | 8.727 35  | 0.111 28 | 14.105 |
|               | MTF(p) | 19.77 | 3.19(−3)        | 4.309 06                 | 0.953 05                 | 8.723 03  | 0.115 05 | 14.100 |
|               | MTF(1) | 20.04 | 2.62(−3)        | —                        | —                        | —         | —        | 14.134 |
| 4000          | MGP    | 22.91 | 6.00(−3)        | 4.591 48                 | 1.397 92                 | 10.133 37 | 0.100 65 | 16.223 |
|               | MTF(p) | 22.83 | 5.99(−3)        | 4.591 10                 | 1.394 70                 | 10.129 05 | 0.104 33 | 16.219 |
|               | MTF(1) | 23.41 | 3.86(−3)        | —                        | —                        | —         | —        | 16.437 |

other physical observables of the BEC, we now calculate the excitation frequency of the compressional collective mode of bosons (characterized by the z-component of the angular momentum  $m' = 0$ ) in a spherically and cylindrically symmetric trap. According to [10, 11, 26], the sum-rule approach of the many-body response theory [20, 21] is used to calculate the excitation frequency. This approach requires the knowledge of the accurate ground-state wavefunction (or the ground-state density of atoms) of the many-body system. As our analytical method provides the accurate density profile, it is expected that our approach will be useful in this perspective. The expression for the excitation frequency of the monopole mode of spherically trapped bosons is given as [10, 12]

$$\frac{\Omega^2}{\omega_{\text{HO}}^2} = 2 \times \left[ \frac{T + U + \frac{9}{4}E_{\text{int}}^{(1)} + \frac{81}{16}E_{\text{int}}^{(2)}}{U} \right]. \quad (28)$$

In the case of the cylindrical trap the expression for the frequency of compressional mode is given as [10]

$$\Omega_{m'=0}^2 = 2 \left( \frac{T_{\perp} + U_{\perp} + \gamma^2(T_z + U_z) + (1 - \gamma/2)^2(E_{\text{int}}^{(1)} + \frac{9}{4}E_{\text{int}}^{(2)})}{\frac{U_{\perp}}{\omega_{\perp}^2} + \gamma^2 \frac{U_z}{\omega_z^2}} \right) \quad (29)$$

where  $\gamma$  is a parameter characterizing the coupling of monopole and quadrupole modes due to axial symmetry of the trap. In equation (29),  $T_{\perp}$  and  $U_{\perp}$  ( $T_z$  and  $U_z$ ) are the transverse components (axial components) of kinetic and potential energies, respectively.

$\Omega_{m'=0}$  will be extremum for the following values of  $\gamma$ :

$$\gamma_+ = -\frac{B}{2} + \frac{1}{2}\sqrt{B^2 + 4C} \quad (30)$$

$$\gamma_- = -\frac{B}{2} - \frac{1}{2}\sqrt{B^2 + 4C} \quad (31)$$

where

$$B = \frac{(2f_2f_4 + f_3f_4/2 - 2f_1f_5 - 2f_3f_5)}{f_3f_5} \quad (32)$$

and

$$C = \frac{f_3}{f_4} \quad (33)$$

$$f_1 = T_{\perp} + U_{\perp}, f_2 = T_z + U_z, f_3 = E_{\text{int}}^{(1)} + \frac{9}{4}E_{\text{int}}^{(2)}, f_4 = U_{\perp}/(\omega_{\perp}^2) \text{ and } f_5 = U_z/(\omega_z^2)$$

Thus for an axially symmetric trap due to the two different values of  $\gamma$  the upper ( $\Omega_u$ ) and lower ( $\Omega_l$ ) branches of collective excitation frequency will be obtained. The ground-state wavefunctions derived in the modified analytical method as mentioned in section 2.2 are used to get the values of excitation frequencies and the results are compared with the numerical MGP and other analytical (MTF(1) and higher order MTF) results.

