Elementary Excitations in Trapped Bose-Einstein Condensed Gases Beyond the Mean-Field Approximation

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(Received 24 July 1998)

Using the hydrodynamic theory of superfluids and the Lee-Huang-Yang equation of state for interacting Bose gases, we derive the first correction to the collective frequencies of a trapped gas, due to effects beyond the mean field approximation. The corresponding frequency shift, which is calculated at zero temperature and for large N, is compared with other corrections due to finite size, nonlinearity, and temperature. We show that for reasonable choices of the relevant parameters of the system, the non-mean-field correction is the leading contribution and amounts to about 1%. The role of the deformation of the trap is also discussed. [S0031-9007(98)07637-6]

PACS numbers: 03.75.Fi, 05.30.Jp, 32.80.Pj, 67.90.+z

The experimental measurements [1–3] of the collective oscillations of Bose-Einstein condensed gases confined in magnetic traps have provided an excellent confirmation of the predictions of mean-field theory (see [4] for a recent theoretical review). The accuracy of the mean-field predictions is not surprising since in these gases the average distance between particles is significantly larger than the range of interatomic forces. Typically, the gas parameter $n(0)a^3$, where $n(0)$ is the density evaluated in the center of the trap, and a is the s-wave scattering length, is smaller than 10^{-4}. According to the theory of Lee, Huang, and Yang (LHY) [5], the first corrections to the mean-field predictions are expected to behave like $\sqrt{a^3n}$ and to be consequently of the order of 1% or less in these systems. While such corrections are too small to be observed in the density profiles or in the release energy, they might be observable in the frequency of the collective excitations where the accuracy of measurements is much higher. For example, an accuracy of $\sim 0.3–0.4\%$ has been already achieved in the experiment of [3].

Measuring effects beyond mean-field theory is a challenging task and would open new perspectives in the many-body investigation of these novel systems. So far the theoretical investigation of these effects has been limited to the equilibrium properties, either including first quantum corrections in analytic form [6,7], or through numerical simulations based on Monte Carlo methods [8]. The purpose of this work is to provide an analytic calculation of the first corrections to the collective frequencies due to non-mean-field effects. These corrections are calculated in the large N limit and at zero temperature.

Our starting point is the hydrodynamic equations of superfluids (see, for example, [9])

$$\frac{\partial}{\partial t} n + \nabla(\mathbf{v}n) = 0 \tag{1}$$

and

$$m \frac{\partial}{\partial t}\mathbf{v} + \nabla\left(\mu + \frac{1}{2} m\mathbf{v}^2\right) = 0 \tag{2}$$

holding at zero temperature. Here n is the density of the system, $\mathbf{v}$ is the velocity field, and μ is the chemical potential. Equations (1) and (2) permit one to describe the low frequency collective excitations also in nonuniform Bose superfluids, provided the density profile varies on a macroscopic scale and one can use the local density approximation for the chemical potential

$$\mu(\mathbf{r}, t) = \mu_l[n(\mathbf{r}, t)] + V_{\rm ext}(\mathbf{r}), \tag{3}$$

where $\mu_l(n)$ is the chemical potential calculated for a uniform gas at density n and $V_{\rm ext}$ is the external confining potential.

In the following we will consider the linearized regime of Eqs. (1) and (2). We write $n(\mathbf{r}, t) = n(\mathbf{r}) + \delta n(\mathbf{r}, t)$ and $\mu(\mathbf{r}, t) = \mu_0 + \delta\mu_l(\mathbf{r}, t)$ with $\delta\mu_l = (\partial\mu_l/\partial n)\delta n$, so that Eqs. (1) and (2) can be rewritten in the useful form

$$m \frac{\partial^2 \delta n}{\partial t^2} - \nabla\left[n\nabla\left(\frac{\partial\mu_l}{\partial n}\,\delta n\right)\right] = 0\,. \tag{4}$$

The ground state density $n(\mathbf{r})$ entering Eq. (4) can be easily calculated by imposing the equilibrium condition $\mu_0 = \mu_\ell(n(\mathbf{r})) + V_{\rm ext}(\mathbf{r})$, where μ_0 is the ground state value of the chemical potential, fixed to ensure the proper normalization of $n(\mathbf{r})$.

