

# Elementary excitations of a trapped Bose gas in the large-gas-parameter regime

Arup Banerjee and Manoranjan P. Singh

*Laser Physics Division, Centre for Advanced Technology, Indore 452013, India*

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We study the effect of going beyond the Gross-Pitaevskii theory on the frequencies of collective oscillations of a trapped Bose gas in the large gas parameter regime. We go beyond the Gross-Pitaevskii regime by including a higher-order term in the interatomic correlation energy. To calculate the frequencies we employ the sum-rule approach of many-body response theory coupled with a variational method for the determination of ground-state properties. We show that going beyond the Gross-Pitaevskii approximation introduces significant corrections to the collective frequencies of the compressional mode.

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## I. INTRODUCTION

The mean-field Gross-Pitaevskii (GP) theory [1] has been quite successful in explaining both static and dynamic properties [2–4] of Bose-Einstein condensates (BEC) produced in alkali-metal atoms [5–7]. The reason for the success of the GP theory is mainly the satisfaction of the dilute gas condition  $na^3 \ll 1$  (where  $n$  is atomic density,  $a$  is the  $s$ -wave scattering length of interatomic potential, and the parameter  $na^3$  is called the gas parameter) in the above-mentioned experiments. Typically the values of the gas parameter in these experiments were in the range of  $10^{-5}$ – $10^{-4}$ . The gas parameter can have a large value when the number of atoms  $N$  in the condensate or the scattering length is large. Thus in the later experiments reported in Refs. [8,9]  $N$  was of the order of  $10^8$  and the corresponding value of the gas parameter was  $10^{-3}$ . On the other hand, in a very recent experiment [10] the maximum value of the peak gas parameter was  $n(0)a^3 \approx 10^{-2}$  [ $n(0)$  is the peak density of the condensate] although the condensate contained only  $10^4$   $^{85}\text{Rb}$  atoms. In this experiment the scattering length  $a$  could be varied continuously from a negative to a very large positive value by exploiting the Feshbach resonance. These kind of condensates, then, naturally raise the question about the validity of the mean-field GP approach. Theoretical investigations of the effects of going beyond the GP (BGP) theory have already been reported in the literature [11–15]. Recently [16] ground-state properties of BEC with large values of the gas parameter (as achieved in the experiments [10]) have been theoretically studied to assess the accuracy of the GP theory. It has been shown that for large values of the gas parameter ( $\approx 10^{-2}$ ) the total energy and the chemical potential are modified significantly by the BGP theory. It is well known that these changes are also reflected in the frequencies of collective excitations which can be measured with a greater accuracy. Therefore, by measuring the frequencies of collective excitations it should be possible to observe the effect of the BGP theory. This has motivated us to calculate the corrections to the frequencies of collective oscillations due to the BGP theory. We focus our attention on the condensates with values of gas parameters, spanning a range similar to that achieved in the experiment [10] and make an assessment of the accuracy of the GP theory in predicting the frequencies of collective oscillations of such condensates.

In the past, corrections to the frequencies of collective oscillations of trapped bosons arising due to the BGP theory have been estimated [17,18] within the Thomas-Fermi (TF) approximation which is valid in the large  $N$  limit (more precisely when  $Na/a_{h0} \gg 1$  is satisfied, where  $a_{h0}$  is the characteristic length of the trapping potential and it is defined in the next section). In the aforesaid references corrections to the frequencies were obtained by solving the time-dependent second-order differential equation perturbatively for the density. Thus the analytical expressions for the fractional change in the frequencies are correct only up to the first order in  $\sqrt{n(0)a^3}$ . It is then expected that these expressions for the corrections will not be accurate in the large-gas-parameter regime, as achieved in the recent experiment [10]. In this paper we also derive an analytical expression for the correction within the TF approximation by making use of the sum-rule approach. We find that the expression for the correction obtained by us is valid for a somewhat larger range of gas parameters than those of Refs. [17,18]. As expected, for very small gas parameters the expression derived by us correctly reduces to those of Refs. [17,18]. We will return to the question of validity of these analytical results later.

