

Collective Excitations of a Trapped Bose-Condensed Gas

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We investigate the low energy excitations of a dilute atomic Bose gas confined in a harmonic trap of frequency ω_0 and interacting with repulsive forces. The dispersion law $\omega = \omega_0(2n^2 + 2n\ell + 3n + \ell)^{1/2}$ for the elementary excitations is obtained for large numbers of atoms in the trap, to be compared with the prediction $\omega = \omega_0(2n + \ell)$ of the noninteracting harmonic oscillator model. Here n is the number of radial nodes and ℓ is the orbital angular momentum. The effects of the kinetic energy pressure are estimated using a sum rule approach. Results are also presented for deformed traps and attractive forces. [S0031-9007(96)01246-X]

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Almost 50 years ago Bogoliubov [1] derived his famous theory for the elementary excitations of a dilute Bose gas. This theory, originally applied to homogeneous systems, is now receiving a novel interest because of the experimental availability of Bose-condensed gases confined in magnetic traps [2–4] (for a review on Bose-Einstein condensation, see, for instance, Ref. [5]). The Bogoliubov theory can be shown [6] to correspond to the linear limit of the time-dependent Gross-Pitaevskii [7] equation for the order parameter Φ :

$$i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) = \left(-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m} |\Phi(\mathbf{r}, t)|^2 \right) \Phi(\mathbf{r}, t). \quad (1)$$

Here V_{ext} is the confining potential and a is the s -wave scattering length. This equation neglects interaction effects arising from the atoms out of the condensate. This is an accurate approximation for a dilute Bose gas at low temperatures, where the depletion of the condensate is negligible. Differently from the homogeneous case, the Gross-Pitaevskii equation in the presence of an external potential admits stationary solutions not only for positive values of the scattering length but also when a is negative. In the latter case a solution of the metastable type is found provided the number of atoms in the trap is not too large [8–11]. This solution does not correspond to a global minimum for the energy due to the occurrence of lower energy collapsed configurations. The solutions of the time-dependent equation (1), after linearization, have the well known RPA structure and have been the object of a recent numerical investigation in the case of a trapped atomic gas [12].

The main purpose of this work is to obtain an explicit, analytic solution of (1), holding when the repulsive interaction is large enough to make the kinetic energy pressure negligible compared to the external and interparticle interaction terms. When applied to the calculation of the ground state this limit corresponds to the Thomas-Fermi approximation and is reached for positive and large values of the adimensional parameter Na/a_{HO} , where $a_{\text{HO}} =$

$(\hbar/m\omega_0)^{1/2}$ is the harmonic oscillator length characterizing the trap and N is the number of atoms. In the study of the elementary excitations this approximation corresponds to the hydrodynamic theory of Bose superfluids accounting for, in homogeneous systems, the propagation of phonons.

In order to discuss the behavior of the elementary excitations in this limit (hereafter called hydrodynamic limit) it is convenient to derive explicit equations for the density $\rho(\mathbf{r}, t) = |\Phi(\mathbf{r}, t)|^2$ and for the velocity field $\mathbf{v}(\mathbf{r}, t) = [\Phi^*(\mathbf{r}, t)\nabla\Phi(\mathbf{r}, t) - \nabla\Phi^*(\mathbf{r}, t)\Phi(\mathbf{r}, t)]/2mi\rho(\mathbf{r}, t)$. These equations can be directly obtained starting from the time-dependent Eq. (1) and take the form

$$\frac{\partial}{\partial t} \rho + \nabla(\mathbf{v}\rho) = 0 \quad (2)$$

and

$$m \frac{\partial}{\partial t} \mathbf{v} + \nabla \left(\delta\mu + \frac{1}{2} m \mathbf{v}^2 \right) = 0, \quad (3)$$

where

$$\delta\mu = V_{\text{ext}} + \frac{4\pi\hbar^2 a}{m} \rho - \frac{\hbar^2}{2m\sqrt{\rho}} \nabla^2 \sqrt{\rho} - \mu \quad (4)$$

is the change of the chemical potential with respect to its ground state value μ . It is worth noting that these equations do not involve any approximation with respect to the Gross-Pitaevskii equation (1) and hold in the linear as well as in the nonlinear regimes. They have the general structure of the dynamic equations of superfluids at zero temperature (see, for example, [13]). In particular, Eq. (3) establishes the irrotational nature of the superfluid flow.