Equations (1)–(4) do not necessarily require that the trapped gas is weakly interacting. It is also worth noticing that the density n entering these equations should not be confused with the density of the condensate, which in general does not obey equations of macroscopic type. Only in the weakly interacting limit, where quantum depletion effects are negligible, can the density of the system be identified with the condensate density. In this case, Eqs. (1)–(4) are equivalent to the time dependent Gross-Pitaevskii equations for the order parameter, evaluated in the large N limit (see, for example, [10]).

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According to LHY theory, the chemical potential of a uniform interacting Bose gas is determined by the low density expansion:

$$\mu_l(n) = gn\left(1 + \frac{32}{3\sqrt{\pi}}\sqrt{a^3 n}\right), \qquad (5)$$

where $g = 4\pi\hbar^2 a/m$ is the interaction coupling constant. Equation (5) represents a major result of many body theory and accounts for nontrivial renormalization effects of the coupling constant. It provides the first correction to the result $\mu = gn$ given by lowest order theory, hereafter called Bogoliubov or mean-field approximation. The LHY equation of state (5) can be derived starting from Bogoliubov theory. In this scheme the energy of the system, including the zero-point motion of elementary excitations, is given by $E = \frac{1}{2}Ngn + \frac{1}{2}\sum_{\mathbf{p}\neq 0}[\epsilon(p) - p^2/2m - gn]$, where $\epsilon(p)$ is the energy of elementary excitations in Bogoliubov theory. The zero point energy contains an ultraviolet divergency at large p which is cured by the proper renormalization $g \to g(1 + g\frac{1}{V}\sum_{\mathbf{p}\neq 0} m/p^2)$ of the coupling constant, so that one finally obtains a convergent result for the energy of the system, yielding result (5) for the chemical potential. It is worth noticing that the LHY correction does not involve additional parameters with respect to Bogoliubov theory, being fixed by the scattering length and by the density.

Using the LHY equation of state (5), the equation for the ground state density can be solved by iteration and one finds the result [6]

$$n(\mathbf{r}) = n_{\mathrm{TF}}(\mathbf{r}) - \alpha n_{\mathrm{TF}}^{3/2}(\mathbf{r}), \qquad (6)$$

where $n_{\mathrm{TF}}(\mathbf{r}) = [\mu_0 - V_{\mathrm{ext}}(\mathbf{r})]/g$ is the so-called Thomas-Fermi result for the ground state density [11] and $\alpha = (32/3\sqrt{\pi})a^{3/2}$.

Notice that in the same scheme the condensate density n_c is given by $n_c(\mathbf{r}) = n_{\mathrm{TF}}(\mathbf{r}) - \frac{5}{4}\alpha n_{\mathrm{TF}}^{3/2}(\mathbf{r})$ which is smaller than the density $n(\mathbf{r})$ and yields [4] the result

$$\frac{N_{\mathrm{out}}}{N} = \frac{5\sqrt{\pi}}{8}\sqrt{a^3 n(0)} \qquad (7)$$

for the quantum depletion of the condensate of an atomic gas confined in a harmonic trap.

Using (5) one can write $(\partial\mu_l/\partial n) = g(1 + 3/2\alpha n_{\mathrm{TF}}^{1/2})$ so that Eq. (4) takes the form

$$m\omega^2\delta n + \nabla(g n_{\mathrm{TF}}\nabla\delta n) = -\frac{1}{2}\nabla^2(\alpha g n_{\mathrm{TF}}^{3/2}\delta n). \qquad (8)$$

Equation (8) provides the appropriate generalization of the zeroth order hydrodynamic (HD) equation

$$m\omega^2\delta n + \nabla(g n_{\mathrm{TF}}\nabla\delta n) = 0 \qquad (9)$$

used in [10] to evaluate the collective frequencies in the large N, Thomas-Fermi approximation. Equation (9) admits analytical solutions if the external potential is harmonic. In particular, for an isotropic trap ($V_{\mathrm{ext}} = \frac{1}{2}m \times \omega_0^2 r^2$) the solutions of (9) obey the dispersion relation [10]

$$\omega(n_r, \ell) = \omega_0(2n_r^2 + 2n_r\ell + 3n_r + \ell)^{1/2}, \qquad (10)$$

where n_r is the number of radial nodes and ℓ is the angular momentum of the excitation. Equation (10) shows that the collective frequencies in the mean-field approximation are fixed, apart from geometrical factors, only by the oscillator frequency, a quantity measured with very high precision in experiments. This is a remarkable feature exhibited by these harmonically trapped gases which allows for a safe investigation of small corrections.