It is well known that the TF approximation does not reproduce the surface region of the density profile of trapped condensates accurately [2]. On the other hand, the collective oscillation frequencies characterizing the response properties of the trapped gas crucially depend on the tail or the surface region of the density profile [19]. Therefore, it becomes necessary to go beyond the TF approximation especially for the calculation of frequencies of collective oscillations [18]. To accomplish this task we make use of the well established variational method [15,20–22] to determine the ground-state densities. The collective oscillation frequencies are then obtained by using the sum-rule approach [23,24] of many-body response theory. In the sum-rule approach the calculation of frequencies requires the knowledge of the ground-state wave function (or the ground-state density) of the many-body system only. Therefore the accuracy of frequencies determined by the sum-rule approach depends on the accuracy of the ground-state wave function (ground-state density) employed for the calculations. Keeping this in mind our aim is also to obtain reasonably accurate ground-state densities of the trapped condensates. To this end we employ the variational approach by using an energy functional of  $N$  interacting

trapped bosons within the local density approximation (LDA) along with a judiciously chosen variational ansatz for the ground-state density [15,22].

The paper is organized in the following manner. In Sec. II we describe the theoretical method for the calculation of the frequencies of collective oscillations. Section III contains the analytical estimate of the corrections to the frequencies within the TF approximation, and the results of our variational calculation. The paper is concluded in Sec. IV.

## II. VARIATIONAL SUM-RULE APPROACH

The central quantity in the variational approach is the energy functional for a condensate of  $N$  bosons, each with mass  $m$ , confined in a trap potential  $V_t(\mathbf{r})$ :

$$E[n] = \int d\mathbf{r} \left[ -\frac{\hbar^2}{2m} \nabla^2 \sqrt{n(\mathbf{r})} + V_t(\mathbf{r})n(\mathbf{r}) + \epsilon(n)n(\mathbf{r}) \right], \quad (1)$$

where the first, the second, and the third terms represent the kinetic energy of bosons, the energy due to the trapping potential, and the energy due to interatomic correlation within the LDA, respectively. Following the usual practice we use the perturbative expansion for  $\epsilon(n)$  in terms of the gas parameter  $na^3$ ,

$$\epsilon(n) = \frac{2\pi\hbar^2 a n}{m} \left[ 1 + \frac{128}{15\sqrt{\pi}} (na^3)^{1/2} + 8 \left( \frac{4\pi}{3} - \sqrt{3} \right) (na^3) \ln(na^3) + O(na^3) \right]. \quad (2)$$

The first term in the above expansion, which corresponds to the energy of the homogenous Bose gas within the mean-field theory as considered in the GP theory, was calculated by Bogoliubov [25]. The second term was obtained by Lee, Huang and Yang (LHY) [26], while the third term was first calculated by Wu [27] using the hard-sphere model for the interatomic potential. Although, it has been emphasized in the literature that the above expansion is valid only for  $na^3 \ll 1$ , it is only recently that the range of validity of the above expansion has been systematically investigated by Giorgini *et al.* [28]. They have used the diffusion Monte Carlo (DMC) method to calculate the ground state of uniform gas of bosons interacting through different model potentials with  $a > 0$ . It has been found that the expansion (2) is valid as long as  $na^3 < 10^{-3}$ . However, for the values of the gas parameter beyond  $10^{-3}$  the inclusion of the logarithmic term leads to a severe mismatch with the DMC simulation results. On the other hand, expansion (2) up to the LHY term gives an accurate representation of the DMC calculations even for the gas parameter of the order of  $10^{-2}$ . Consequently, we do not consider the logarithmic term in the expansion (2) for all the calculations in this study.

The trapping potential  $V_t(\mathbf{r})$  is taken to be axially symmetric characterized by two angular frequencies  $\omega_\perp^0$  and  $\omega_z^0$  ( $\omega_x^0 = \omega_y^0 = \omega_\perp^0 \neq \omega_z^0$ ). It is given by

$$V_t(\mathbf{r}) = \frac{m\omega_\perp^0{}^2}{2} (x^2 + y^2 + \lambda_0^2 z^2), \quad (3)$$

where  $\lambda_0 = \omega_z^0/\omega_\perp^0$  is the anisotropy parameter of the trapping potential ( $\lambda_0 = 1$  corresponds to a spherically symmetric trap).

The ground-state properties which are needed to calculate the collective frequencies are determined by minimizing the energy functional (1) with respect to the density  $n(\mathbf{r})$  [29] satisfying the normalization condition

$$\int n(\mathbf{r}) d\mathbf{r} = N. \quad (4)$$

To implement the variational scheme we take the ansatz for the ground-state density as [15,22]

$$n(\mathbf{r}_1) = \frac{p}{2\pi\Gamma\left(\frac{3}{2p}\right)} \lambda^{1/2} \left( \frac{\omega_\perp}{\omega_\perp^0} \right)^{3/2} e^{-(\omega_\perp/\omega_\perp^0)^p (r_{1\perp}^2 + \lambda_0^2 z_1^2)^p}, \quad (5)$$

