Properties of trapped Bose gas with vortices in large-gas-parameter regime

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We study the properties of vortex states of a trapped Bose gas in the large-gas-parameter regime. To test the validity of the Gross-Pitaevskii theory in this regime for vortex states, we compare the results of the Gross-Pitaevskii and the modified Gross-Pitaevskii calculations for the total energy, chemical potential, density profile, and frequency shift of the quadrupole modes of the collective oscillations of a harmonically trapped condensate carrying a single quantized vortex. We find that in the large-gas-parameter regime, two calculations give substantially different results for all the properties mentioned above.

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I. INTRODUCTION

The mean-field Gross-Pitaevskii (GP) theory [1] has been quite successful in describing both static and dynamic properties of Bose-Einstein condensates (BEC) of alkali-metal atoms confined in magnetic or optical traps [2–6]. It is well known that the GP theory is valid for condensates satisfying the dilute gas condition $na^3 \ll 1$ (where n is the atomic density, a is the s-wave scattering length of the interatomic potential, and the parameter $x=na^3$ is called the gas parameter). Physically it implies that an interacting atomic gas can be considered to be dilute when the average distance between the atoms ($\propto n^{-1/3}$) is much larger than the range of the atomic potential ($\propto a$). Moreover, under this condition the detailed shape of the interatomic potential is not required, rather the boson-boson interaction can be simulated by a pseudopotential which is completely characterized by the scattering length a. It is important to note here that in some recent theoretical studies it was shown that as long as $x \leqslant 10^{-3}$, the GP theory produces accurate results for both static [7–10] and dynamic properties [11,12]. Typically, the values of the gas parameter in most of the experiments were in the range of $10^{-4}-10^{-5}$ and therefore the GP theory works very well in predicting the properties of these trapped condensates. However, in a recent experiment, condensates with peak gas parameter, of the order of 10^{-2} have been achieved by enhancing the scattering length a with the help of Fesbach resonance [13]. For condensates with such large values of the gas parameter, the question of validity of the GP theory has been raised and tested [10,12] by employing modified GP (MGP) theory within the local-density approximation. These studies clearly show that for large values of the gas parameter ($\approx 10^{-2}$), both ground-state (energy, chemical potential) and dynamic properties (frequencies of collective oscillations) are significantly modified by the MGP theory.

The vortex states in trapped condensates play an important role in establishing the superfluid properties of BEC [2,3]. It is then natural to ask how the properties of vortex states are modified in the large-gas-parameter regime. This has motivated us to study the properties of trapped condensates with vortex states in the large-gas-parameter regime. To describe the condensates in the large-gas-parameter regime, we employ the MGP theory that is considered to be applicable in this regime. By comparing the MGP results with the corresponding GP numbers, we make a systematic assessment of the corrections introduced by the MGP calculations over the GP results. In this paper, we consider condensates with the values of the gas parameter spanning a range similar to that achieved in the experiment of Cornish *et al.* [13]. The results presented in this paper can be divided into two parts. In the first part, we focus our attention on the modifications of the energy, chemical potential, and the density profile of BEC with a single quantized vortex in the large-gas-parameter regime.

The quantized vortex state not only affects the static properties of the condensate, but it also modifies the dynamic properties. For example, the presence of a quantized vortex state leads to splitting of the two modes of the quadrupole oscillations with opposite values of the third component of angular momentum, which are degenerate in the absence of a quantized vortex state [14–19]. The vortex state breaks the time-reversal symmetry, which in turn results in the removal of the degeneracy of the two modes of oscillations carrying opposite values of angular momentum. Therefore, splitting of the two quadrupole modes of collective oscillations can be employed to detect the presence of quantized vortex states in BEC [19] as the measurement of frequencies of the collective oscillations can be carried out with high precision. In the second part of this paper, we focus our attention on the effect of the large gas parameter on the splitting of the two degenerate quadrupole modes due to the presence of a vortex state. We calculate and compare the results for the frequency shift caused by the splitting between the two quadrupole modes by employing the GP and the MGP equations in the large-gas-parameter regime.

For the purpose of calculation, we use the variational approach [20] with a quite accurate variational ansatz for the wave function of a harmonically trapped condensate with a quantized vortex line along the z axis, and the frequency shifts of the quadrupole modes are then obtained by employing the well established sum-rule approach [21–23].

The paper is organized in the following manner. In Sec. II, we describe the theoretical methods employed in this paper and briefly describe the MGP theory followed by the variational method employed to obtain the wave function of the vortex state and other physical observables mentioned above and the sum-rule approach for the calculation of frequencies of collective oscillations. Sec. III is devoted to a discussion of the results. The paper is concluded in Sec. IV.

II. THEORY

The ground-state energy functional associated with a condensate of N bosons each with mass m confined in a trap potential $V_t(\mathbf{r})$ can be written as [7]

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

where $\Psi(\mathbf{r})$ is the condensate wave function (order parameter) and $n(\mathbf{r})$ represents the corresponding density and it is given by $n(\mathbf{r})=|\Psi(\mathbf{r})|^2$. The condensate wave function $\Psi(\mathbf{r})$ can be determined by minimizing the above energy functional. In the above equation, the first, second, and third terms represent the kinetic energy of bosons, the energy due to the trapping potential, and the interatomic interaction energy within the local-density approximation (LDA), respectively. To go beyond the GP theory, we make use of the perturbative expansion for $\epsilon(n)$ in terms of the gas parameter na^3,