The density ρ_0 relative to the ground state is obtained setting $\mathbf{v} = 0$ and $\delta\mu = 0$. This yields the equation

$$V_{\text{ext}}(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m} \rho_0 - \frac{\hbar^2}{2m\sqrt{\rho_0}} \nabla^2 \sqrt{\rho_0} - \mu = 0 \quad (5)$$

which, as expected, coincides with the Gross-Pitaevskii equation for the order parameter $\Phi_0 = \sqrt{\rho_0}$ of the ground state. The chemical potential μ is fixed by imposing the proper normalization to the density ρ_0 . When the number of atoms in the trap is sufficiently large the density profile $\rho_0(\mathbf{r})$ becomes smooth, and the kinetic energy pressure

term $\frac{\hbar^2}{2m\sqrt{\rho_0}}\nabla^2\sqrt{\rho_0}$ can be neglected with respect to the interaction terms of Eq. (5). The ground state density then takes the well known Thomas-Fermi form,

$$\rho_0(\mathbf{r}) = \frac{m}{4\pi\hbar^2 a} [\mu - V_{\text{ext}}(\mathbf{r})], \quad (6)$$

if $\mu \geq V_{\text{ext}}(\mathbf{r})$ and is equal to zero elsewhere. This approximation provides an accurate description of the solution of the Gross-Pitaevskii equation (5), except in the surface region where the exact solution vanishes smoothly. It can be used to calculate correctly the potential energy when N is large. It cannot be used instead to evaluate the kinetic energy, which requires a more accurate knowledge of the order parameter in the boundary region [14]. The distance from the boundary where the Thomas-Fermi approximation starts failing goes the same as $(a_{\text{HO}}^4/R)^{1/3}$ [9,14], where R is the radius of the boundary (see below).

In the following we will neglect [15] the kinetic energy pressure also in the solution of the time-dependent equations (2)–(4). This yields the simple expression $\delta\mu = 4\pi\hbar^2 a(\rho - \rho_0)/m$ for the change of the chemical potential [see Eqs. (4) and (5)]. Assuming for simplicity an isotropic harmonic oscillator potential $V_{\text{ext}}(\mathbf{r}) = \omega_0^2 r^2/2m$, the equations of motion (2) and (3), after linearization, can be written in the useful form

$$\omega^2 \delta\rho = -\frac{1}{2}\omega_0^2 \nabla(R^2 - r^2)\nabla\delta\rho, \quad (7)$$

where $\delta\rho(\mathbf{r})\exp(-i\omega t) = \rho(\mathbf{r}, t) - \rho_0(\mathbf{r})$ and $R^2 = 2\mu/m\omega_0^2$ fixes the boundary of the system where the density (6) vanishes. In the absence of the external trap the same procedure yields the well known equation $\omega^2 \delta\rho = -c^2 \nabla^2 \delta\rho$, where $c = (4\pi\hbar^2 a \rho_0/m^2)^{1/2}$ is the sound velocity of the homogeneous Bose gas.

The solutions of the hydrodynamic equations (7) are defined in the interval $0 \leq r \leq R$ and have the form

$$\delta\rho(\mathbf{r}) = P_\ell^{(2n)}(r/R)r^\ell Y_{\ell m}(\theta, \phi), \quad (8)$$

where $P_\ell^{(2n)}(t) = 1 + \alpha_2 t^2 + \dots + \alpha_{2n} t^{2n}$ are polynomials of degree $2n$, containing only even powers of t , and satisfying the orthogonality condition $\int_0^1 P_\ell^{(2n)}(t)P_{\ell'}^{(2n')}(t)t^{2\ell+2}dt = 0$ if $n \neq n'$. The parameters ℓ and m label the angular momentum of the excitation and its z component, respectively. The coefficients α_{2k} satisfy the recurrence relation $\alpha_{2k+2} = -\alpha_{2k}(n-k) \times (2\ell+2k+3+2n)/(k+1)(2\ell+2k+3)$. The dispersion law of the normal modes is given by the formula

$$\omega(n, \ell) = \omega_0(2n^2 + 2n\ell + 3n + \ell)^{1/2} \quad (9)$$

which represents the main result of the present work, holding in the limit $Na/a_{\text{HO}} \gg 1$. It should be compared with the prediction of the harmonic oscillator (HO) model in the absence of interparticle interactions:

$$\omega_{\text{HO}} = \omega_0(2n + \ell). \quad (10)$$

Of particular interest is the case of the lowest radial modes ($n = 0$), also called surface excitations, for which we predict the dispersion law

$$\omega(n = 0) = \sqrt{\ell}\omega_0. \quad (11)$$

The frequency of these modes lies systematically below the harmonic oscillator result $\omega_{\text{HO}}(n = 0) = \ell\omega_0$. This behavior should be taken into account in the determination of the critical frequency $\omega_{\text{cr}} = \min_\ell[\omega(\ell)/\ell]$ needed to generate a rotational instability [11,16], and might provide a competitive mechanism with respect to the creation of a vortex line. Notice that in the dipole case ($\ell = 1$) both the hydrodynamic and harmonic oscillator predictions coincide with the oscillator frequency ω_0 . This follows from the fact that in an external harmonic potential the lowest dipole mode corresponds to the oscillation of the center of mass, and is, consequently, unaffected by the interatomic forces.

