Many-body approach to low-lying collective excitations in a BEC approaching collapse

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Abstract

An approximate many-body theory incorporating two-body correlations has been employed to calculate low-lying collective multipole frequencies in a Bose-Einstein condensate containing A bosons, for different values of the interaction parameter $\lambda = \frac{A a_s}{a_{ho}}$. Significant difference from the variational estimate of the Gross-Pitaevskii equation has been found near the collapse region. This is attributed to two-body correlations and finite range attraction of the realistic interatomic interaction. A large deviation from the hydrodynamic model is also seen for the second monopole breathing mode and the quadrupole mode for large positive λ.

Low-lying collective excitations of a Bose-Einstein condensate can provide valuable information about the interactions and stability of the condensate, as the dimensionless interaction parameter $\lambda = \frac{A a_s}{a_{ho}}$ decreases from a large positive (repulsive interaction) value to negative (attractive interaction) values. Starting from the Gross-Pitaevskii (GP) equation, and using a sum rule approach, Stringari [1] obtained analytic expressions in terms of expectation values of kinetic energy (E_{kin}) and harmonic confining potentials (E_{ho}), for the monopole (ω_M) and quadrupole (ω_Q) frequencies. In Fig.1 of Ref.[1], variational estimates [2, 3] were plotted against λ, which shows a sharp change for both ω_M and ω_Q as λ approaches the variational critical value $\lambda_{cr}^{GP,var} = -0.671$ [3]. Note that this provides an upper bound. Furthermore, numerical calculation of E_{kin} by the GP equation close to the collapse region involves large errors. Hence, it is desirable to calculate the low-lying excitation frequencies directly using a many-body approach, which can

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handle a finite range interaction instead of the contact interaction in the GP equation.

In the present work, we calculate low-lying collective excitation frequencies of a dilute Bose-Einstein condensate (BEC), using the many-body potential harmonics expansion (PHE) approach [4]. Only two-body correlations are relevant in the dilute many-body system. Hence the (ij)-Faddeev component of the many-body wave function, is a function of the relative separation ($\vec{r}_{ij}$) and a global length called hyperradius (r) only. In the PHE method, one expands the Faddeev component (ψ_{ij}), corresponding to the (ij)-interacting pair of the condensate containing A atoms, in the corresponding potential harmonics (PH) basis [5] (which is the subset of the full hyperspherical harmonics (HH) basis [6], needed for the expansion of the two-body potential $V(\vec{r}_{ij})$)

$$\psi_{ij}(\vec{r}_{ij}, r) = r^{\frac{-(3A-4)}{2}} \Sigma_K P_{2K+l}^{lm}(\Omega_{ij}) u_K^l(r). \tag{1}$$

Here, l and m are the orbital angular momentum of the system and its projection and Ω_{ij} represents the full set of hyperangles for the (ij)-partition. A closed analytic expression can be obtained for the PH, $P_{2K+l}^{lm}(\Omega_{ij})$ [5]. The expansion (1) is, in general, very slow due to the fact that the lowest order PH is a constant and does not represent the strong short-range correlation of the interacting pair, arising from the very short range repulsion of the interatomic interaction. To enhance the expansion we introduce a short-range correlation function $\eta(r_{ij})$, in analogy with atomic systems [7, 8]. This is obtained as the zero energy solution of the two-body Schrödinger equation with the chosen two-body potential [9], corresponding to the appropriate s-wave scattering length (a_s). Thus we replace expansion (1) by [10]

$$\psi_{ij}(\vec{r}_{ij}, r) = r^{\frac{-(3A-4)}{2}} \Sigma_K P_{2K+l}^{lm}(\Omega_{ij}) u_K^l(r) \eta(r_{ij}). \tag{2}$$

Substitution of this expansion in the many-body Schrödinger equation and projection on a particular PH gives rise to a system of coupled differential equation (CDE) in r [4, 10], which is solved numerically using hyperspherical adiabatic approximation (HAA) [11]. Details of the procedure can be found in ref. [10].