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

The first term in the above expansion, which corresponds to the energy of the homogeneous Bose gas within the mean-field theory as considered in the GP theory, was calculated by Bogoliubov [24]. The second term was obtained by Lee, Huang, and Yang (LHY) [25], while the third term was first calculated by Wu [26] 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.* [27]. They have used the diffusion Monte Carlo (DMC) method to calculate the ground state of a 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 a 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 performed 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 ω_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 energy functional (1) can be easily generalized to include the vortex states. In this paper, we consider condensates with a vortex line along the z axis and all the atoms are flowing around it. The wave function for such a state can be written as [28]

$$\Psi(\mathbf{r}) = \psi(\mathbf{r})e^{i\kappa\phi}, \quad (4)$$

where ϕ is the angle around the z axis and κ is an integer denoting the quantum circulation, and the total angular momentum along the z axis is given by $N\hbar\kappa$. Substituting the above complex wave function [Eq. (4)] in Eq. (1), we get the MGP energy functional for the condensates with a vortex state as [28]

$$E[\psi] = \int d\mathbf{r}\left[\frac{\hbar^2}{2m}|\nabla\psi|^2 + \frac{\hbar^2\kappa^2}{2mr_\perp^2}|\psi|^2 + v_{\text{ext}}(\mathbf{r})|\psi|^2 + \epsilon(n)|\psi|^2\right]. \quad (5)$$

In the above equation, $r_\perp=\sqrt{x^2+y^2}$ denotes the transverse radius and the density $n(\mathbf{r})=|\psi(\mathbf{r})|^2$. The presence of a centrifugal term due to the vortex state makes the above functional different from Eq. (1). The GP energy functional for the vortex states can be obtained from the above functional by neglecting the LHY and the logarithmic terms in $\epsilon(n)$. The minimization of the above functional with respect to $\psi(\mathbf{r})$ with the constraint

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

leads to the MGP equation for the condensate with a vortex state,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{\hbar^2\kappa^2}{2mr_\perp^2} + V_t(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m}|\psi|^2 \times\left(1 + \frac{32a^{3/2}}{3\pi^{1/2}}|\psi|\right)\right]\psi(\mathbf{r}) = \mu\psi(\mathbf{r}), \quad (7)$$

where μ is the chemical potential arising from the constraint condition given by Eq. (6). The GP equation for the vortex state can be obtained from Eq. (7) by neglecting the interaction energy term proportional to $|\psi|^3$ from the left-hand side of this equation. It is not possible to find an exact solution to Eq. (7). Consequently, various numerical techniques have been developed to solve the above nonlinear Schrödinger equation for studying the properties of trapped BEC [29,30]. In this paper, we use the variational method to obtain the wave function (or the density) and other relevant physical observables of the condensate. The main advantage of this method is that with a suitable choice for the form of the wave function, one can get quite accurate results with less computational effort. In our earlier work [9,12,20], we demonstrated the applicability of the variational method by calculating the ground-state properties and the collective oscillation frequencies of condensates both with the GP and the MGP equations for a wide range of values of particle number and scattering length.

Following Ref. [20], the variational form for the wave function of the condensate with a quantized vortex state is chosen as

$$\psi(\mathbf{r}_1) = A r_{1\perp}^{q} e^{-(1/2)(\omega_\perp/\omega_\perp^0)^p (r_{1\perp}^2 + \lambda z_1^2)^p}, \tag{8}$$

where q, λ, $\omega_\perp$, and p are the variational parameters which are obtained by minimizing the energy functional given by Eq. (5) with respect to these parameters. In the above equation, we use 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. (6) it can be seen that

$$n(\mathbf{r}) = \frac{N}{a_{h0}^3} n(\mathbf{r}_1). \tag{9}$$

The above variational form for the wave function has already been shown to describe the state of the dilute Bose gas with a quantized vortex confined in a trap quite accurately for a wide range of particle numbers [20]. In this paper, we extend the applicability of this wave function in the large-gas-parameter regime also.

The proportionality factor A in Eq. (8) is determined by the normalization condition [Eq. (6)]

$$A^2 = \frac{\sqrt{\lambda} p \Gamma(3/2+q)}{\pi^{3/2}\Gamma(1+q)\Gamma((3/2+q)/2p)} \left(\frac{\omega_\perp}{\omega_\perp^0}\right)^{(3/2+q)}. \tag{10}$$

Using this variational form for the wave function, physical observables can be expressed analytically in terms of the four variational parameters. For example, the total energy $E_1 = E/\hbar\omega_\perp^0$ and the chemical potential $\mu_1 = \mu/\hbar\omega_\perp^0$ can be written as

$$\frac{E_1}{N} = T + U + E_{\rm rot} + E_{\rm int}^1 + E_{\rm int}^2 \tag{11}$$

and

$$\mu_1 = T + U + E_{\rm rot} + 2E_{\rm int}^1 + \frac{5E_{\rm int}^2}{2}, \tag{12}$$

respectively. Here T, U, and $E_{\rm rot}$ denote the average kinetic, trapping potential, and the rotational energies per particle, respectively. The term $E_{\rm int}^1$ gives the interaction energy per particle in the mean-field approximation as considered in the GP theory, while $E_{\rm int}^2$ gives the correction due to the LHY term in the expansion (2) resulting in the MGP functional. The analytical expressions for these energy components are

$$T = \frac{\omega_\perp(1+2q)[(1+2p)(1+\lambda/2)+q(2p+2q+\lambda)]\Gamma((1+2q)/2p)}{\omega_\perp^0 4(3+2q)\Gamma((3+2q)/2p)}, \tag{13}$$

$$U = \frac{\omega_\perp^0(1+q+\lambda_0^2/2\lambda)\Gamma((5+2q)/2p)}{\omega_\perp(3+2q)\Gamma((3+2q)/2p)}, \tag{14}$$

$$E_{\rm rot} = \frac{\kappa^2\omega_\perp(1+2q)\Gamma((1+2q)/2p)}{4\omega_\perp^0 q\Gamma((3+2q)/2p)}, \tag{15}$$