For a fixed value of N the accuracy of prediction (9) is expected to become lower and lower as n and ℓ increase. In fact, the high energy states are associated with rapid variations of the density in space, and, consequently, the kinetic energy contribution in Eq. (4) cannot be neglected any longer. The energy range where our prediction (9) is expected to be accurate corresponds to values smaller than the chemical potential μ . For large values of n and ℓ , the correct dispersion law will approach the harmonic oscillator result (10).

The effects of the kinetic energy pressure, ignored in the hydrodynamic approximation, can be investigated by calculating the energy of the collective mode through a sum rule approach [17] based on the ratio

$$\hbar^2 \omega^2 = m_3/m_1 \quad (12)$$

between the cubic energy weighted and the energy weighted moments of the dynamic structure factor $m_p = \sum_n |\langle 0|F|n\rangle|^2 (\hbar\omega_n)^p$. Here $\hbar\omega_n$ is the excitation energy of the state $|n\rangle$ and F is a general excitation operator. The moments m_1 and m_3 can be reduced in the form of commutators involving the Hamiltonian of the system. One finds $m_1 = \frac{1}{2}\langle 0|[F^\dagger, [H, F]]0\rangle$ and $m_3 = \frac{1}{2}\langle 0[[F^\dagger, H], [H, [H, F]]]0\rangle$. Equation (12) provides, in general, a rigorous upper bound to the energy of the lowest state excited by F . The sum rule approach has the merit of providing useful information on the dynamic behavior of the system using only the knowledge of the ground state. By evaluating explicitly the commutators with the Hamiltonian [18]

$$H = \sum_i \frac{p_i^2}{2m} + \sum_i \frac{1}{2} m\omega_0^2 r_i^2 + \frac{4\pi\hbar^2 a}{m} \sum_{i<j} \delta(\mathbf{r}_i - \mathbf{r}_j), \quad (13)$$

we find, in the case of the surface ($n = 0$) operator $F = \sum_i r_i^\ell Y_{\ell m}(\theta_i, \phi_i)$, the results

$$m_1 = \frac{\hbar^2}{8m\pi} \ell(2\ell + 1) \int r^{2\ell-2} \rho d\mathbf{r} \quad (14)$$

and

$$m_3 = \frac{\hbar^4}{8m^2\pi} \ell(2\ell + 1) \left(\ell m \omega_0^2 \int r^{2\ell-2} \rho d\mathbf{r} + \ell(\ell - 1) \times \frac{\hbar^2}{m} \int |\nabla\sqrt{\rho}|^2 r^{2\ell-4} d\mathbf{r} \right), \quad (15)$$

and the excitation frequency (12) takes the form

$$\omega^2(n=0) = \omega_0^2 \ell [1 + (\ell - 1)\beta_\ell], \quad (16)$$

where $\beta_\ell = \hbar^2 \int |\nabla \sqrt{\rho}|^2 r^{2\ell-4} d\mathbf{r} / m^2 \omega_0^2 \int r^{2\ell-2} \rho d\mathbf{r}$. For the most relevant quadrupole ($n=0, \ell=2$) case, we find

$$\omega_Q = \sqrt{2} \omega_0 (1 + E_{\text{kin}}/E_{\text{ho}})^{1/2}, \quad (17)$$

where E_{kin} and E_{ho} are, respectively, the expectation value of the kinetic and harmonic potential energies in the ground state. In the absence of interparticle interactions, one has $E_{\text{kin}} = E_{\text{ho}}$, and hence one recovers the harmonic oscillator result $\omega = 2\omega_0$ of Eq. (10). On the other hand, when the interaction is repulsive and the number of atoms is sufficiently large, the kinetic energy term can be neglected and one obtains the hydrodynamic prediction $\omega = \sqrt{2} \omega_0$ of Eq. (11). The knowledge of the kinetic energy relative to the ground state then permits the estimation of the quadrupole excitation energy in the general case. For higher multipolarities the determination of the coefficient β_ℓ of Eq. (16) requires the knowledge of finer details of the ground state. A simple estimate can be obtained using the Gaussian approximation for the wave function of the condensate, yielding $\beta_\ell = E_{\text{kin}}/E_{\text{ho}}$, independent of ℓ .

