Collective and single-particle excitations of trapped Bose gas with very large particle number

M.L. Lekala, B. Chakrabarti, T.K. Das, G.J. Rampho, S.A. Sofianos, R.M. Adam, S.K. Haldar

1 Physics Department, University of South Africa, P.O. Box 392, Pretoria 0003, South Africa. Tel.: +27-12-4298640 Fax.: +27-12-4299633.
2 The Abdus Salam International Centre for Theoretical Physics, I-34100, Trieste, Italy.
3 Department of Physics, University of Calcutta, 92 A.P.C. Road, Kolkata 700084, India.
4 Square Kilometer Array Radiotelescope, The Park, Park Rd., Pinelands 7405, South Africa.
5 Theoretical Physics Division, Physical Research Laboratory, Navarangpura, Ahmedabad-380 009, India.

We study the collective and single particle excitations of trapped Bose gas with the realistic van der waals interaction for very large particle number (\(N \sim 10^7 - 10^8\)) in an external harmonic trap, using the correlated two-body basis functions for expansion of the full many-body wave function. We calculate the ground state energy and one-body density and compare our results with those obtained using mean-field approaches. The effect of different \(C_6\) parameter has been critically examined for wide range of particle number \(N \sim 3 - 10^7\) which rigorously show how the shape dependent approximation starts to develop with gradual increase in particle number. We calculate the one-body density for various particle number with several choices of \(C_6\) parameters which justify the use of shape-dependent two-body interaction in the many-body calculation. We also present an extensive study of the excitation spectrum over a wide range of energy and observe that the low-lying excitations are of collective nature, where the effect of interaction is quite important. For large particle number limit, these are well described by the hydrodynamic (HD) model and the results are in good agreement with experimental results. Though only the modes with lower multipolarity and frequency have been detected in the experiments, the excitations at high energy and higher angular momentum are specially important as they determine the thermodynamic properties.

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I. INTRODUCTION

Laboratory realization of gaseous Bose-Einstein condensates (BEC) [1-3] and subsequent experiments characterizing low-lying collective excitations [4] have prompted various theoretical investigations [5-7]. Unlike the phenomena such as superfluidity of liquid helium, the atomic vapour is very dilute and the fundamental interaction is characterized by the \(s\)-wave scattering length \(a_s\). Thus even with the interaction the system is quite easy for theoretical understanding. The standard theory for BEC in a dilute atomic vapour, basically uses Gross-Pitaevskii (GP) equation [8] which is the nonlinear Schrödinger equation with the inter-atomic interaction modelled by an \(s\)-wave scattering length. The exact shape of the inter-particle interaction and inter-atomic correlations are ignored in this picture. The elementary excitations of BEC in finite harmonically confined dilute Bose gas have been studied using the GP equation [9]. Later the low-lying collective excitations have also been studied by the temperature dependent Hartree approximation [10] and the results are in good agreement with experimental results [4]. Though only the modes with lower multipolarity and frequency have been detected in the experiments, the excitations at high energy and higher angular momentum are specially important as they determine the thermodynamic properties.

In the present manuscript we report the ground state properties, collective excitations both at low and high energy for up to \(N \sim 10^7 - 10^8\) atoms in the trap. We choose the van der Waals interaction as the inter-atomic interaction as in our earlier calculations. Even for small finite sized system we have observed that ground state energy depends on the exact shape of the potentials, all of them giving the same scattering length [11]. We have also observed that our calculated ground state energy separately depends on \(N\) and \(a_s\) and not on the effective interaction \(Na_s\) as claimed by the mean-field theory [8]. We utilize the two-body correlated basis function and expand the many-body condensate wave function in it. Thus our present treatment also incorporates the effect of pair-wise correlations and we are few steps ahead of
the mean-field theory. It also allows us to calculate the correlation energy as a function of atom number. We also compare our results in such large particle number limit with GP, modified GP (MGP) [8], and Thomas-Fermi (TF) approximation [8] for wide range of \( N a_0^3 \).

Most of the theoretical studies of dilute inhomogeneous Bose gases use the shape independent approximation where the true interatomic interaction is replaced by contact \( \delta \)-potential [8]. Later, the shapeless potential assumption has been tested theoretically in several important issues [11–15]. Although the conclusions of all the past works are qualitatively same, quantitative disagreements exist. All the earlier works in this direction consider truly finite number of particles and use standard short ranged 2-body potential. Here we use the realistic van der Waals potential with a short ranged hard core and long attractive tail parameterized by \( C_6 \) parameter. We thoroughly investigate the effect of long attractive tail (by gradually increasing \( C_6 \), adjusting the cutoff radius \( r_c \) such that they produce the same scattering length \( a_s = 100 \) Bohr, which mimics the JILA experiment) on the ground state energy and one-body density for wide range of particle number \( N \sim 3 \times 10^7 \). Appreciable dependence on \( C_6 \), particularly for larger number of particles, nicely justify the use of shape-dependent potential in the many-body calculation. The effects of shape dependence of the two-body potential obviously increases with the number of interacting pairs, i.e. with \( N \). We therefore first calculate the ground state energy and one body density for a small number of particles, which agree with the shape independent mean-field theory results, establishing the validity of our method.