$$E_{\rm int}^1 = 2N\tilde{a}\left(\frac{\omega_\perp}{\omega_\perp^0}\right)^{3/2} \frac{p\sqrt{\lambda}\Gamma^2(q+3/2)\Gamma(2q+1)\Gamma((4q+3)/2p)}{2^{(4q+3)/2p}\sqrt{\pi}\Gamma^2((2q+3)/2p)\Gamma^2(q+1)\Gamma(2q+3/2)}, \tag{16}$$

and

$$E_{\rm int}^2 = \frac{128}{15\sqrt{2}\pi}\frac{2\sqrt{2}}{\pi^{9/4}} N^{3/2}\tilde{a}^{5/2}\left(\frac{\omega_\perp}{\omega_\perp^0}\right)^{9/4}\left(\frac{2}{5}\right)^{(5q+3/2p)} p^{3/2}\lambda^{3/4}\frac{\Gamma^{5/2}(q+3/2)\Gamma(5q/2+1)\Gamma((5q+3)/2p)}{\Gamma^{5/2}((2q+3)/2p)\Gamma^{5/2}(q+1)\Gamma((5q+3)/2)}, \tag{17}$$

where $\tilde{a} = a/a_{ho}$ and $\Gamma(m)$ is the gamma function. It is easy to check that the above energy components correctly reduce to the expressions derived in [9] for the case of condensates without a quantized vortex by setting κ and q equal to zero. For particular values of N and $\tilde{a}$, the parameters $\omega_\perp$, q, λ, and p are obtained by minimizing the energy given by Eq. (11) and Eqs. (13)–(17).

Having described the variational method for obtaining the wave function and other physical observables, we now describe the sum-rule approach of many-body response theory for the calculation of frequencies of the collective oscillations. The main advantage of this approach is that the calculation of frequencies requires the knowledge of the ground-state wave function (or the ground-state density) of the many-body system only. This method has been extensively applied to calculate the frequencies of the collective oscillations of trapped atomic gases [3]. In this paper, we follow the sum-rule approach developed in Ref. [16] for the calculation of the splitting of the quadrupole modes of the collective oscillations.

The collective excitations of any many-body system are generally probed by applying an external excitation field. For the excitation operators F_+ and F_- exciting two quadrupole modes with opposite angular momentum, respectively, the

corresponding strength functions are given by [22,23]

$$S_{\pm}(E) = \sum_n |\langle 0|F_{\pm}|n\rangle|^2 \delta(E - E_n), \tag{18}$$

where $|0\rangle$ denotes the ground state of the system and $E_n - E_0$ is the excitation energy of the eigenstate $|n\rangle$ of the Hamiltonian H relative to the ground-state energy E_0. The pth order moments of the strength function can be defined as

$$m_p^{\pm} = \int E^p [S_+(E) \pm S_-(E)] dE. \tag{19}$$

These moments provide various energy-weighted sum rules, which are employed to obtain the frequencies of the collective oscillations. An important property of these moments is that, for a given p, some of the moments can be expressed in terms of the commutators of the excitation operators with the Hamiltonian H. Some of the energy-weighted sum rules which are relevant for this paper are

$$m_0^- = \langle 0|[F^\dagger, F]|0\rangle,$$

$$m_1^+ = \langle 0|[F^\dagger, [H, F]]|0\rangle,$$

$$m_2^- = \langle 0|[[F^\dagger, H], [H, F]]|0\rangle,$$

$$m_3^+ = \langle 0|[[F^\dagger, H], [H, [H, F]]]|0\rangle, \tag{20}$$

where $[,]$ represents the commutator between the corresponding operators.

These expressions can be used to calculate the frequency shifts of the quadrupole oscillations of a trapped condensate. For the quadrupole case, we will consider the modes excited by the operators

$$F_{\pm} = (x \pm iy)^2 \tag{21}$$

carrying angular momentum $m_z = \pm 2$, where m_z represents the z component of angular momentum of the elementary excitation. In order to use the above expressions for the calculation of the shift in frequencies of quadrupole modes, we now assume that the moments m_p^+ (m_p^-) are exhausted by a single excitation with frequency ω_+ (ω_-) and the corresponding strength is σ_+ (σ_-). Under such a single-mode approximation, the strength distributions can be written as

$$S_{\pm}(E) = \sigma_{\pm} \delta(E - \hbar\, \omega_{\pm}). \tag{22}$$

Moreover, the vanishing of m_0^- [as given by the first moment of Eq. (20)] due to the commutator of F_+ and F_- being zero leads to the result $\sigma_+ = \sigma_- = \sigma$. We note here that the single-mode approximation is well suited for the condensates with a large number of atoms N and positive scattering length a [16]. Using Eqs. (22) and (19), we obtain the following expression for the difference between the two frequencies:

$$\hbar\, \delta = \hbar\, (\omega_+ - \omega_-) = \frac{m_2^-}{m_1^+}. \tag{23}$$

Furthermore, the individual frequencies of the quadrupole oscillations can be determined by using Eq. (23) along with the expression for the square of the mean frequency, as given in Ref. [31],

$$\hbar^2 \left(\frac{\omega_+ + \omega_-}{2} \right)^2 = \frac{m_3^+}{m_1^+} - \frac{3}{4} (\hbar\, \delta)^2. \tag{24}$$

In the next section, we calculate the moments m_1^+, m_2^-, and m_3^+ in terms of some averages over the vortex state wave function, and we use Eqs. (23) and (24) to determine the frequency shifts between the two quadrupole modes due to the presence of a quantized vortex in a trapped condensate falling in the large-gas-parameter regime.