In the HAA, the coupling potential matrix together with the diagonal hyper-centrifugal repulsion is diagonalised to get the effective potential, $\omega_o(r)$, as the lowest

eigenvalue of the matrix for a particular value of r. Collective motion of the condensate in the hyperradial space takes place in the effective potential $\omega_o(r)$. Ground state in this well gives the ground state energy (E_{00}) of the condensate corresponding to $n = 0$, $l = 0$. Here E_{nl} is the energy in oscillator units ($o.u.$) of the nth radial excitation of the lth surface mode. Hyperradial excitations corresponding to the breathing mode for $l = 0$, give the monopole frequencies as $\omega_{Mn} = (E_{n0} - E_{00})$. For $l \neq 0$, we get the surface modes. Numerical calculation of the off-diagonal potential matrix elements for $l \neq 0$ is fraught with large inaccuracies and its numerical computation is very slow. On the other hand the diagonal hypercentrifugal term is very large for large A and contributes most to the potential matrix. Hence we disregard $l > 0$ contributions to the off-diagonal matrix elements. For non-zero orbital angular momentum, we thus get the effective potential $\omega_l(r)$ in the hyperradial space. The ground state in this potential is the ground state of the lth surface mode E_{0l} and n^{th} radial excitations provide E_{nl}. The lowest monopole and quadrupole frequencies are given by $\omega_M = E_{10} - E_{00}$ and $\omega_Q = E_{02} - E_{00}$. The s-wave scattering length (a_s) has been chosen as 2.09783×10^{-4} $o.u.$ for repulsive interaction and -1.39217×10^{-4} $o.u.$ for attractive interaction. The interatomic interaction is chosen as the van der Waals potential with a hard core of radius r_c, $viz.$, $V(r_{ij}) = \infty$ for $r_{ij} < r_c$ and $= -\frac{C_6}{r_{ij}^6}$ for $r_{ij} \geq r_c$. The value of C_6 is chosen to be appropriate for rubidium atoms. The value of r_c is adjusted to get the desired value of a_s [12]. All quantities are expressed in oscillator units ($o.u.$) appropriate for the JILA experiment with ^{85}Rb [13]. The PHE equation is then solved numerically for different A to calculate E_{nl} for different values of λ.

In Fig.1 we plot calculated ω_M and ω_Q as a function of the dimensionless interaction parameter λ. For comparison we include the variational estimates from the GP equation [1]. We have also included results of a numerical solution of the GP equation [14]. However calculation of E_{kin} and E_{int} using the GP program have large errors for values of λ close to collapse for attractive condensates as also for large positive λ. This is shown by the lack of agreement with the virial identity involving E_{kin}, E_{int} and E_{ho}, $viz.$ $2E_{kin} - 2E_{ho} + 3E_{int} = 0$ [15]. Hence in Fig.1, the curves obtained by a numerical solution of the GP equation is shown only in the region where it is reliable. It is seen that

3

for positive values of λ, all the three curves for the monopole frequency are close to each other. Results of PHE and variational estimates are almost indistinguishable. However for negative λ, ω_M by the PHE method drops faster as λ approaches the critical value $\lambda_{cr} = -0.461$. Note that while GP equation predicts a critical value of -0.571 (variational estimate is -0.671) [15], experimental critical number is $-0.459\pm0.012\pm0.054$ [13]. The prediction by the PHE method agrees well with this value [16]. As the attractive condensate approaches collapse, with λ approaching λ_{cr} from the right, the condensate becomes softer (more compressible) and the breathing mode easier.
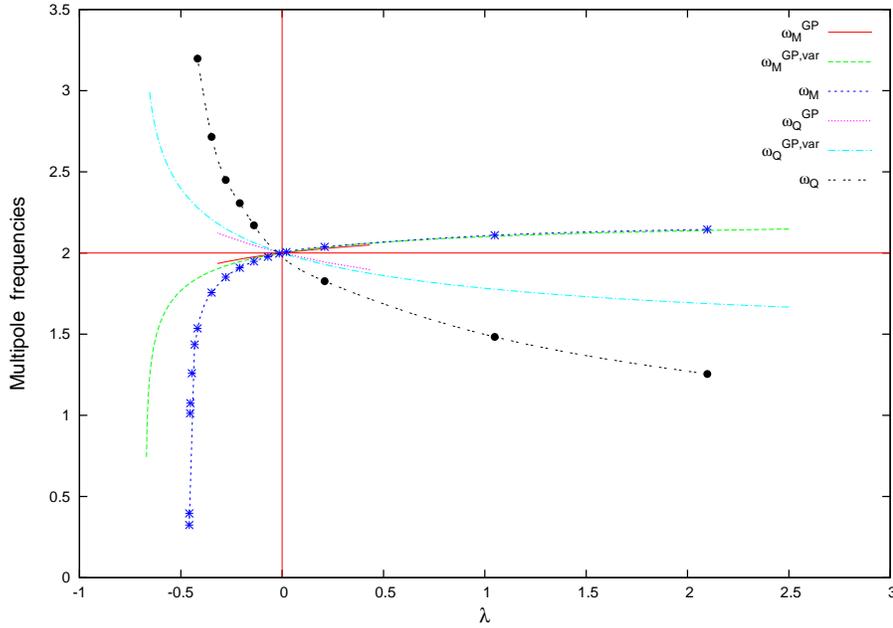

Figure 1: Calculated monopole (ω_M) and quadrupole (ω_Q) frequencies as functions of λ. Superscripts GP, GP,var and PHE correspond respectively to numerical solution of the GP equation, its variational estimate, and the present calculation.