where  $\lambda$ ,  $\omega_\perp$ , and  $p$  are the variational parameters which are obtained by minimizing  $E[n]$  with respect to these parameters. In the above equation we have used the scaled coordinates  $\mathbf{r}_1 = \mathbf{r}/a_{ho}$  with  $a_{ho} = (\hbar/m\omega_\perp^0)^{1/2}$ . We note that  $n(\mathbf{r}_1)$  is normalized to unity and from Eq. (4) it can be seen that

$$n(\mathbf{r}) = \frac{N}{a_{ho}^3} n(\mathbf{r}_1). \quad (6)$$

We make this choice of variational form for the density as it has been shown convincingly that this ansatz is capable of describing the ground state of Bose gas in a trap quite accurately both within [22] and beyond [15] the GP theory for a wide range of particle numbers. Using this variational form the physical observables can be expressed analytically in terms of three variational parameters [15]. The total energy  $E_1 = E/\hbar\omega_\perp^0$  can be written as [15]

$$\frac{E_1}{N} = T + U + E_{int}^1 + E_{int}^2. \quad (7)$$

Here  $T$  and  $U$  denote the average kinetic and the trapping potential energies per particle, respectively. The term  $E_{int}^1$  gives the interaction energy per particle in the mean-field approximation as considered in the GP theory while  $E_{int}^2$  gives the correction in the interaction energy due to the LHY term in the expansion (2) arising from the BGP theory.

The ground-state energy components obtained from the variational calculation are employed to compute the frequencies of collective oscillations by using the sum-rule approach of many-body response theory. In the following we briefly

outline the sum-rule approach and present some of the results which are relevant for the present work.

According to the basic result of the sum-rule approach [23,24] the upper bound of the lowest excitation energy is given by

$$\hbar\Omega_{ex} = \sqrt{\frac{m_3}{m_1}}, \quad (8)$$

where

$$m_p = \sum_n |\langle 0|F|n\rangle|^2 (\hbar\omega_{n0})^p \quad (9)$$

is the  $p$ th order moment of the excitation energy associated with the excitation operator  $F$  and  $\Omega_{ex}$  is the frequency of excitation. Here  $\hbar\omega_{n0} = E_n - E_0$  is the excitation energy of eigenstate  $|n\rangle$  of the Hamiltonian  $H$  of the system. The upper bound given by Eq. (8) is close to the exact lowest excited state when this state is highly collective, that is, when the oscillator strength is almost exhausted by a single mode. This condition is satisfied by the trapped bosons in most of the cases. Moreover, Eq. (8) can be used for computation of the excitation energies by exploiting the fact that the moments  $m_1$  and  $m_3$  can be expressed as expectation values of the commutators between  $F$  and  $H$  in the ground state  $|0\rangle$  [23,24],

$$\begin{aligned} m_1 &= \frac{1}{2} \langle 0 | [F^\dagger, [H, F]] | 0 \rangle, \\ m_3 &= \frac{1}{2} \langle 0 | [[F^\dagger, H], [H, [H, F]]] | 0 \rangle. \end{aligned} \quad (10)$$

The main advantage of the sum-rule approach is that it allows us to calculate the dynamic properties such as the excitation frequencies of many-body systems, with the knowledge of ground state  $|0\rangle$  (or the ground-state density) only. Thus, with the knowledge of a reasonably accurate ground-state density we calculate the expectation values given in Eq. (10) to determine the frequencies of collective oscillations. It is worth mentioning that the sum-rule approach has been extensively used to calculate collective frequencies of the trapped condensate [30,31].

For the purpose of calculation one needs to choose an appropriate excitation operator  $F$ . In this paper we concentrate only on the compressional collective mode characterized by the  $z$  component of angular momentum index,  $m' = 0$ . For the axially symmetric trap the mode  $m' = 0$  involves coupling of the monopole ( $l = 0$ ) and the quadrupole ( $l = 2$ ) modes. Following Kimura *et al.* [31] the operator  $F$  for the excitation of the  $m' = 0$  collective mode is written as

$$F = \sum_i (x_i^2 + y_i^2 - \alpha z_i^2), \quad (11)$$

where  $\alpha$  is a parameter characterizing the coupling of the two modes due to the axial symmetry of the trap. This parameter is obtained by making the excitation energy given by

Eq. (8) extremal. Here, we note that  $F$  given above can also be used to describe excitation of the monopole ( $\alpha = -1$ ) and the quadrupole ( $\alpha = 2$ ) modes separately. For a spherically symmetric trap ( $\lambda_0 = 1$ ) the two modes get decoupled and  $\alpha = -1$  and  $\alpha = 2$  correspond to the minimum and the maximum values of the excitation energies, respectively.