III. RESULTS AND DISCUSSION

A. Ground-state properties

We begin this section with a comparison of our results obtained by the variational method with the corresponding numbers of Ref. [32] calculated by solving the MGP equation with the help of the steepest-descent method. We make this comparison to check the accuracy of the variational approach, as it has been shown in Ref. [32] that their MGP results are in very good agreement with the results of *ab initio* variational Monte Carlo calculations both in the presence and in the absence of a vortex state. At this point we note that in addition to the comparison with the *ab initio* results, the virial relation among the different energy components also provides a way of checking the correctness and the accuracy of the variational solutions. For the MGP theory, in the presence of a single quantized vortex the virial relation is given by

$$2T - 2U + 2E_{\rm rot} + 3E_{\rm int}^1 + \frac{9}{2} E_{\rm int}^2 = 0. \tag{25}$$

This expression has been derived by using the variational nature of the ground-state energy and the scaling transformation $n(\mathbf{r}_\eta) \rightarrow \eta^3 n(\mathbf{r})$. In all our calculations, the virial relation given above is satisfied up to the sixth decimal place or better. This indicates that the variational method employed in this paper yields quite accurate results for condensates with a vortex state in the large-gas-parameter regime.

For the purpose of comparison, we calculate the total energy, individual energy components given by Eqs. (13)–(17) and the chemical potential of harmonically trapped ^{87}Rb condensates carrying a single vortex state ($\kappa = 1$). In accordance with Ref. [32], we consider a disk-shaped trap with $\lambda_0 = \sqrt{8}$ and $\omega_z^0 = 2\pi \times 220$ Hz confining $N = 500$ condensate atoms and the scattering length is chosen to be $a = 0.151\,55 a_{ho}$ $[a_{ho} = (\hbar/m\omega_\perp^0)^{1/2}]$. The results of this calculation are shown in Table I along with the corresponding numbers of Ref. [32] in parentheses. It can be clearly seen from Table I that the numbers obtained by the variational method are very close to the corresponding results of Ref. [32]. In particular, our numbers for the total energy, the trap energy, and both components of interaction energy are slightly higher, (of the order of 1%) than those of Ref. [32]. On the other hand, our results for the kinetic and the rotational energies are appreciably lower and higher, respectively, than the corresponding num-

TABLE I. Results for the chemical potential and the energies in units of $\hbar\omega_{\perp}^{0}$ obtained from the GP and the MGP calculations for the condensate of $N=500$ ^{85}Rb atoms carrying a single vortex ($\kappa=1$). The condensate is trapped in an anisotropic trap with $\lambda_0=\sqrt{8}$ and $\omega_z^0=2\pi\times 220$ Hz. The scattering length is $\tilde{a}=a/a_{ho}=0.151\,55$. Numbers in parentheses are the results of Ref. [32]

	μ_1	E_1/N	T/N	U/N	$E_{\rm int}^1/N$	$E_{\rm int}^2/N$	$E_{\rm rot}/N$
GP	13.334	9.889	0.3926	5.8056	3.445		0.2463
	(13.187)	(9.7836)	(0.4251)	(5.7427)	(3.4039)		(0.2119)
MGP	15.811	11.443	0.3405	7.1248	2.4999	1.2454	0.2324
	(15.623)	(11.305)	(0.37692)	(7.0377)	(2.4824)	(1.2233)	(0.1849)

bers reported in Ref. [32]. Despite this difference between the results for the kinetic and the rotational energies, the results for the total energy and the chemical potential obtained by two methods match quite well. Moreover, we find that for the above choice of N and a, the MGP results for the total energy and the chemical potential are approximately 19% and 16%, respectively, higher than the corresponding GP numbers. To gain further insight, we compare the density profiles obtained by these two methods in Fig. 1 both for the GP and the MGP cases. Once again we find a good overall agreement. There are some differences in the core region. The density attains its maximum more rapidly for the steepest-descent method described in Ref. [32]. As a result of this, the peak values and peak positions of the density profiles obtained by the two methods are somewhat different. On the other hand, the tail regions of the density profiles obtained by the two methods match quite well. These results along with our earlier work [9,12,20] clearly demonstrate the applicability of the variational approach in calculating the properties of condensates both with and without a quantized vortex state in the large-gas-parameter regime.