Study of collective excitations both at low and high energies at such large particle number limit is quite interesting for the following reason. The excitations at high energy are expected to be of single-particle nature. However laboratory BEC is a strongly inhomogeneous system due to the external trap and may significantly differ from the uniform Bose gas where only phonons are present at low energy. Thus the study of transition from low-lying collective excitations to single-particle excitations by the correlated many-body method using the realistic interaction is itself interesting. In the limit of large particle number, ignoring the kinetic energy term in the GP equation one gets the TF approximation. In the same limit the collective excitations are described by the hydrodynamic (HD) model [5, 8] of superfluidity, eigenfrequencies are calculated by a simple analytic formula. It is already shown that the HD approximation provides excellent description only for the low-lying elementary excitations. At the opposite end, the Hartree-Fock theory correctly predicts the single particle nature. Thus our present complete many-body calculation can be treated as a bridge between the two extreme cases and will explore better understanding from the collective to single particle regime.

The paper is organized as follows. In Sec. II we discuss the correlated potential harmonic basis for large particle number. Sec. III mainly considers the ground state properties and comparison with the mean-field results are provided. The validity of shape independent approximation and the justification of the choice of realistic potential in the many-body calculation is presented in Sec. IV. Sec. V deals with the calculation of collective excitations both at low and high energies. Sec. VI concludes with a summary.

II. FORMALISM

A. Potential harmonic expansion of the many-body equation

In the present work we calculate the ground state energy, low-lying and high-lying collective excitation frequencies of a dilute BEC for quite a large number of bosons \( N \sim 10^7 \times 10^5 \) using the potential harmonics expansion method (PHEM) [16]. The most fundamental feature of PHEM is that the two-body correlations are relevant in the many-body system and the \((ij)\) Faddeev component of the \(N\)-body wave function is a function of the relative separation \( \vec{r}_{ij} \) and a global length called hyperradius \( r \). We have already successfully utilized the two-body correlated basis function for the description of the dilute BEC [17]. So in the present description we only point out the essential part of PHEM which is required for the completeness and clarity of the manuscript. For the detailed formulation we refer the reader to our earlier published works [18–20].

In the PHEM, we expand the two-body Faddeev component \( \phi_{ij} \) corresponding to the \((ij)\) interacting pair of the condensate with \( N = N + 1 \) bosons in the potential harmonic (PH) basis as

\[
\phi_{ij}(\vec{r}_{ij}, r) = r^{-\left(\frac{3N+1}{2}\right)} \sum_K P_{2K+\ell} \left(\Omega_N^{ij}\right) u_K(r),
\]