On the other hand the quadrupole frequency (ω_Q) shows a greater deviation from the variational estimate – both for positive and negative values of λ. Since $\lambda_{cr} = -0.461$, it is natural that both monopole and quadrupole frequencies calculated by PHE method have rapid changes as λ approaches -0.461. The difference between the collective excitation frequencies calculated by PHE and GP equation can be attributed to the two-body correlations and finite range interactions. As the condensate approaches collapse, its

size decreases rapidly [16], so that the finite range interatomic attractions of the realistic atom-atom potential dominate and correlations play a more important role. Although for small values of $|\lambda|$ use of an effective interaction in terms of a_s is adequate, the strong correlations arising from the attractive part of the realistic atom-atom interaction produces discernible effects [17, 18, 19, 20] for λ approaching λ_{cr}. One can also qualitatively interpret the dependence of ω_Q on λ as follows. The two-body correlation disallows proximity of two interacting atoms in the repulsive case. Again in the $l = 2$ state the atoms are further apart compared to the $l = 0$ state. It is therefore easier (*i.e.* excitation energy is lower) for the condensate to jump from $l = 0$ to $l = 2$ state, when two-body correlations are included than when they are excluded (as in the GP equation). The inverse is true for the attractive case. The results obtained in the present work are in conformity with these arguments. Further discussions on the behaviour of ω_Q for large positive λ will be taken up together with those of higher excitation frequencies, after we present them.
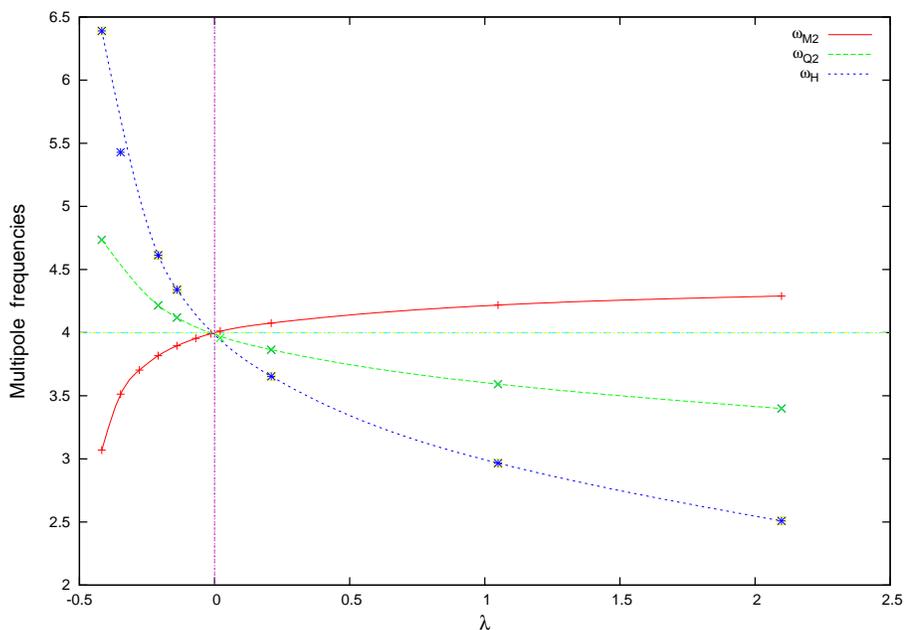

Figure 2: Higher order multipole frequencies calculated by PHE method, as functions of λ.