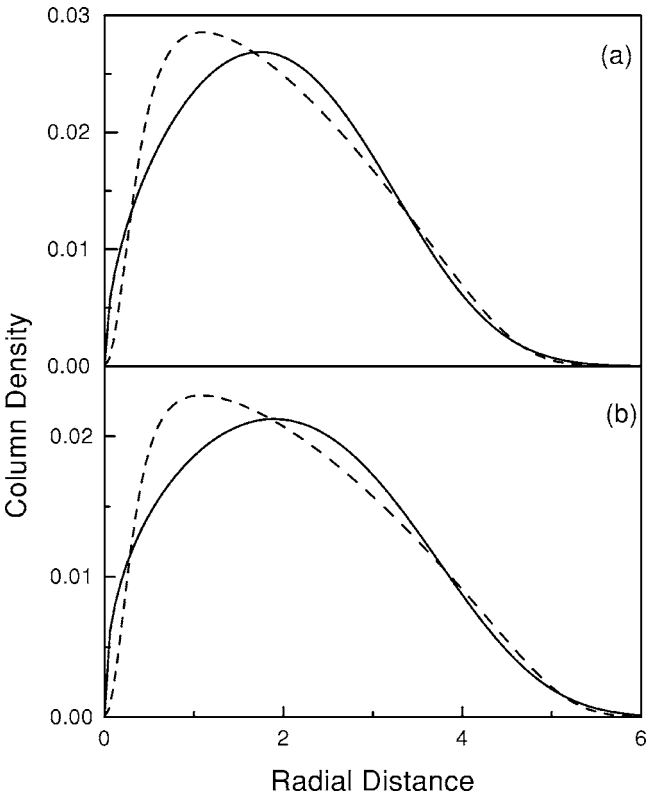

FIG. 1. Comparison of (a) GP and (b) MGP column density profiles as a function of the radial distance $r_{\perp}$, obtained by our variational formalism (solid lines) with the ones obtained by the method of steepest-descent in Ref. [32] (dashed lines) for a vortex state. The calculations are performed for a condensate of $N=500$ ^{85}Rb atoms trapped in an anisotropic trap with $\lambda_0=\sqrt{8}$ and $\omega_z^0=2\pi\times 220$ Hz. The scattering length is $\tilde{a}=a/a_{ho}=0.151\,55$.

Now we focus our attention on the application of the MGP theory to the condensates with a single quantized vortex for larger values of the gas parameter as achieved in the experiment of Cornish *et al.* [13]. In accordance with the experiment, we consider $N=10^4$ ^{85}Rb atoms confined in an anisotropic trap with frequencies $\omega_{\perp}^0=2\pi\times 17.5$ Hz and $\omega_z^0=2\pi\times 6.9$ Hz and the scattering length is varied from $a=1400a_0$ to $a=10\,000a_0$, where a_0 is the Bohr radius of hydrogen atom. We note here that this range of values of the scattering length falls in the large-gas-parameter regime as the maximum value of a corresponds to the peak gas parameter $x_{\rm peak}\approx 10^{-2}$. In Table II, we show the MGP results for the total energy and the chemical potential and compare them with the corresponding GP numbers. It clearly shows that the difference between the MGP and the GP results increases with the increase in the scattering length. For $a/a_0=1400$, the differences in the total energy and the chemical potential are approximately 3% and 4%, respectively. On the other hand, for the maximum value of $a/a_0=10\,000$, the MGP results for the total energy and the chemical potential are higher by around 26% and 30%, respectively, over the corresponding GP numbers. From these results, we conclude

TABLE II. Results for the chemical potential and the total energy per unit number of bosons in units of $\hbar\omega_{\perp}^{0}$ obtained from the GP and the MGP calculations for the condensate of $N=10^4$ ^{85}Rb atoms carrying a single vortex ($\kappa=1$). The condensate is trapped in an anisotropic trap with $\lambda_0=0.39$ and $\omega_{\perp}^0=2\pi\times 17.5$ Hz.

	GP		MGP	
a/a_0	μ_1	E_1/N	μ_1	E_1/N
1400	10.223	7.545	10.621	7.790
3000	13.649	9.955	14.898	10.739
8000	19.955	14.422	24.798	17.528
10000	21.774	15.715	28.223	19.871

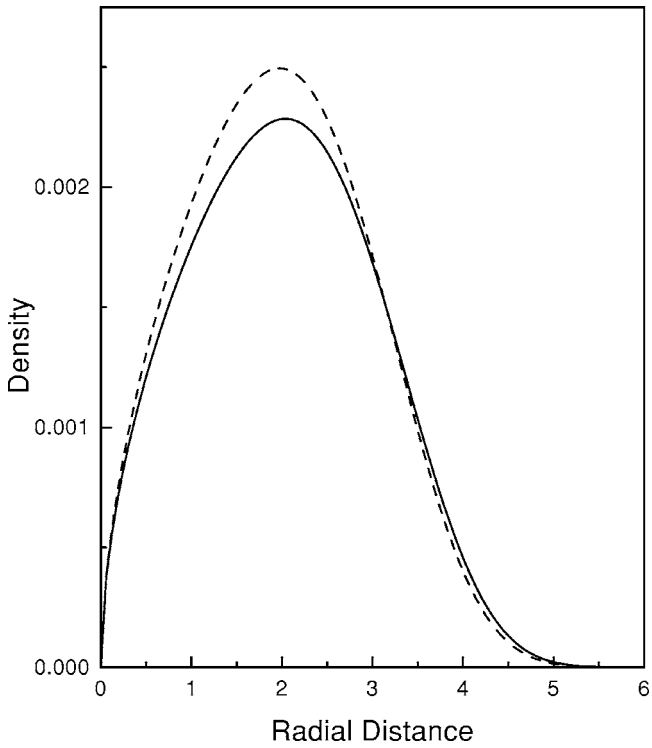

FIG. 2. Comparison of the GP (dashed line) and the MGP (solid line) density profiles of a vortex state with $\kappa=1$ as a function of the radial distance $r_\perp$ (in units of a_{ho}) from the z axis for $N=10^4$ ^{85}Rb atoms trapped in an anisotropic trap with $\lambda_0=0.39$ and $\omega_\perp^0=2\pi\times 17.5$ Hz. The scattering length $a/a_0=1400$.