Once the solutions of (9) are known, Eq. (8) can be easily solved by treating its right-hand side as a small perturbation. One finds that the corresponding frequency shifts obey the general equation

$$\frac{\delta\omega}{\omega} = -\frac{\alpha g}{4m\omega^2}\frac{\int d^3\mathbf{r}\,(\nabla^2\delta n^*)\delta n n_{\mathrm{TF}}^{3/2}}{\int d^3\mathbf{r}\,\delta n^*\delta n}, \qquad (11)$$

where δn are the solutions of (9) and ω are the corresponding frequencies. The integrals of (11) extend to the region where the Thomas-Fermi density is positive.

In the absence of trapping, the gas is uniform and the solutions of Eqs. (8) and (9) have the form $\delta n \sim e^{iqz}$ and exhibit a phonon dispersion $\omega = cq$. In this case Eq. (8) [or, equivalently, (11)] gives the Beliaev result [12] $\delta c/c = 8\sqrt{a^3 n/\pi}$ for the shift of the sound velocity with respect to the Bogoliubov value $c = \sqrt{gn/m}$, calculated at the density n. Notice that even in the uniform case n differs from n_{TF} because of Eq. (6). The shift of the sound velocity is consistent with the change in the compressibility $mc^2 = n\partial\mu/\partial n$ associated with the LHY correction in the equation of state (5).

Equation (11) shows that the so-called "surface" oscillations $\delta n = r^\ell Y_{\ell m}$, satisfying the condition $\nabla^2\delta n = 0$, are not affected by the LHY correction. For spherical trapping these solutions obey the dispersion law $\omega = \sqrt{\ell}\,\omega_0$, which is simply obtained setting $n_r = 0$ in (10).

In order to observe effects beyond mean field, one has consequently to focus on compressional modes, which are sensitive to the equation of state. The lowest mode in a spherical trap is the monopole (breathing) oscillation ($n_r = 1, \ell = 0$), characterized by the zeroth order dispersion $\omega = \sqrt{5}\,\omega_0$ and by density oscillations of the form $\delta n \sim (r^2 - 3/5R^2)$. In this case Eq. (11) yields

$$\frac{\delta\omega_M}{\omega_M} = \frac{63\sqrt{\pi}}{128}\sqrt{a^3 n(0)}, \qquad (12)$$

showing that the fractional shift of the monopole frequency is proportional to the square root of the gas parameter evaluated in the center of the trap. This correction exhibits the same dependence on the gas parameter as the quantum depletion of the condensate, although the coefficient of proportionality slightly differs in the two cases. It is useful to write the gas parameter in terms of the relevant parameters of the system as [4]

$$a^3 n(0) = \frac{15^{2/5}}{8\pi}\left(N^{1/6}\frac{a}{a_{\mathrm{ho}}}\right)^{12/5}, \qquad (13)$$

where N is the number of atoms in the trap and $a_{\rm ho} = (\hbar/m\omega_0)^{1/2}$ is the oscillator length. Using, for example, $N = 10^6$ and $a/a_{\rm ho} = 6 \times 10^{-3}$, we predict a fractional shift of 1%. A similar value is found for the quantum depletion of the condensate. Equation (13) shows that in order to enhance the value of the gas parameter it is more effective to increase the value of the ratio $a/a_{\rm ho}$ rather than the value of N which enter the equation with a much lower power. In practice, however, it is not easy to obtain large values of $a^3n(0)$ and hence large frequency shifts. So far the achievement of high densities is in fact limited by three-body recombinations.

The above shift of the monopole frequency should be compared with other corrections which might be relevant in actual experiments, like finite size, nonlinearity, and thermal effects. Finite size effects arise because even in the mean-field scheme the Thomas-Fermi value $\sqrt{5}\,\omega_0$ holds only in the large-N limit. These corrections arise from the "quantum pressure term" in the equation for the velocity field, which is ignored in Eq. (2), and can be calculated by a proper perturbation procedure in the Gross-Pitaevskii equation. Using a sum rule approach one obtains the following result for the leading correction to the monopole oscillation in the large N limit and isotropic trapping [13]

$$\frac{\delta\omega_M}{\omega_M} = -\frac{7}{6}\left(\frac{a_{\rm ho}}{R}\right)^4 \log\left(\frac{R}{Ca_{\rm ho}}\right), \tag{14}$$

where $C = 1.3$ is a dimensionless parameter and $R = a_{\rm ho}(15Na/a_{\rm ho})^{1/5}$ is the radius of the system. For the surface quadrupole mode, one finds that the fractional shift has opposite sign and is larger by a factor of 5.