Using the energy functional given by Eq. (1) along with the expansion (2) we find after a tedious although straightforward algebra the following expressions for the moments  $m_1$  and  $m_3$ :

$$m_1 = \frac{4\hbar^2}{m^2} \left( \frac{U_\perp}{(\omega_\perp^0)^2} + \alpha^2 \frac{U_z}{(\omega_z^0)^2} \right), \quad (12)$$

$$\begin{aligned} m_3 &= \frac{8\hbar^4}{m^2} \left[ T_\perp + U_\perp + \alpha^2 (T_z + U_z) \right. \\ &\quad \left. + (1 - \alpha/2)^2 \left( E_{int}^1 + \frac{9}{4} E_{int}^2 \right) \right]. \end{aligned} \quad (13)$$

In the above equations  $T_\perp$  and  $U_\perp$  ( $T_z$  and  $U_z$ ) are the transverse components ( $z$  component) of the kinetic and potential energies, respectively. By substituting Eqs. (12) and (13) in Eq. (8) we get the following expression for the frequency of the  $m' = 0$  mode

$$\begin{aligned} \Omega_{m'=0}^2 &= 2 \left( \frac{T_\perp + U_\perp + \alpha^2 (T_z + U_z) + (1 - \alpha/2)^2 \left( E_{int}^1 + \frac{9}{4} E_{int}^2 \right)}{\frac{U_\perp}{(\omega_\perp^0)^2} + \alpha^2 \frac{U_z}{(\omega_z^0)^2}} \right). \end{aligned} \quad (14)$$

The frequency of collective oscillations is determined by substituting the values of energy components from the variational calculation and making  $\Omega_{m'=0}^2$  extremal with respect to  $\alpha$ . The variation with respect to  $\alpha$  leads to a quadratic equation in  $\alpha$  and the two roots, corresponding to the maximum ( $\alpha_+$ ) and the minimum ( $\alpha_-$ ) values of  $\Omega_{m'=0}^2$ , are

$$\alpha_\pm = -\frac{B}{2} \pm \frac{1}{2} \sqrt{B^2 + 4C}, \quad (15)$$

with

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

and

$$C = \frac{f_4}{f_5}, \quad (16)$$

where  $f_1 = T_\perp + U_\perp$ ,  $f_2 = T_z + U_z$ ,  $f_3 = E_{int}^1 + \frac{9}{4} E_{int}^2$ ,  $f_4 = U_\perp / (\omega_\perp^0)^2$ , and  $f_5 = U_z / (\omega_z^0)^2$ . In the next section we first apply these results to estimate analytically the correction to

the collective frequency due to the LHY term within the TF approximation followed by the results of our variational calculation.

### III. RESULTS AND DISCUSSION

#### A. Analytical estimate within TF approximation

Before discussing the results of our variational calculation we present the analytical estimate of collective frequencies within the TF approximation. We generalize the perturbative results of Refs. [17,18] and also discuss the validity regime of these results. For convenience we consider the case of a spherically symmetric trap ( $\lambda_0=1$ ). Generalization for the axially symmetric trap is straightforward. It is easy to verify that for spherically symmetric trap  $B=-1$  and  $C=2$  and the two roots are  $\alpha=2$  and  $\alpha=-1$  corresponding to the quadrupole and the monopole modes, respectively. It is well known that the frequency of the quadrupole mode is not affected by the LHY term [17]. Therefore we focus our attention on the monopole mode. By substituting  $\alpha=-1$  in Eq. (14) the frequency of the monopole mode of bosons in a spherical trap ( $U=U_\perp+U_z$ ) within the TF approximation ( $T_\perp=T_z=0$ ) can be written as

$$\frac{\Omega^2}{(\omega_\perp^0)^2} = \left[ \frac{U + \frac{9}{4}E_{int}^1 + \frac{81}{16}E_{int}^2}{U} \right]. \quad (17)$$

Hereafter we drop for convenience the subscript  $m'=0$  in  $\Omega$ . To eliminate  $U$  from the above equation we make use of the virial relation [15]

$$2T - 2U + 3E_{int}^1 + \frac{9}{2}E_{int}^2 = 0, \quad (18)$$

and obtain within the TF approximation

$$\frac{\Omega^2}{(\omega_\perp^0)^2} = \left[ \frac{\frac{15}{4}E_{int}^1 + \frac{117}{16}E_{int}^2}{\frac{3}{2}E_{int}^1 + \frac{9}{4}E_{int}^2} \right]. \quad (19)$$