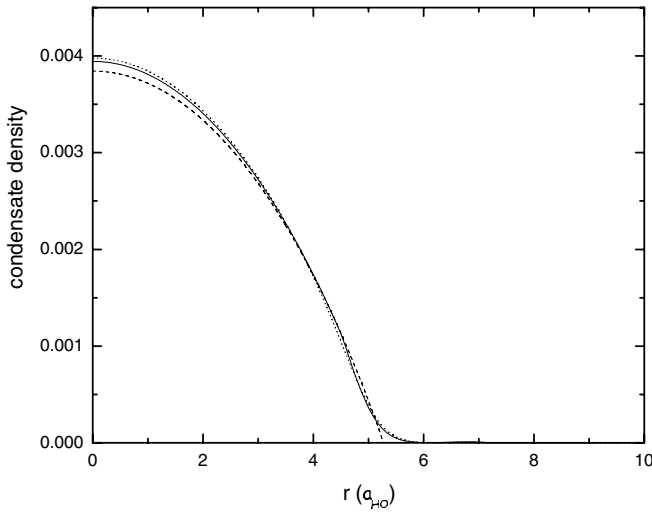
### 3. Results and Discussion

#### 3.1. Ground-state properties

In this section, a comparison of analytical results obtained by solving the MTF equation (along with the fitted model function) with the corresponding numerical results from the MGP equation has been provided for a spherically and cylindrically symmetric trapped atomic condensate. The chemical potential ( $\mu$ ), peak gas parameter ( $x_{\text{pk}}$ ) and the individual energy components of the  $^{85}\text{Rb}$  condensate have been given in table 1 for  $10^4$  atoms confined in a spherical trap. The oscillator angular frequency is given as  $\omega_{\text{HO}}/2\pi = (\omega_{\perp}^2\omega_z)^{1/3}/2\pi = 12.83$  Hz [7], where  $\omega_{\perp}/2\pi = 17.5$  Hz and  $\omega_z/2\pi = 6.9$  Hz are the radial and axial frequencies associated with the external potential of the axially symmetric trap used in [1]. Use of the model function at the surface of the trap enables us to calculate the kinetic energy of the system accurately using the modified analytical method ( $\Psi_{\text{MTF}(p)}$  + model function fitting). All other energy components such as the interaction energies ( $E_{\text{int}}^{(1)}$  and  $E_{\text{int}}^{(2)}$ ), kinetic energy ( $T$ ) and the trap potential energy ( $U$ ), are calculated both using the modified analytical methods and by numerically solving the MGP equation. It can be clearly seen from table 1 that the results obtained by our modified analytical method are very close to the corresponding MGP results. In particular, our results for both the components of interaction energies and the trap energy match very well, the differences being less than 1%. Our analytical results for the kinetic energies are slightly higher (of the order of 3%) than those of the numerical MGP values. The MGP results for total energies are approximately 0.04% higher than the corresponding modified analytical values. To gain further insight, we compare the density profile for a spherical

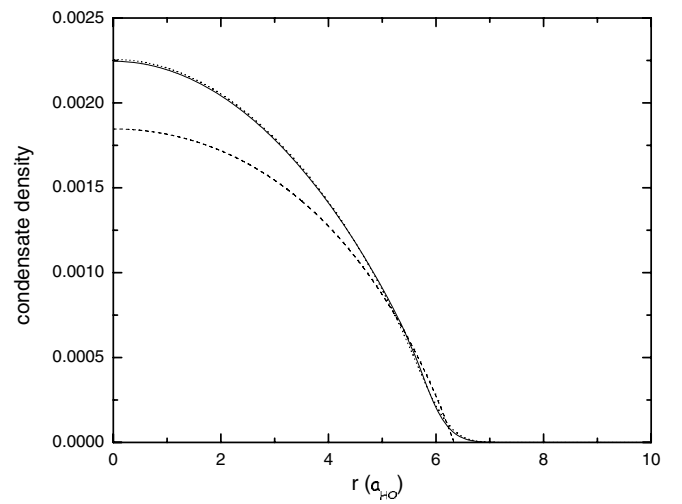
**Table 2.** Results for the ground-state properties of  $10^4$   $^{85}\text{Rb}$  atoms in a cylindrical trap in different approaches with  $\frac{\omega_{\perp}}{2\pi} = 17.5$  Hz and  $\lambda = 0.39$ . Energies are in units of  $\hbar\omega_{\perp}$ .