where \( \Omega_N^{ij} \) corresponds to the full set of hyperangles for the \(ij\)th partition and \( \ell \) and \( m_\ell \) are the orbital angular momentum of the system and its projection. In the hyperspherical coordinate, the variables are characterized by the hyperradius \( r^2 = \sum_{i=1}^N \zeta_i^2 \) (\( \zeta_i \), \( i = 1,N \) being the Jacobi vectors describing the relative motion) and \((3N - 1) \) hyperangles [21]. However for the potential harmonic expansion method of weakly interacting BEC, as the two-body correlations are only dominating, we assume that when the \((ij)\) pair of atoms interact, the rest of the atoms are inert spectators [18]. As all the degrees of freedom coming from the \((N - 1)\) inert spectators are frozen, the number of quantum numbers becomes effectively four irrespective of the number of bosons, these are orbital angular momentum \( \ell \), azimuthal \( m_\ell \), the grand orbital angular momentum \( 2K + \ell \), and the energy quantum number. The closed analytic expression for PH, \( P_{2K+\ell}^{m_\ell} \left(\Omega_N^{ij}\right) \) can be found in the Ref. [16]. It has been mentioned in our earlier works that the above expansion is in general very slow as the lowest order PH is a constant.
and does not represent the strong-range repulsion of the interatomic interaction. Therefore we introduced a short-range correlation \( \eta(r_{ij}) \) which is obtained as the zero-energy solution of the two-body Schrödinger equation
\[
\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr_{ij}^2} + V(r_{ij})\right] \eta(r_{ij}) = 0,
\]
with the chosen two-body potential \( V(r_{ij}) \) [20] and correspond to the appropriate s-wave scattering length \( a_s \) as described in next section. The expansion (Eq. (1)) now takes the form
\[
\phi_{ij}(\vec{r}_{ij}, r) = r^{-(3N-4)/2} \sum_{K} P_{2K+\ell}^{\alpha\beta}(\Omega_{ij}^N) u_{K}^\ell(r) \eta(r_{ij}).
\]
Substituting this expansion (Eq. (3)) in the many-body Schrödinger equation, one gets a set of coupled differential equations (CDE) in \( r \). The coupling potential matrix element \( V_{KK'} \) is given by
\[
V_{KK'}(r) = \frac{1}{\sqrt{\hbar^2 \kappa^2 \kappa_0^4}} \int_{1}^{+1} P_{\kappa}^{\alpha\beta}(z) V \left( r \sqrt{(1+z)/2} \right) \times P_{\kappa'}^{\alpha\beta}(z) \eta \left( r \sqrt{(1+z)/2} \right) W_\ell(z) dz,
\]
where \( P_{\kappa}^{\alpha\beta}(z) \), \( \hbar^2 \kappa^2 \) and \( W_\ell(z) \) are the Jacobi polynomial, its norm and weight function respectively, with \( \alpha = (3N - 8)/2 \) and \( \beta = \ell + \frac{1}{2} \). The CDE is solved using hyperspherical adiabatic approximation (HAA) [22]. The HAA basically reduces the whole 3N dimensional problem to an effective one dimensional one. In HAA, the coupled potential matrix \( V_{KK'} \) along with the diagonal hypercentrifugal repulsion is diagonalized to get an effective potential \( \omega_0(r) \) as the lowest eigen value of the matrix for a particular value of \( r \).

The basic length scale for a harmonic oscillator trap of frequency \( \omega_0 \) is \( a_0 = \hbar/(m \omega_0) \). For the typical experimental BEC, \( a_0 \) is of the order of \( 10^4 a_0 \). However, the effective potential in hyperspherical space due to the hypercentrifugal repulsion together with the harmonic oscillator trap has a minimum at about \( \sqrt{3N} a_0 \). As an example, with \( N \approx 10^4 \), the minimum of the effective potential will be near about \( 10^6 a_0 \) which is almost \( 10^5 \) times larger than the typical range of the interatomic interaction. This shows that for such a typical case, the entire contribution to \( V_{KK'}(r) \) in the integral in Eq. (4) comes from an extremely narrow interval of \( z \)-integration (\( \approx 10^{-16} \)). The integral in Eq. (4) also varies rapidly within this narrow interval because of the following reason. The integrand contains the Jacobi polynomial \( P_{\kappa}^{\alpha\beta}(z) \) and its weight function \( W_\ell(z) = (1 - z)^\alpha (1 + z)^\beta \) [23]. For large \( N \), both \( P_{\kappa}^{\alpha\beta}(z) \) and \( W_\ell(z) \) change very rapidly with respect to \( z \). \( W_\ell(z) \) varies from zero at \( z = -1 \) to a maximum of \( \approx 2^\alpha \) at \( z_m = (\beta - \alpha)/(\beta + \alpha) \) and then rapidly reaching a value about \( 10^{-10} \) of the peak value at \( z = -1 + 0.003 \). Although the peak value \( 2^\alpha \) is extremely large for large \( N \), partial cancellation results from the factor \( [\hbar K_h^{\alpha\beta} h_{KK'}^{\alpha\beta}]^{-1/2} \) [23]. Thus, any standard quadrature to evaluate the integrand in Eq. (4) gives essentially zero for \( N > 50 \). Usually we solve this problem by splitting the interval \( z \in [-1, 1] \) into \( n \) gradually increasing subintervals and evaluating the integral in each subinterval using a 32-point Gauss-Legendre quadrature. This permits us to evaluate \( V_{KK'}(r) \) for \( N \) up to 15000 with an accuracy of one part in \( 10^5 \) [24].