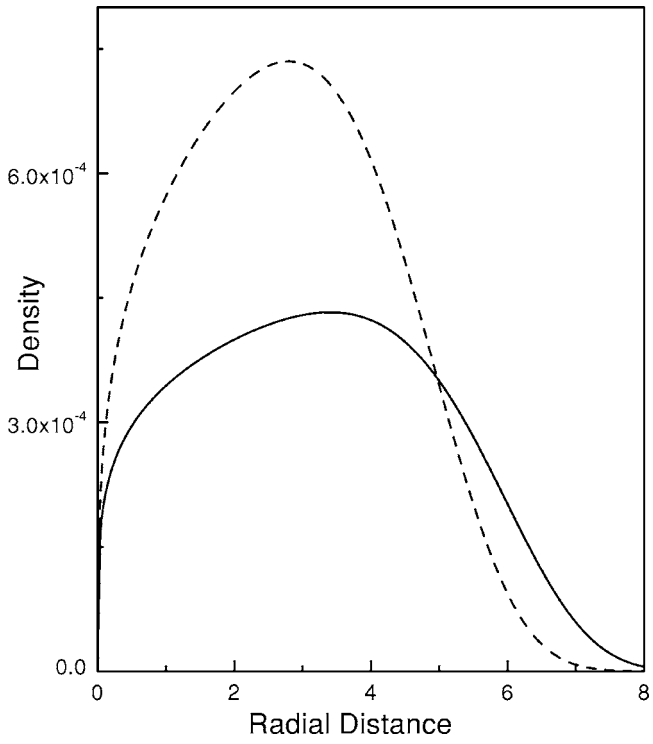

FIG. 3. Same as Fig. 2 but with the scattering length $a/a_0=10\,000$.

that in the large-gas-parameter regime the MGP results for the condensates with a single quantized vortex are substantially altered as compared to the corresponding GP results. It is important to note here that although the MGP corrections to the total energy and the individual components are significant, the MGP calculation of critical angular velocity Ω_c for the formation of the vortex state given by [28]

$$\frac{\Omega_c}{\omega_\perp^0}=\kappa^{-1}[(E_1/N)_\kappa-(E_1/N)_0] \tag{26}$$

yields results that are nominally different from their GP counterparts. For example, corresponding to $a/a_0=10\,000$ we obtain $\Omega_c=0.325\omega_\perp^0$ and $\Omega_c=0.335\omega_\perp^0$ for a single vortex with $\kappa=1$ by employing the MGP and the GP calculations, respectively. This observation regarding the small change in value of critical angular velocity was also made in Ref. [32], however for a much lower value of the gas parameter. Our results clearly show that the MGP calculation does not provide any sizable correction to the critical angular velocity Ω_c even for very large values of the gas parameter.

Having estimated the corrections introduced by the MGP calculation over the GP results for the total energy and the chemical potential, now we wish to present the results for the density profile obtained by the MGP and the GP calculations and compare them to study the effect of a large gas parameter on the density profile. In Figs. 2 and 3, we show the density profiles of condensates with a single vortex for the values of scattering length $a/a_0=1400$ and $a/a_0=10\,000$, respectively, obtained by the MGP and the GP calculations. It can be clearly seen from these two figures that for $a/a_0=1400$, the MGP calculation leads to a slight modification in the density profile over the GP result. On the other hand, for $a/a_0=10\,000$ the MGP density profile is substantially different from the corresponding GP density profile. Due to the repulsive nature of the LHY term in the MGP equation, bosons in the condensate are pushed outward resulting in an increase in the size of the condensate and a decrease in the value of the peak density in comparison to the GP case. Furthermore, it is evident from Fig. 3 that the values of the peak density n_{peak} and the transverse distance $r_{1\perp}^{\text{peak}}$ at which densities become maximum are significantly different in the GP and the MGP calculations. To show the difference in the MGP and the GP density profiles in a more quantitative manner, we plot in Figs. 4 and 5 the peak density n_{peak} and the corresponding peak position $r_{1\perp}^{\text{peak}}$, respectively, as functions of the scattering length. From the variational form of the wave function given by Eq. (4), it is easy to verify that the density peaks at

$$r_{1\perp}^{\text{peak}}=\sqrt{\frac{\omega_\perp^0}{\omega_\perp}}\left(\frac{q}{p}\right)^{1/2p} \tag{27}$$

and the expression for the peak density is given by

$$n_{\text{peak}}=A^2\left(\frac{\omega_\perp^0}{\omega_\perp}\right)^q\left(\frac{q}{p}\right)^{q/p}e^{-q/p}. \tag{28}$$

The values of variational parameters $\omega_\perp$, λ, p, and q which are obtained by minimization of the energy are then used to

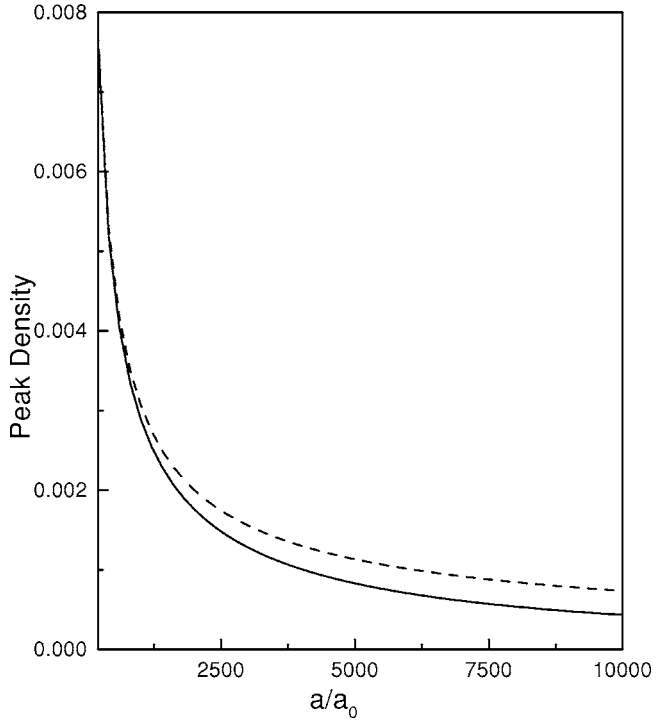

FIG. 4. The peak density n_{peak} as a function of the scattering length a/a_0 of a condensate with a quantized vortex of quantum of circulation $\kappa=1$. The solid line corresponds to the MGP result and the dashed line is obtained with the GP calculation. The trap parameters are the same as Fig. 2.