In Fig.2 we present the multipole frequencies which are degenerate with a value of 4 in the non-interacting case, *viz.*, $\omega_{M2} = E_{2,0} - E_{0,0}$, $\omega_{Q2} = E_{1,2} - E_{0,0}$ and

$\omega_H = E_{0,4} - E_{0,0}$. As expected from the softness of the condensate , the second breathing mode frequency ω_{M2} is larger than 4 for positive λ and less than 4 for negative λ, decreasing sharply as $\lambda \to \lambda_{cr}$. This once again shows that the condensate becomes softer as $\lambda \to \lambda_{cr}$, and harder and more rigid as λ increases to large positive values. On the ther hand, both ω_{Q2} and ω_H are less than 4 for $\lambda > 0$ and greater than 4 for $\lambda < 0$. Both increase sharply as $\lambda \to \lambda_{cr}$, ω_H increasing much faster than ω_{Q2}. As positive λ increases, the condensate becomes less compressible (more rigid) costing less energy for rotational excitations. Hence the spacing between the rotational levels decrease. For negative λ close to λ_{cr}, ω_H is much larger than ω_{Q2}. This shows that for such soft condensates, the first breathing mode of $l = 2$ surface mode is easier to excite than the ground state of the $l = 4$ surface mode, although they are degenerate in the non-interacting limit. This is consistent with the general picture and intuition. One can also note that $\omega_{Q2} - \omega_Q = E_{1,2} - E_{0,2}$ decreases rapidly from 2 as λ decreases from zero to λ_{cr}. This again shows the softness of the $l = 2$ surface mode of the attractive condensate.

We next come back to a discussion of our results as compared with those by the GP equation and the hydrodynamic model, as also with available experimental results. As mentioned earlier, results using the numerical solution [14] of the GP equation are not reliable for almost all values of λ except small $|\lambda|$. Moreover ω_M and ω_Q given in terms of E_{kin} and E_{ho} are rigorous upper bounds for the frequency of the lowest states excited by the appropriate multipole operator [1]. The upper bounds get further upwardly shifted for the variational estimate. The PHE result for ω_Q is lower than the variational estimate; hence it is consistent with this requirement. Using the hydrodynamic model Stringari also derived a dispersion law for the frequencies of the normal modes [1], $viz.$, $\omega(n, l) = \omega_0(2n^2 + 2nl + 3n + l)^{1/2}$, where ω_0 is the frequency of the spherically symmetric trap. This is valid in the limit $\lambda >> 1$, where kinetic energy contribution can be disregarded. While the PHE result for ω_M is very close to this estimate, that for ω_Q is close to but less than this limit. Available experimental results [21, 22, 23, 24] are for axially symmetric traps only – measured ω for $m = \pm 2$ and $m = 0$ agree well with the GP equation and the hydrodynamic model estimates for the deformed trap. Since accuracy of the hydrodynamic model estimate is expected to decrease as n and l increase, due

to the neglect of the kinetic energy contribution [1] and ω_M calculated by PHE agrees remarkably well with that from the GP equation, it is important to have accurate measurement of ω_Q for the spherical trap. The experimental procedure of ref. [24] can be utilized for this purpose, since it is suitable for any geometry of the trap. This technique uses the optical dipole force of a rapidly scanning laser beam to excite surface modes by inducing deformations of the trap potential.

More remarkable is the disagreement of the second breathing mode (ω_{M2}). The PHE predicts a value > 4 for positive λ, while the $\lambda >> 1$ limit by the hydrodynamic model gives $\sqrt{14}$. One expects that the system becomes less and less compressible as positive λ increases. Consequently one would expect $\omega_{M2} > 4$ for positive λ, which disagrees with the hydrodynamic model prediction. This is an indication that the kinetic energy contribution can no longer be disregarded for such excitation energies. To resolve the issue, one needs a precise measurement of ω_{M2}. The higher mode can be excited by an appropriate frequency of the laser beam.

In summary, we have investigated monopole, quadrupole and hexadecapole frequencies (corresponding to $l = 0$, 2 and 4 respectively) of the collective motion of Bose-Einstein condensates by a many-body approach based on hyperspherical harmonics method. We include the most important two-body correlations, disregarding higher-body correlations. We notice that two-body correlations and the finite range attraction of a realistic two-body interaction make the attractive condensate softer compared with the use of a contact interaction. This is consistent with intuitive expectations. Consequently our results differ appreciably from those by the GP equation in the collapse region for an attractive condensate. The effect of two-body correlations become increasingly more relevant as the condensate approaches collapse. For repulsive condensates the monopole frequency agrees very well with the the GP estimate, while the quadrupole frequency differs by about 10% of the asymptotic value. For the second breathing mode the PHE result is greater than the non-interacting value, as expected intuitively, for $\lambda > 0$. This is in sharp contrast with the asymptotic ($\lambda >> 1$) GP estimate of $\sqrt{14}$, indicating that the disregard of kinetic energy terms in the hydrodynamical model is not valid for such excitation levels. This calls for precise measurements of these multipole frequencies.

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