We note that the expression given by Eq. (19) is exact within the TF limit. To derive an analytical expression for the frequency we express  $E_{int}^1$  and  $E_{int}^2$  in terms of parameter  $x = \sqrt{n(0)a^3}$ . This is done by using the analytical expressions for the total energy and chemical potential [2,15] obtained within the TF approximation with the LHY term included in the expansion  $\epsilon(n)$ . These expressions are

$$\begin{aligned} E_{int}^1 &= \frac{2}{7}\mu_{TF} - \frac{9}{16}\mu_{TF}x, \\ E_{int}^2 &= \frac{5}{8}\mu_{TF}x, \end{aligned} \quad (20)$$

where  $\mu_{TF}$  is the chemical potential of trapped bosons obtained within the TF approximation [2]. It is important to

note that the expressions for  $E_{int}^1$  and  $E_{int}^2$  given above [Eq. (20)] are approximate in nature and neglect terms of order  $O(na^3)$  and, thus, expected to be valid in the small gas parameter regime. It has been recently shown [16] that the expressions in Eq. (20) are not valid for very large gas parameters and lead to results which differ considerably from the exact results. In the large-gas-parameter regime one needs to solve the nonlinear equation of the density more accurately with the help of numerical methods. Consequently, to compute the frequencies of collective oscillation (for that matter any observable) in the large-gas-parameter regime within the TF approximation one needs a noniterative or non-perturbative method to solve the nonlinear equation. In this paper we take a different route to achieve this goal. Instead of solving the time-dependent differential equation for the density (or the time-dependent GP equation) we exploit the sum-rule approach of the many-body response theory along with the accurate ground-state density determined variationally to compute the frequencies of collective oscillations. We describe the results of such a calculation in the next subsection.

Now by substituting Eq. (20) in Eq. (19) we get following expression for the frequency of the monopole collective mode within the BGP theory:

$$\frac{\Omega}{\omega_0} = \left[ \frac{5 \left( 1 + \frac{147}{64}x \right)}{1 + \frac{21}{16}x} \right]^{1/2}, \quad (21)$$

where  $\omega_0$  is the angular frequency of the spherically symmetric trap. In the limit of  $x \rightarrow 0$  the above expression [Eq. (21)] correctly reduces to the mean-field result  $\Omega_{mf} = \sqrt{5}\omega_0$  within the TF approximation [30].

It is customary to define the fractional change in the frequency as [17,18]

$$\delta = \frac{1}{2} \left( \frac{\Omega^2 - \Omega_{mf}^2}{\Omega_{mf}^2} \right). \quad (22)$$

By using Eq. (21) we get

$$\delta = \frac{\frac{63}{128}x}{1 + \frac{21}{16}x}. \quad (23)$$

In the limit of  $x \ll 1$  we recover the results of Refs. [17,18]. Figure 1 shows the fractional change  $\delta$  as a function of the dimensionless parameter  $a/a_0$  (where  $a_0$  is the Bohr radius of hydrogen atom) for  $N=10^4$   $^{85}\text{Rb}$  atoms trapped in a spherical trap with  $\omega_0/2\pi = [(\omega_\perp^0)^2 \omega_z^0]^{1/3}/2\pi = 12.83$  Hz, where  $\omega_\perp^0 = 2\pi \times 17.5$  Hz and  $\omega_z^0 = 2\pi \times 6.9$  Hz [10]. The values of the parameter  $a/a_0$  are chosen such that the condition for the TF approximation, that is,  $Na/a_{h0} \gg 1$  is satisfied. Moreover, as discussed above Eq. (20) [and hence Eq. (21)] is valid only for small gas parameter values and accord-



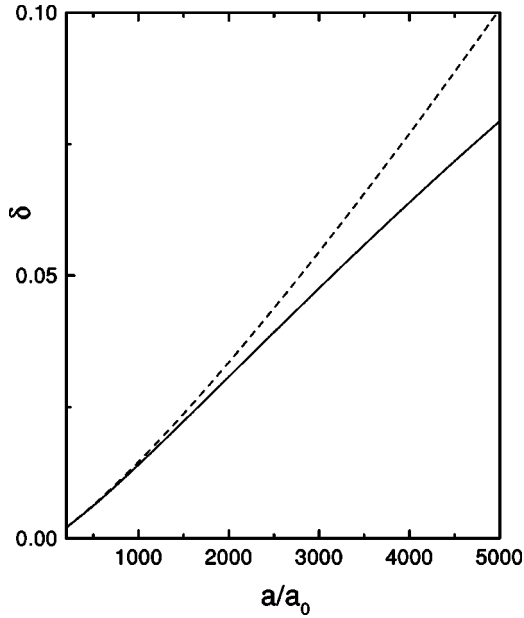


FIG. 1. Fractional shift of the frequency of  $m'=0$  mode in a spherically symmetric trap with  $\omega_0 = 2\pi \times 12.83$  Hz. The solid line corresponds to Eq. (23) and the dashed line shows the results of Refs. [17,18].