| $a$ ( $a_0$ ) |        | $\mu$ | $x_{\text{pk}}$ | $E_{\text{int}}^{(1)}$ | $E_{\text{int}}^{(2)}$ | $U/N$    | $T/N$    | $E/N$  |
|---------------|--------|-------|-----------------|------------------------|------------------------|----------|----------|--------|
| 1400          | MGP    | 10.21 | 5.73(−4)        | 2.519 75               | 0.234 93               | 4.443 94 | 0.131 33 | 7.325  |
|               | MTF(p) | 10.11 | 5.68(−4)        | 2.516 06               | 0.231 16               | 4.431 05 | 0.136 65 | 7.315  |
|               | MTF(1) | 10.14 | 5.52(−4)        | —                      | —                      | —        | —        | 7.205  |
| 3000          | MGP    | 14.51 | 3.19(−3)        | 3.147 00               | 0.691 25               | 6.373 39 | 0.097 59 | 10.309 |
|               | MTF(p) | 14.42 | 3.18(−3)        | 3.144 92               | 0.689 65               | 6.369 16 | 0.100 98 | 10.304 |
|               | MTF(1) | 14.63 | 2.61(−3)        | —                      | —                      | —        | —        | 10.319 |
| 4000          | MGP    | 16.76 | 5.99(−3)        | 3.333 94               | 1.014 95               | 7.372 65 | 0.088 12 | 11.809 |
|               | MTF(p) | 16.67 | 5.98(−3)        | 3.330 87               | 1.013 65               | 7.367 43 | 0.090 43 | 11.802 |
|               | MTF(1) | 17.09 | 3.85(−3)        | —                      | —                      | —        | —        | 11.998 |

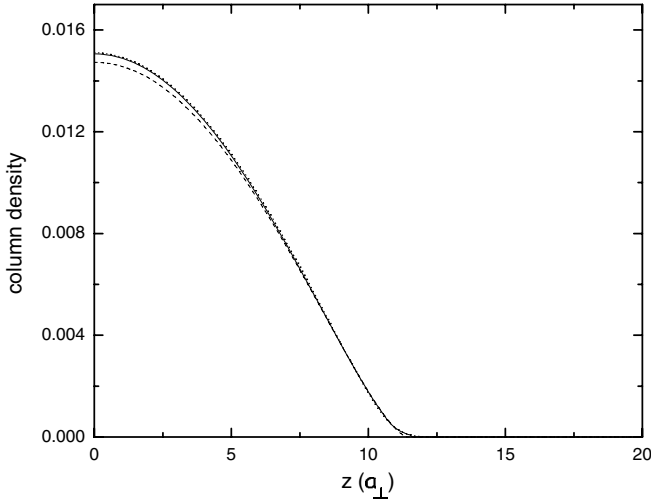
**Figure 1.** Condensate densities of  $10^4$   $^{85}\text{Rb}$  atoms at  $a = 1400 a_0$  as a function of the radial distance from the centre of the spherically symmetric trap with  $\omega_{\text{HO}}/2\pi = 12.83$  Hz. The horizontal axis is scaled in harmonic oscillator length unit given by  $a_{\text{HO}} = (\frac{\hbar}{m\omega_{\text{HO}}})^{1/2}$ . The vertical axis is multiplied by  $a_{\text{HO}}^3/N$ . The solid line represents the modified analytical, the dotted line gives the MGP and the dashed line gives the MTF(1) results.

trap obtained from the modified analytical method (solid line) and the numerical MGP (dotted line) method in figures 1 and 2 for  $a = 1400a_0$  and  $3000a_0$ , respectively. The density of atoms obtained in the MTF(1) [9, 12] (dashed line) approach is also plotted. We find excellent overall agreement between our complete analytical density of atoms with the MGP results in the central region as well as in the surface region of the trap. However, the curve for MTF(1) differs significantly from the other two curves. We have not plotted here the density of ground-state atoms obtained in the MTF(p) approach but these are in very good agreement with the numerical MGP results (except at the edges of the trap) as shown previously (figures 1–3 in [12]).