In a similar way, starting from Eq. (12), one can determine the frequency of the compression modes. For the lowest monopole mode ($n=1, \ell=0$), excited by the operator $F = \sum_i r_i^2$, we find

$$m_1 = \frac{2\hbar^2}{m} N \langle r^2 \rangle \quad (18)$$

and

$$m_3 = \frac{2\hbar^4}{m^2} (4E_{\text{kin}} + 4E_{\text{ho}} + 9E_{\text{int}}), \quad (19)$$

where $E_{\text{int}} = 2\pi\hbar^2 a/m \int d\mathbf{r} \rho_0^2(r)$ is the interaction energy. Using the virial identity $2E_{\text{kin}} - 2E_{\text{ho}} + 3E_{\text{int}} = 0$, holding for the ground state, we finally obtain the following result for the monopole frequency:

$$\omega_M = \omega_0 (5 - E_{\text{kin}}/E_{\text{ho}})^{1/2}, \quad (20)$$

yielding the value $\omega = 2\omega_0$ in the harmonic oscillator model and $\omega = \sqrt{5} \omega_0$ in the large N limit, where $E_{\text{kin}}/E_{\text{ho}}$ tends to zero. We stress again that results (16)–(20) provide a rigorous upper bound to the frequency of the lowest states excited by the corresponding multipole operators.

Predictions (17) and (20) can be compared with the results recently obtained in Ref. [12] by solving numerically the time-dependent Gross-Pitaevskii equations for a trapped atomic gas interacting with repulsive forces. The conditions of Ref. [12] correspond to the value $\mu = 4.3\omega_0$ for the chemical potential and to the value 0.18 for the ratio between the kinetic and harmonic oscillator energies. This yields, using Eqs. (17) and (20), the values $\omega_Q = 1.54\omega_0$ and $\omega_M = 2.20\omega_0$, in excellent agreement with the findings of [12] ($1.53\omega_0$ and $2.19\omega_0$, respectively).

The above results for the dispersion law can be generalized to the case of a deformed trap. This is particularly relevant since the available magnetic traps are often highly anisotropic. Let us consider the case of a harmonic oscillator trap with axial symmetry along the z axis: $V_{\text{ext}} = m\omega_\perp^2 s^2/2 + m\omega_z^2 z^2/2$, where $s = (x^2 + y^2)^{1/2}$ is the radial variable in the x - y plane. In this case the relevant differential equation (7) should be replaced by

$$\omega^2 \delta\rho = -\frac{1}{2} \nabla[\omega_\perp^2 (S^2 - s^2) + \omega_z^2 (Z^2 - z^2)] \nabla \delta\rho, \quad (21)$$

with $m\omega_\perp^2 S^2/2 = m\omega_z^2 Z^2/2 \equiv \mu$.

Because of the axial symmetry of the trap, the third component m of the angular momentum is still a good quantum number. However, the dispersion law will depend on m . Explicit results are available in some particular cases. For example, functions of the form $\delta\rho = r^\ell Y_{\ell m}(\theta, \phi)$ are still solutions of Eq. (21) for $m = \pm\ell$ and $m = \pm(\ell - 1)$. The resulting dispersion laws are

$$\omega^2(m = \pm\ell) = \ell\omega_\perp^2 \quad (22)$$

and

$$\omega^2(m = \pm(\ell - 1)) = (\ell - 1)\omega_\perp^2 + \omega_z^2. \quad (23)$$

Equations (22) and (23) provide a full description of the dipole excitation ($\ell=1$) whose frequencies coincide, as expected, with the unperturbed harmonic oscillator values $\omega_D(m = \pm 1) = \omega_\perp$ and $\omega_D(m = 0) = \omega_z$. However, for the quadrupole ($\ell=2$) mode, Eqs. (22) and (23) account only for the $m = \pm 2$ ($\omega = \sqrt{2} \omega_\perp$) and $m = \pm 1$ [$\omega = (\omega_\perp^2 + \omega_z^2)^{1/2}$] components. The solution with $m=0$ involves a coupling with the monopole ($n=1, \ell=0$) excitation, and the dispersion law of the two decoupled modes is given by