It is worth noticing that the corrections to the Thomas-Fermi value due to non-mean-field (12) and finite size (14) effects depend on different combinations of the relevant parameters of the system. In fact, finite size effects depend on the combination $Na/a_{\rm ho}$, while non-mean-field effects depend on $N^{1/6}a/a_{\rm ho}$. In the thermodynamic limit, where $N \to \infty$ and $\omega_0 \to 0$, with the product $N\omega_0^3$ kept constant, finite size corrections go to zero, while the gas parameter (13) has a finite value [4]. The large N, thermodynamic limit is reasonably well realized in experiments. For example, using the same values for N and $a/a_{\rm ho}$ employed above, one finds that the finite size shift (14) of the monopole frequency is much smaller ($\sim$0.1%) than the non-mean-field correction (12). In general, finite size effects are negligible if the condition $N \gg (a_{\rm ho}/a)^2 \log(R/a_{\rm ho})$ is satisfied.

Nonlinearity is another important effect to discuss. In fact, in actual experiments the amplitude of the oscillation cannot be made arbitrarily small. The effects of nonlinearity have been investigated in details in [14] in the framework of the Thomas-Fermi approximation. The leading corrections to the frequency shift can be written in the form $\delta\omega/\omega = A^2\delta$, where A is the fractional amplitude of the oscillation of the atomic cloud confined in the trap and the coefficient δ can be calculated in an explicit way [14]. For the monopole mode in the spherical trap, one has $\delta = -1/6$ so that for fractional amplitudes less than 10%, the effects of nonlinearity are very small.

In addition to finite size and nonlinearity effects, one should also take into account that experiments are carried out at finite temperature. At present there is no fully reliable theory to account for the temperature dependence of the collective frequencies of these trapped gases. However, one expects that these effects should vanish very rapidly when kT is smaller than the chemical potential. A rough estimate of the thermal effect can be obtained by assuming that the shift of the real part of ω is of the same order as its imaginary part which is responsible for the damping of the oscillation. This might provide an experimental control of the thermal effect on the frequency shift.

Finally, an important question concerns the role of the anisotropy of the confining potential. In fact, most of the magnetic traps are at present nonspherical. For an axially deformed trap of the form $V_{\rm ext} = \frac{1}{2}m\omega_\perp^2 r_\perp^2 + \frac{1}{2}m\omega_z^2 z^2$, where $r_\perp = (x^2 + y^2)^{1/2}$ is the radial coordinate, the HD Eq. (9) admits several interesting solutions. In addition to the dipole (center of mass) oscillation, the excitations so far investigated experimentally are the $m = 2$ quadrupole mode, whose density varies as $\delta n \sim r^2 Y_{22}$, and the $m = 0$ oscillations resulting from the coupling between the quadrupole and the monopole modes (notice that the zth component, m, of angular momentum is still a good quantum number in axially deformed systems). The $m = 2$ quadrupole mode has frequency $\omega = \sqrt{2}\,\omega_\perp$ and is not affected by non-mean-field effects since $\nabla^2\delta n = 0$. Conversely, the decoupled frequencies of the $m = 0$ modes are given by [10]

$$s^2 = \frac{\omega^2}{\omega_\perp^2} = 2 + \frac{3}{2}\lambda^2 \pm \frac{1}{2}(9\lambda^4 - 16\lambda^2 + 16)^{1/2}, \tag{15}$$

where $\lambda = \omega_z/\omega_\perp$ characterizes the asymmetry of the trap. The corresponding density oscillations have the form $\delta n \sim -2\mu(s^2 - 2)/m\omega^2 + r_\perp^2 + (s^2 - 4)z^2$. After some length, but straightforward algebra, one finds

$$\frac{\delta\omega}{\omega} = \frac{63\sqrt{\pi}}{128}\sqrt{a^3n(0)}\,f_\pm(\lambda) \tag{16}$$

for the frequency shift of the $m = 0$ modes where

$$\begin{aligned} f_\pm(\lambda) &= \frac{5}{3}\frac{(s^2 - 2)^2}{(3s^4 - 20s^2 + 40)} \\ &= \frac{1}{2} \pm \frac{8 + \lambda^2}{6\sqrt{9\lambda^4 - 16\lambda^2 + 16}}, \end{aligned} \tag{17}$$

and the index $\pm$ refers to the higher (+) and lower (−) solutions of Eq. (15). Notice that for a spherical trap ($\lambda = 1$) the solutions of (15) are $s^2 = 5$ (monopole) and