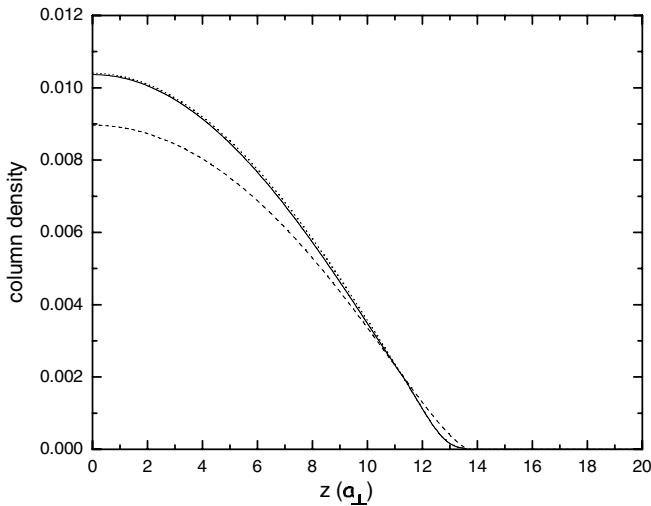
The ground-state properties (similar as in table 1) for the cylindrical trap are shown in table 2. Here also, the MTF(p) wavefunctions fitted with the model functions are used for calculating different components of the total energy. The agreement between the energy components obtained in the numerical MGP and our modified analytical method is very

**Figure 2.** Condensate densities of  $10^4$   $^{85}\text{Rb}$  atoms at  $a = 3000 a_0$  as a function of the radial distance from the centre of the spherically symmetric trap with  $\omega_{\text{HO}}/2\pi = 12.83$  Hz. The horizontal and vertical axes scaling are the same as in figure 1. The solid line represents the modified analytical, the dotted line gives the MGP and the dashed line gives the MTF(1) results.

good. In the case of the kinetic energy, the agreement is within 4% and for the other energy components the agreement is within 1%. The analytical values of  $\mu$  obtained in the higher order MTF approach become closer to the MGP values as the scattering length ( $a$ ) increases, since in this case the interaction energy grows over the kinetic energy. We also find good agreement between the MTF(p) and MGP values of the peak gas parameter. However, MTF(1) results deviate from MGP results as  $a$  increases. Throughout this calculation we have checked that the virial relation (as given in equation (24)) is satisfied up to the fourth decimal place or better for both types of trap. This proves that not only the total energy but also its different components can be accurately reproduced in our modified analytical method. In figures 3 and 4, we show the column densities (already defined in equation (15)) in different approaches for  $a = 1400a_0$  and  $a = 3000a_0$ , respectively. The dotted, solid and dashed lines correspond to the MGP, modified analytical and MTF(1) results, respectively. The modified analytical and MGP results almost coincide. The agreement between the two curves is also good in the surface



**Figure 3.** Column densities of  $10^4$   $^{85}\text{Rb}$  atoms at  $a = 1400 a_0$  as a function of axial distance for a cylindrical trap with  $\omega_{\perp}/2\pi = 17.5$  Hz and  $\lambda = 0.39$ . The horizontal axis is scaled in harmonic oscillator length unit given by  $a_{\perp} = (\hbar/m\omega_{\perp})^{1/2}$ . The vertical axis is multiplied by  $2 \times a_{\perp}^3/N$ . The solid line represents the modified analytical, the dotted line gives the MGP and the dashed line gives the MTF(1) results.