$$\omega^2(m=0) = \omega_\perp^2 \left(2 + \frac{3}{2}\lambda^2 \mp \frac{1}{2}\sqrt{9\lambda^4 - 16\lambda^2 + 16} \right), \quad (24)$$

with $\lambda = \omega_z/\omega_\perp$. When $\lambda \rightarrow 1$, one recovers the original solutions (17) and (20) corresponding, respectively, to the quadrupole and monopole excitations in a spherical trap. When $\lambda \gg 1$ (disk-type geometry) the two solutions approach the frequencies $\sqrt{10/3} \omega_\perp$ and $\sqrt{3} \omega_z$, respectively. On the other hand, when $\lambda \ll 1$ (cigar-type geometry), the two frequencies become $\sqrt{5/2} \omega_z$ and $2\omega_\perp$.

For systems interacting with attractive forces ($a < 0$) the hydrodynamic results discussed above do not provide an adequate description of the dispersion law, and, in this case, the sum rule approach becomes particularly useful. The kinetic energy contribution E_{kin} entering Eqs. (17) and (20) can never be neglected, being larger than E_{ho} , and the monopole mode turns out to be located below the quadrupole one. Physically, this reflects the tendency of the system to become more compressible. In Fig. 1, we show the behavior of the monopole and quadrupole frequencies obtained using Eqs. (17) and (20) as a function of the adimensional parameter Na/a_{HO} . The ratio

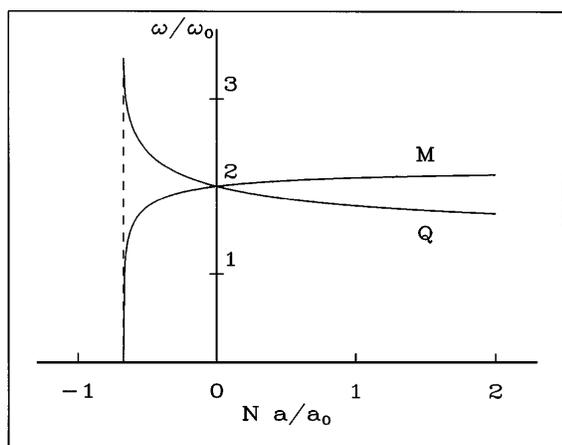


FIG. 1. Quadrupole (Q) and monopole (M) frequencies as a function of the adimensional parameter Na/a_0 , calculated using Eqs. (17) and (20).

$E_{\text{kin}}/E_{\text{ho}}$ has been estimated using a variational calculation of the ground state based on Gaussian trial wave functions for the order parameter [9,10]. One can see that, while the energy of the quadrupole excitation is enhanced at negative scattering lengths, the monopole mode becomes softer. The upper bound (20) for the monopole energy vanishes when $E_{\text{kin}} = 5E_{\text{ho}}$. This coincides exactly with the condition for the onset of instability predicted by the use of Gaussian trial wave functions in the variational calculation ($Na/a_{\text{HO}} = -0.67$ [10]). It is, however, worth noting that the results shown in the figure provide only a semiquantitative estimate of the excitation frequencies. In fact, the onset of instability obtained from the exact solution [8] of the Gross-Pitaevskii equation ($Na/a_{\text{HO}} \sim -0.57$) differs from the Gaussian estimate. Furthermore, one should keep in mind that the estimates (17) and (20), being based on the ratio (12), provide only an upper bound to the frequency of the lowest excitations.

In conclusion, we have derived a systematic investigation of the collective excitations of a Bose-condensed gas confined in an external trap. We have obtained analytic results for the dispersion law of both surface and compression modes employing the hydrodynamic approximation and the sum approach. Our work reveals the key role played by the interatomic forces which introduce a rich structure in the dynamic behavior of these new many-body systems.

After submitting this paper, we have received a preprint [19] reporting the first experimental measurements of the lowest collective modes of a gas of ^{87}Rb atoms trapped in an anisotropic potential ($\lambda = \sqrt{8}$). The experimental results are in good agreement with our predictions $\omega = 1.4\omega_{\perp}$ and $1.8\omega_{\perp}$ for the lowest $m = 2$ [Eq. (22)] and $m = 0$ [Eq. (24)] frequencies. The same results also agree well with the predictions of the recent numerical calculations of Refs. [20] and [21]. A similar experiment has been carried out on a gas of sodium atoms confined in cigar-type trap [22]. The measured frequency is in

very close agreement with the lowest solution of Eq. (24) ($\sqrt{5/2}\omega_z$ for small values of λ).

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