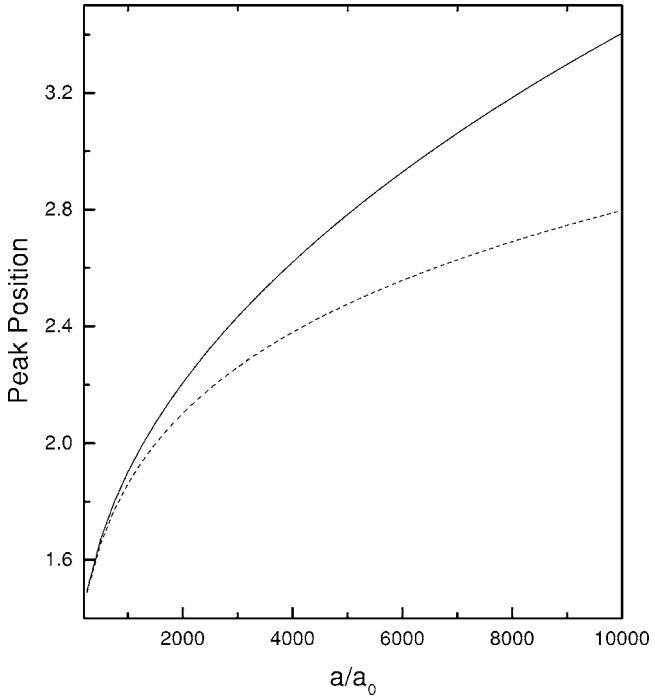

FIG. 5. The peak position $r_{1\perp}^{\text{peak}}$ (in unit of a_{ho}) as a function of the scattering length a/a_0 of a condensate with a quantized vortex of quantum of circulation $\kappa=1$. The solid line corresponds to the MGP result and the dashed line is obtained with the GP calculation. The trap parameters are the same as Fig. 2.

calculate $r_{1\perp}^{\text{peak}}$ and n_{peak} by using Eqs. (27) and (28), respectively. From Fig. 4, we observe that with both MGP and the GP calculations, the peak density shows a decreasing trend with increasing a/a_0 due to greater repulsion between the bosons. As mentioned above for the MGP calculation, the second term in the interatomic potential corresponds to more repulsion, which results in a higher reduction in the peak density as compared to the GP case. The difference between the MGP and the GP peak densities increases with increasing scattering length. For example, as a/a_0 is scanned from 1400 to 10 000, the difference between the GP and the MGP results grows from around 7% to 37%. In contrast to this, $r_{1\perp}^{\text{peak}}$ increases as the scattering length is increased in conformity with the fact that the size of the condensate grows as the repulsive interaction goes up. However, like peak density, the difference between the results for $r_{1\perp}^{\text{peak}}$ obtained by the MGP and the GP calculations also increases with increasing value of a/a_0. For $a/a_0=1400$ and $a/a_0=10\,000$, the differences in the MGP and the GP values of $r_{1\perp}^{\text{peak}}$ are found to be approximately 3% and 22%, respectively. Furthermore, we also notice from Figs. 2 and 3 that the depth and the size of the vortex hole around the z axis obtained by the GP calculation are significantly greater than the MGP case in the large-gas-parameter regime. The size of the hole can be characterized by the transverse radial distance r_c at which the density first reaches e^{-1} times its peak value n_{peak} [33]. For $a/a_0=1400$, the GP value of r_c is just 7% higher than the MGP result. On the other hand, for $a/a_0=10\,000$, the GP value of r_c becomes 66% more than the corresponding MGP number. This large change in the size of the vortex hole can be clearly seen from Fig. 3. These results indicate that in the large-gas-parameter regime, the GP calculation yields highly overestimated values of the size of the hole.

Thus we conclude that in the presence of a vortex, the MGP results for the properties such as total energy, chemical potential, and the density profile differ significantly in comparison to the GP predictions in the large-gas-parameter regime. On the other hand, the MGP results for the critical angular velocity Ω_c change nominally over the GP numbers. In the next section, we discuss the results for the splitting of the quadrupole modes of the collective oscillations due to the presence of a vortex in the large-gas-parameter regime.

B. Splitting of quadrupole modes

To calculate the frequency shifts of the quadrupole modes characterized by the components of angular momentum $m_z=2$ and $m_z=-2$, respectively, first we need to evaluate the moments m_1^+, m_2^-, and m_3^+. For excitation operators given by Eq. (21), the commutators in Eq. (20) can be evaluated to give the following expressions for the moments [16,31]:

$$m_1^+ = \frac{8\hbar^2}{m}\langle 0|x^2+y^2|0\rangle,$$

$$m_2^- = \frac{16\hbar^3}{m^2}\langle 0|xp_y - yp_x|0\rangle,$$

$$m_3^+ = \frac{16\hbar^4(\omega_\perp^0)^2}{m}\left[\langle 0|x^2+y^2|0\rangle + \frac{\langle 0|p_x^2+p_y^2|0\rangle}{m^2(\omega_\perp^0)^2}\right], \quad (29)$$

where p_i is the ith component of the linear momentum vector $\mathbf{p}$ and $|0\rangle$ represents the wave function of the vortex state obtained by solving the time-independent MGP or GP equations [Eq. (7)]. In deriving the above equations, the relation $F_+^\dagger = F_-$ has been used. It is worth noticing that the moments up to third-order do not depend on the boson-boson coupling parameter (two-body interaction) explicitly. This is because the energies within the LDA do not contribute to moments up to third order for the excitation operators satisfying $\nabla^2 F_\pm = 0$ [34]. Now, use of moments m_1^+ and m_2^- of Eq. (29) along with Eq. (23) yields the result

$$\delta = \frac{2}{m}\frac{N\hbar\,\kappa}{\langle r_\perp^2\rangle}, \quad (30)$$

where $\langle r_\perp^2\rangle$ is the transverse size of the condensate determined by the average

$$\langle r_\perp^2\rangle = \int (x^2+y^2)n(\mathbf{r})d\mathbf{r}. \quad (31)$$