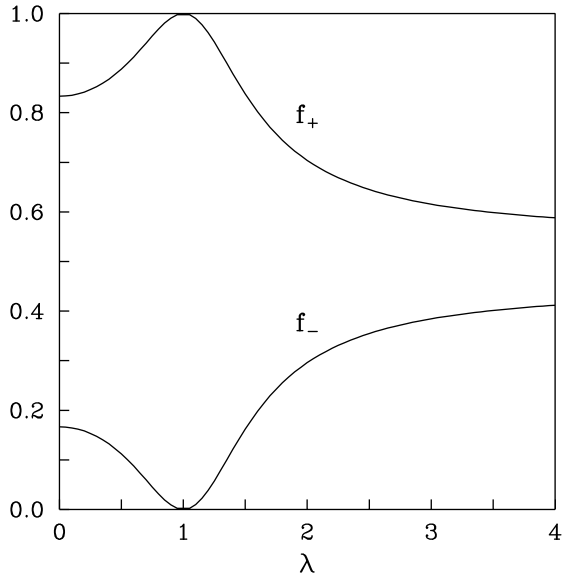

FIG. 1. Functions f_+ and f_- relative to the higher and lower $m = 0$ modes [see Eq. (17)], as a function of the deformation parameter $\lambda = \omega_z/\omega_\perp$.

$s^2 = 2$ (quadrupole). In the first case one finds $f_+ = 1$ and one recovers result (12) for the breathing mode, while in the second case there is no shift. In Fig. 1 we show the functions f_+ and f_- relative to the two modes as a function of the deformation parameter λ.

Another important consequence of the use of deformed trap concerns the effects of nonlinearity. It has been shown [14] that these effects can be amplified or reduced by changing the value of λ. For example, choosing $\lambda = 1.40$ one finds that the nonlinearity coefficient δ of the high lying solution of (15) vanishes. For this mode one finds $s^2 = 7.1$ and $f_+ = 0.88$. Another interesting case is obtained choosing $\lambda = \sqrt{8}$. In this case the nonlinear effect is vanishingly small for the low energy solution. For this mode one finds $s^2 = 3.2$ and $f_- = 0.38$.

The largest values of the gas parameter have been so far reached for cigar trap configurations $\lambda \ll 1$. In this case the frequency shift of the lower mode with dispersion $s^2 = 5\lambda^2/2$ is reduced significantly [$f_-(0) = 1/6$] with respect to the case of the $\lambda = 1$ breathing mode [$f_+(1) = 1$]. Conversely, the higher mode, which corresponds to a compressional radial oscillation with dispersion $s^2 = 4$, exhibits only a small reduction [$f_+(0) = 5/6$]. It is also worth pointing out that for this mode the nonlinear effect vanishes as [14] $\delta\omega/\omega = -0.0938\lambda^2 A^2$. Finite size effects are also vanishing in the same limit. The fact that nonlinear and finite size effects vanish for $\lambda \to 0$ reflects the occurrence of a hidden symmetry [15] of the Gross-Pitaevskii equation characterizing the radial compressional mode in two-dimensional gases and might be used to improve the accuracy of measurements. One should, however, notice that, for small values of λ, the trapped gases exhibit, in addition to the radial excitations, also a low-lying branch of axial modes [16]. This could produce a "parametric" instability [17] of the compressional radial oscillation due to decay into two or more axial excitations.

In conclusion, in this Letter we have derived the first corrections to the collective frequencies of trapped Bose gases arising from effects beyond mean-field theory. We have shown that with reasonable choices of the parameters these effects, although small, might be visible experimentally. Their direct observation would represent an important achievement in the study of many-body effects associated with Bose-Einstein condensation.

We thank E. Cornell, J. Dalibard, W. Ketterle, and D. Stamper-Kurn for stimulating discussions. This research was supported by the Istituto Nazionale per la Fisica delle Materia through the Advanced Research Project on BEC.

Note added.—After this paper was submitted for publication, a preprint by Braaten and Pearson [18] appeared where the authors, using a different method, obtained the same expressions for the frequency shifts.

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