ingly we have restricted ourselves to  $a/a_0 = 5000$ . It is evident from Fig. 1 that the correction to the monopole frequency due to the inclusion of the LHY term in the interatomic correlation energy obtained by us is slightly lower than the corresponding results of Refs. [17,18]. In particular for  $a/a_0 = 5000$  we obtain a 7% change in the monopole frequency as compared to the correction of 9% predicted in Refs. [17,18]. It is only for very small values of  $x$  (less than  $10^{-3}$ ) that fractional corrections obtained in Refs. [17,18] match with Eq. (23).

### B. Variational results

Before discussing the results for the excitation frequencies obtained by the variational method, we first demonstrate that this method is capable of yielding sufficiently accurate results for the ground-state properties of BEC even for large gas parameter values, as achieved in the experiment of Cornish *et al.* [10]. The parameters used in this calculation are similar to the ones used in the previous section. We present these results in Tables I and II for the spherically symmetric and the axially symmetric traps, respectively. To check the accuracy, we compare our variational results with those of Ref. [16] (presented in parentheses in Tables I and II) obtained by numerically solving the modified GP equation. The results in Tables I and II clearly show that the variational method gives quite accurate results for the ground-state properties as they compare very well with the numbers of Ref. [16]. Therefore the variational method is indeed suitable for describing the ground-state properties even in the regime of large gas parameters. The accuracy of our variational results was further checked by verifying that the generalized virial relation as given in Eq. (18) is satisfied. In all the variational calculations the virial relation was satisfied up to

TABLE I. Results for the ground-state properties of  $^{85}\text{Rb}$  atoms trapped in an isotropic trap with  $\omega_\perp^0/2\pi = 17.5$  Hz. Total energy  $E_1/N$  and chemical potential  $\mu_1$  are in units of  $\hbar\omega_\perp^0$ . Numbers in parentheses are results of Ref. [16]. The values of parameter  $Na/a_{h0}$  given in the second column signify the importance of the interaction energy over the kinetic energy.

$a/a_0$	$Na/a_{h0}$	$E_1/N$	$\mu_1$
1400	243.38	10.03 (10.01)	14.05 (13.97)
3000	522.0	14.14 (14.10)	19.92 (19.84)
8000	1392.0	23.52 (23.43)	33.54 (33.38)
10000	1740	26.75 (26.63)	38.24 (38.06)

the fifth decimal place or better. This indicates that not only the total energy but its different components are also obtained accurately by the variational method, which is quite crucial for the calculation of the frequencies of collective oscillations.

Now we focus our attention on the results for the frequencies of collective oscillations of trapped bosons. Figures. 2 and 3 show the upper ( $\Omega_u$ ) and the lower ( $\Omega_l$ ) frequencies, respectively, associated with the breathing mode as a function of the dimensionless parameter  $a/a_0$ . The results presented in Figs. 2 and 3 correspond to the axially symmetric trap which is more relevant from the experimental point of view. Notice that the maximum value of the parameter  $a/a_0$  is chosen to be  $10^4$  in accordance with the experimental number [10] and the corresponding value of the peak gas parameter is  $\approx 10^{-2}$ . For comparison we also show in these figures the corresponding results obtained within the GP theory. It is important to note here that the GP results shown in Figs. 2 and 3 are also obtained variationally by dropping the LHY term from the expansion (2) and thus, retaining only the first term. The results corresponding to the GP case obtained by us match quite well with those already reported

TABLE II. Results for the ground-state properties of  $^{85}\text{Rb}$  atoms trapped in an axially symmetric trap with  $\omega_\perp^0/2\pi = 17.5$  Hz and  $\lambda_0 = 0.39$ . Total energy  $E_1/N$  and chemical potential  $\mu_1$  are in units of  $\hbar\omega_\perp^0$ . The numbers in parentheses are results of Ref. [16]. The values of parameter  $Na/a_{h0}$  given in the second column signify the importance of the interaction energy over the kinetic energy.