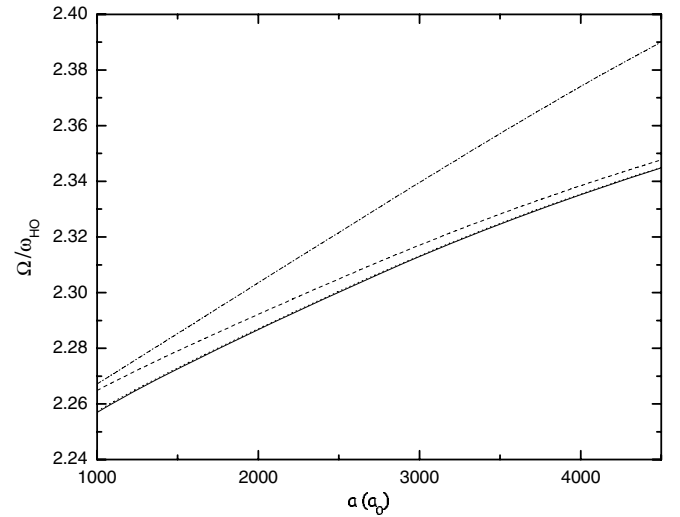


**Figure 4.** Column densities of  $10^4$   $^{85}\text{Rb}$  atoms at  $a = 3000 a_0$  as a function of the axial distance for a cylindrical trap. The horizontal and vertical axes scaling are the same as in figure 3. The solid line represents the modified analytical, the dotted line gives the MGP and the dashed line gives the MTF(1) results.

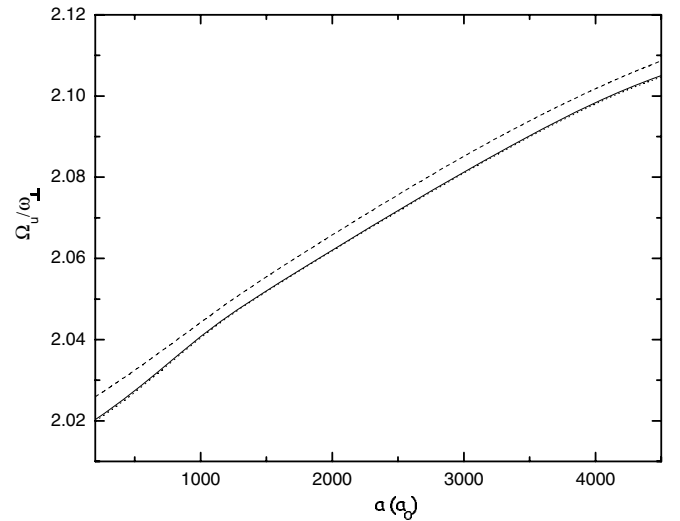
region. However, the MTF(1) curve deviates from these two curves significantly.

### 3.2. Frequencies of collective excitation

In this section, we have presented the frequencies of collective excitation obtained in different analytical and numerical approaches. Figure 5 shows the excitation frequencies of the monopole mode of the spherically trapped bosons as a function of the dimensionless parameter  $a/a_0$  obtained by solving the MGP equation numerically (dotted line), the MTF(p) (dashed line) and the modified analytical (solid line) approach. The results for MTF(1) method (taken from equation (21) of [9])



**Figure 5.** The frequencies (in units of  $\omega_{HO}$ ) of the monopole mode excitation as a function of  $a/a_0$  of  $10^4$   $^{85}\text{Rb}$  atoms confined in a spherical trap with the parameter the same as given in figure 1. The solid, dotted, dashed and dashed-dotted lines represent the modified analytical, MGP, MTF(p) and MTF(1) results, respectively.