It is important to note that although the frequency shift does not explicitly depend on the boson-boson coupling parameter, implicit dependence on the two-body interaction enters through the wave function or the density of the condensate, which crucially depends on the nature of the boson-boson interaction. We have already observed that the transverse sizes of the condensate obtained by employing the MGP and the GP equations differ significantly in the large-gas-parameter regime. Consequently, the MGP and the GP frequency shifts of the two quadrupole modes will also vary significantly in this regime. We show the results for the MGP and the GP frequency shifts as a function of the scattering length in Fig. 6. The frequency shift between the two quadrupole modes decreases with the increase in the scattering length due to the fact that higher values of the scattering length correspond to greater repulsive interaction between the bosons, resulting in condensates with larger values of the transverse size. For up to around $a/a_0 = 1000$, the GP and the MGP frequency shifts are nearly identical, and as the scattering length is increased beyond this value, the difference between the two results starts growing. For example, at the maximum value of the scattering length ($a/a_0 = 10\,000$), we find that the GP frequency shift is around 26% higher in comparison to the MGP result.

Finally, we note that the quadrupole frequencies $\omega_\pm$ can be obtained from Eq. (24) and the expressions for m_1^+ and m_3^+ given in Eq. (29). For the values of the gas parameter considered in this paper, the transverse kinetic energy $\langle 0|p_x^2+p_y^2|0\rangle$ is much smaller than the transverse radius $\langle 0|x^2+y^2|0\rangle$ of the condensate with a vortex state and thus it can be neglected in m_3^+. As a result of this, under the single-mode approximation [Eq. (22)] the expressions for the quadrupole frequencies are given by

$$\omega_\pm = \sqrt{2}\omega_\perp^0 \pm \frac{\delta}{2}. \quad (32)$$

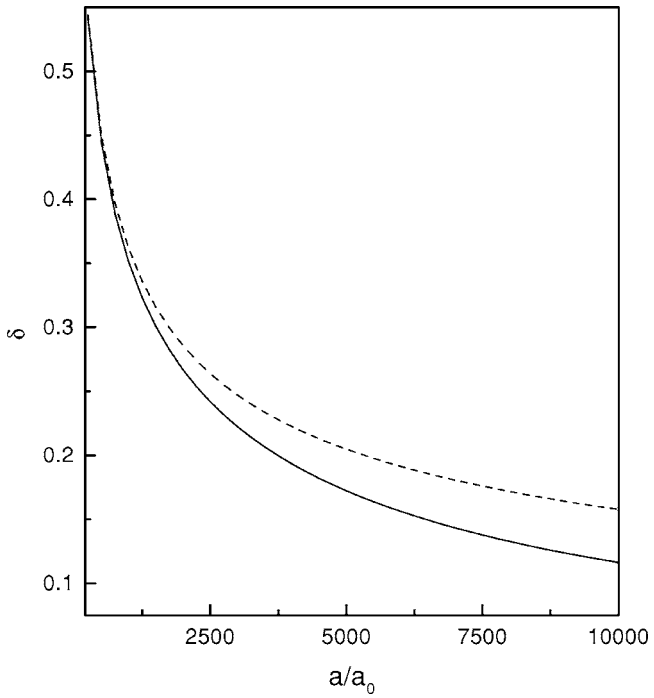

FIG. 6. The frequency shift (in unit of $\omega_\perp^0$) of the quadrupole oscillations of a condensate due to the presence of a single quantized vortex ($\kappa=1$) as a function of the scattering length a/a_0. The solid line corresponds to the MGP result and the dashed line is obtained with the GP calculation. The trap parameters are the same as Fig. 2.

From the above results, we conclude that in the large-gas-parameter regime, the MGP and the GP results for the frequency shift of the two quadrupole modes and also the individual frequencies of the two modes are substantially different for the values of scattering lengths which are achieved by tuning the Fesbach resonance.

IV. CONCLUSION

In this paper, we have studied the properties of BEC with a single quantized vortex in the large-gas-parameter regime. For this purpose, we have employed the MGP theory, which has been obtained by including the second term (LHY term) in the perturbative expansion of the interatomic interaction energy per particle obtained from the ground-state energy of uniform Bose gas. We have used the variational approach to solve the MGP equation by employing a suitable ansatz for the wave function of a condensate with a quantized vortex. The wave function obtained by the variational approach is then employed to calculate the static properties such as the total energy, chemical potential, and the density profile for a wide range of scattering length lying well within the large-gas-parameter regime. The correctness and accuracies of our solutions are checked by verifying the generalized virial relation and also by comparing them with the solutions obtained by the steepest-descent method. By using the wave function of the vortex state and the sum-rule approach, we have also calculated the frequency shift of the two quadrupole modes of the collective oscillations arising due to the

presence of a quantized vortex. We have studied the effect of large gas parameter on the frequency shift. To test the accuracy of GP theory, we have made a detailed comparison of the results of the GP and the MGP calculations for all the observables mentioned above. We have found that the MGP calculations introduce sizable corrections in all the properties, except for the critical angular frequency, of the condensates lying in the large-gas-parameter regime. These changes are quite large in magnitude and therefore can easily be observed in measurements involving condensates with large gas parameter as achieved in Ref. [13]. The comparison of the results obtained in this paper with the experimental results will also test the validity of the GP theory for the description of condensates with large gas parameter.

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