$a/a_0$	$Na/a_{h0}$	$E_1/N$	$\mu_1$
1400	284.25	7.36 (7.33)	10.25 (10.22)
3000	609.0	10.35 (10.31)	14.55 (14.51)
8000	1624.0	17.18 (17.09)	24.49 (24.38)
10000	2030.0	19.53 (19.43)	27.92 (27.79)

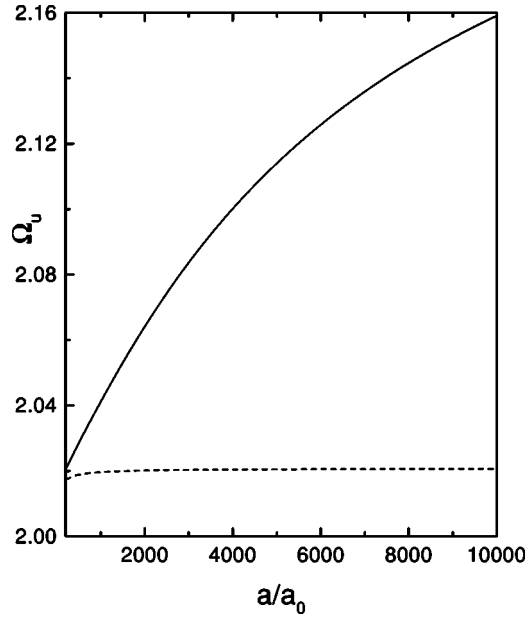


FIG. 2. The frequencies (in units of  $\omega_{\perp}^0$ ) of the upper branch of the collective mode  $m'=0$  of  $10^4$   $^{85}\text{Rb}$  atoms confined in an axially symmetric trap with  $\lambda_0=0.39$  and  $\omega_{\perp}^0=2\pi\times 17.5$  Hz. The solid line represents results for the BGP case while the corresponding GP results are shown by the dashed line.

in the literature [30–38]. It can be clearly seen from Fig. 2 that for small values of the gas parameter the numbers obtained within the GP and the BGP theory are quite close. The difference between these two results, however, increases with  $a$ . For example, for  $a/a_0=8000$  the BGP number for  $\Omega_u$  is 6% higher than the corresponding mean-field GP result. Thus we conclude that the introduction of the LHY term in the interatomic correlation energy results in a significant correction to the upper frequency  $\Omega_u$  of  $m'=0$  mode of the

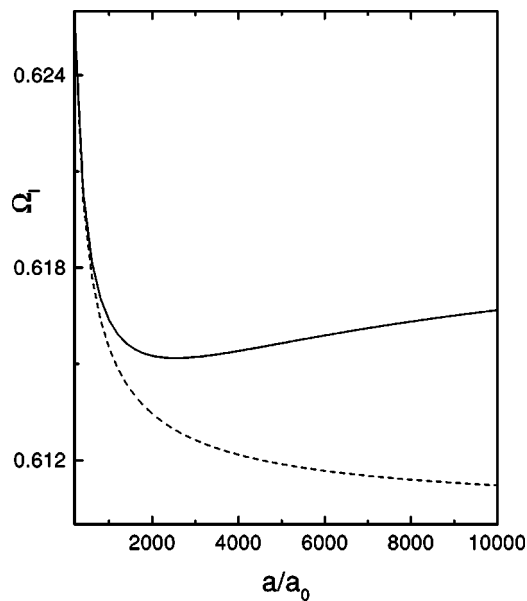


FIG. 3. The frequencies (in units of  $\omega_{\perp}^0$ ) of the lower branch of collective mode  $m'=0$ . The parameters are the same as in Fig. 2

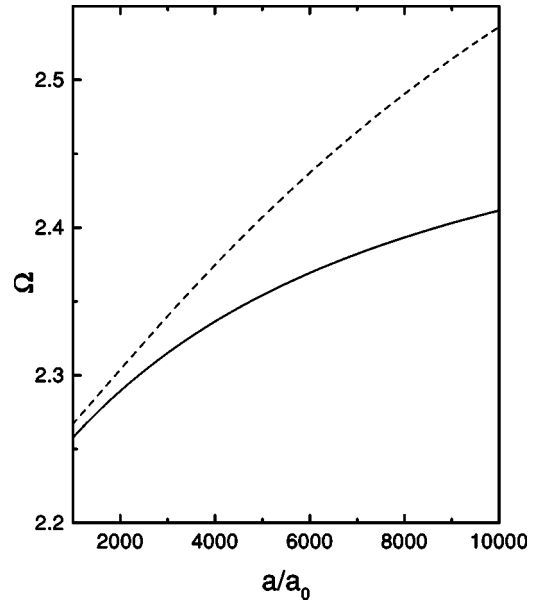


FIG. 4. The frequencies (in units of  $\omega_0$ ) of the monopole mode of  $10^4$   $^{85}\text{Rb}$  atoms confined in a spherically symmetric trap with parameters the same as Fig. 1. The solid line represents results for the BGP case and the dashed line shows results obtained from Eq. (21).