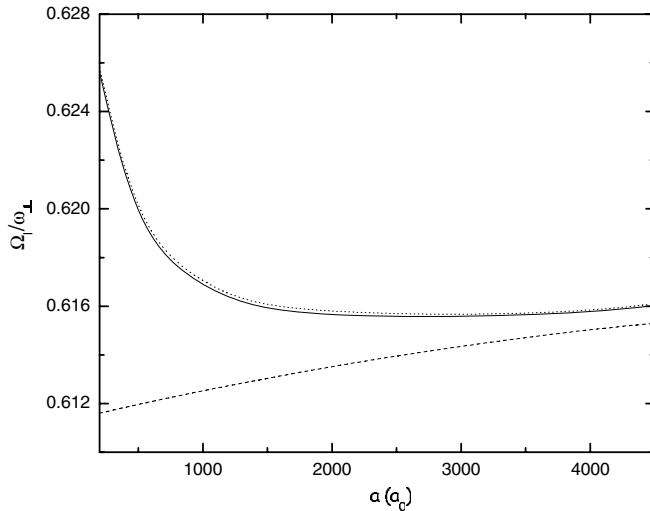


**Figure 6.** The excitation frequencies (in units of  $\omega_{\perp}$ ) of the upper branch of the compressional mode ( $\Omega_u$ ) as a function of  $a/a_0$  of  $10^4$   $^{85}\text{Rb}$  atoms confined in a cylindrical trap with the trap parameters the same as given in figure 3. The solid, dotted and dashed lines correspond to the modified analytical, the MGP and the MTF(p) results respectively.

are also plotted (dashed-dotted line). It can be seen the both the results for MTF(1) and MTF(p) are systematically higher than the MGP values and the agreement between MGP and MTF(p) becomes better but that between MTF(1) and MGP becomes worse with increasing  $a$ . Our results for modified analytical method almost coincide (agreement is within 0.02%) with the MGP results for the monopole mode of the excitation frequency for the small as well as large values of scattering length.

Let us now focus our attention on the lower ( $\Omega_l$ ) and the upper ( $\Omega_u$ ) (associated with the  $\gamma_+$  and  $\gamma_-$  values, respectively) branches of the compressional mode. The results presented in figures 6 and 7 correspond to the cylindrically symmetric trap.





**Figure 7.** The excitation frequencies (in units of  $\omega_{\perp}$ ) of the lower branch of the compressional mode ( $\Omega_l$ ) as a function of  $a/a_0$  of  $10^4$   $^{85}\text{Rb}$  atoms confined in a cylindrical trap. The solid, dotted and dashed lines correspond to the modified analytical, the MGP and the MTF(p) results, respectively.

In these two figures the frequencies obtained from the MGP (dotted line), MTF(p) (dashed line) and modified analytical (solid line) approaches are plotted. Figure 6 shows the variation of  $\Omega_u$  with  $a/a_0$ . The MGP and modified analytical curves are in very good agreement (of the order of 0.03%). The MTF(p) values are slightly higher than the other two results. The lower branch of the compressional mode  $\Omega_l$  is shown in figure 7. Here also, the modified analytical and MGP results are very close (within 0.04%) to each other. The MTF(p) curve for  $\Omega_l$  is much lower than the other two curves as the kinetic energy part actively contributes in the expression for  $\Omega_l$ . Thus the values of collective excitation frequencies depend on the correct values of ground-state densities of the condensate in particular at the surface. The modified analytical method (higher order MTF approach+model function fitting) described in this paper gives the correct asymptotic values of ground state density of atoms at the surface of the trap and hence the correct values of different components of energy as well as the excitation frequency. Therefore this approach provides an appropriate analytical method for getting the ground state as well as the dynamical properties of an atomic BEC.

#### 4. Conclusion

In summary, we have developed a complete analytical method for obtaining the solution of the MTF equation for a spherically and cylindrically trapped BEC. The ground-state properties, e.g., the chemical potential and the peak gas parameter obtained in the higher order MTF [MTF(p)] approach are in very good agreement with those obtained by solving the

MGP equation numerically for the  $^{85}\text{Rb}$  BEC containing  $10^4$  atoms in the peak gas parameter range  $10^{-3} < x_{\text{pk}} < 10^{-2}$ . The agreement becomes better with the increase in  $a$  or  $x_{\text{pk}}$ . Since in the surface region the MTF approximation turns out to be inadequate to give the density of atoms in the condensate, we have fitted a model function with the wave function obtained from the higher order iterative method (the MTF(p) approach) at the edges of the trap. Using this modified analytical wavefunction we have been able to calculate the kinetic energy of the system correctly. It has been shown that all the components of energy and hence the frequencies of collective excitation obtained from the numerical solution of the MGP equation can be reproduced correctly by using this modified analytical method for the gas parameter lying in the range  $10^{-3} < x_{\text{pk}} < 10^{-2}$ . The accuracy of these calculations has been checked by keeping the virial relation satisfied within the limit  $\leq 10^{-4}$ .

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