collective oscillations. Considering the accuracy of current experiments [9] in measuring the frequencies of the collective excitations, it should be possible to observe these corrections experimentally. It is also important to note that the frequency  $\Omega_u$  obtained within the GP theory remains almost constant with the increase in the parameter  $a/a_0$ . In contrast, the BGP theory predicts  $\Omega_u$  growing monotonically with  $a/a_0$ . Therefore a signature of the predictions of the BGP theory can be observed by measuring  $a/a_0$  dependence of the excitation frequency  $\Omega_u$ .

Next we focus our attention on the lower frequency  $\Omega_l$  of the breathing mode which is shown in Fig. 3. For small values of the gas parameter the frequency of the lower branch obtained via GP theory is very close to the corresponding BGP theory result. In the same regime of the gas parameter the frequency  $\Omega_l$  decreases with the gas parameter both for the GP and the BGP cases. The decrease of the lower frequency with an increase in the gas parameter value has already been theoretically predicted [30,32,34,37] and experimentally verified as well [39]. However, in contrast to the GP case, the frequency of the lower branch for the BGP case starts increasing, albeit slowly, after a critical value of  $a/a_0 \approx 2200$ . It is also noteworthy that the change in the frequency  $\Omega_l$  obtained from the BGP theory is considerably lower than that in the upper frequency  $\Omega_u$ . For example, for  $N=10^4$  and  $a/a_0=8000$  the change in the lower frequency is just 0.8% while that in the upper frequency is 6%.

We conclude this section by making a comparison of the frequencies obtained by using the analytical expression as given in Eq. (21) with the results obtained by the variational approach. The comparison is shown in Fig. 4 where we plot the frequency of the monopole mode of a condensate in a spherically symmetric trap as a function of  $a/a_0$  obtained

using Eq. (21) (dashed line) and using the variational method (solid line). The range of values of  $a/a_0$  is chosen such that the TF approximation (i.e.,  $Na/a_{h0} \gg 1$ ) is satisfied. Accordingly the minimum value of  $a/a_0$  in Fig. 4 is chosen to be  $10^3$  which corresponds to  $Na/a_{h0} = 174$ . It can be seen that the results obtained using Eq. (21) are systematically higher than the corresponding results from variational calculation and the difference between the two grows as the value of the gas parameter is increased. Moreover, we also note that the two results are reasonably close for values of  $a/a_0$  of the order of 3500 [ $n(0)a^3 \approx 3.77 \times 10^{-3}$ ]. Therefore, we emphasize that the correction obtained within the TF approximation as given by Eq. (21) is valid as long as the gas parameter is of the order of  $10^{-3}$ . As discussed earlier, for condensates with the values of the gas parameter beyond  $10^{-3}$  one needs to evaluate  $E_{int}^1$  and  $E_{int}^2$  in a nonperturbative manner. The variational approach employed in this paper accomplishes exactly this task.

#### IV. CONCLUSION

In this paper we have calculated the frequencies of the collective excitation of a trapped condensate in the large-gas-parameter regime using the BGP theory. To go beyond the GP theory we have included a higher-order term (the LHY

term) in the interatomic correlation energy obtained from the ground-state energy of a uniform Bose gas. The calculations of the frequencies were performed by employing the sum-rule approach of many-body response theory along with the variational method to obtain the ground-state energy components. We have also derived an analytical expression for the corrections to the frequencies of the compressional mode valid for small gas parameters within the TF approximation. The results of our variational calculations clearly show that for large gas parameter values, the frequencies of the compressional mode characterized by the index  $m'=0$  are significantly altered. Although the change in the lower branch of the  $m'=0$  mode,  $\Omega_l$ , is small, we observe a new qualitative feature. The frequency  $\Omega_l$  increases slowly as the gas parameter exceeds a critical value in contrast to a monotonically decrease predicted within the GP theory. It would be very interesting to verify the predictions of the BGP theory by measuring collective excitation frequencies for condensates with large gas parameter as reported in Ref. [10].

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