### B. Extension to \( N \to \infty \) limit

As pointed out earlier, the experimental BEC treats up to \( 10^8 \) atoms in the trap. But the numerical code mentioned above can treat only up to 15000 atoms which is far from the experimental situation. To circumvent the problem and extend the correlated many-body technique to quite large number of atoms we recently made a direct mathematical transformation [25]. This basically transforms the PHEM into a two-variable integro differential equation. With this transformation, the Jacobi polynomial \( P_{\kappa}^{\alpha\beta}(z) \) can be replaced with the associated Laguerre polynomial as discussed in the following. In our initial attempt we applied the CPHEM using the Laguerre polynomial (CPHEM) for the order of \( 10^6 \) atoms only for the ground state [25]. We utilize a mathematical relation \( \beta \to \infty \) to transform Jacobi polynomials into associated Laguerre polynomials [23]. An outline of the derivation, including derivation of the relations between Jacobi and associated Laguerre polynomials in the limit \( \alpha \to \infty \) are as follows. Starting from the mathematical relation [23]
\[
\lim_{\beta \to \infty} P_{n}^{\alpha\beta}(1 - \frac{2x}{\beta}) = L_{n}^{\alpha}(x),
\]
interchanging \( \beta \) and \( \alpha \) and using the relation [23]
\[
P_{n}^{\alpha\beta}(-x) = (-1)^n P_{n}^{\beta\alpha}(x),
\]
we obtain
\[
\lim_{\alpha \to \infty} P_{n}^{\alpha\beta}(\frac{2x}{\alpha} - 1) = (-1)^n L_{n}^{\beta}(x).
\]
Substituting \( x = \zeta^2 = \alpha (r_{ij}/r)^2 \) and \( z = 2(r_{ij}/r)^2 - 1 \), we get
\[
\lim_{\alpha \to \infty} P_{K}^{\alpha\beta}(z) = (-1)^K L_{K}^{\beta}(\zeta^2).
\]
This relation has been used in evaluating \( f_{KK'} \) appearing in the CDE for large \( \alpha \) [25]. In this limit, the weight function \( W_\ell(z) \) of the Jacobi polynomial transforms as
\[
W_\ell(z) = (1 - z)^\alpha (1 + z)^\beta = \frac{2^{\alpha+\beta}}{\alpha^\beta} \zeta^{2\beta} \left( 1 - \frac{\zeta^2}{\alpha} \right)^\alpha.
\]
In the limit \( \alpha \to \infty \), the last factor becomes \( e^{-\zeta^2} \). Hence for large \( \alpha \),
\[
W_\ell(z) = \frac{2^{\alpha+\beta}}{\alpha^\beta} \zeta^{2\beta} e^{-\zeta^2}.
\]
This has the correct functional form for the weight function of associated Laguerre polynomial $L^\alpha_K(x)$. Substituting equations (8) and (10) in equation (4), and using the explicit expression of the norm of the Jacobi polynomial [23] we obtain

$$V_{K,K'}(r) = A_c \int_{x_{\min}}^{x_{\max}} L^\beta_K(x) V(r \sqrt{\alpha}/\alpha) \eta(r \sqrt{\alpha}) \times L^\beta_{K'}(x)^2 \alpha e^{-x^2} dx$$

where $x_{\min} = (r_c/r)^2 \alpha$, $r_c$ is the hard core radius of our chosen realistic van der Waals potential and

$$A_c = \left( -\frac{(K+K')\alpha^3}{\alpha^3} \right) \left[ \frac{2K + \alpha + \beta + 1}{\alpha} \frac{2K' + \alpha + \beta + 1}{\alpha} \right] \times \left[ \frac{\Gamma(K+1)}{\Gamma(K'+1)} \frac{\Gamma(K')}{\Gamma(K'+K+1)} \right] \times \left[ \frac{\Gamma(K + \alpha + \beta + 1)}{\Gamma(K' + \alpha + 1)} \right]^{1/2}.$$

### III. RESULTS FOR GROUND STATE ENERGY WITH $N \simeq 10^7 - 10^8$ ATOMS IN THE EXTERNAL TRAP

Throughout our calculation we keep the system parameters which correspond to the JILA trap [1]. The mass $m = 87$ amu, trap frequency $\omega_{ho} = 2\pi \times 77.78$ Hz and the scattering length $a_s = 100$ Bohr. As a unit of length we choose the oscillator unit (o.u.) of length $a_{ho} = \sqrt{\hbar/m\omega_{ho}}$ and the energy unit as the harmonic oscillator energy $\hbar \omega_{ho}$. For the mean-field GP equation, the two-body potential is chosen as the zero-range potential $V(r) = 4\pi \hbar^2 m \omega_{ho} \delta(r)$, where $a_s$ is the $s$-wave scattering length [8]. It is shape-independent and completely ignores the energy dependence of scattering amplitude. We choose the realistic van der Waals interaction as

$$V(r_{ij}) = -\frac{C_6}{r_{ij}^6}, \quad r_{ij} > a_s$$

$$= \infty, \quad r_{ij} \leq a_s$$

with $C_6 = 6.489755 \times 10^{-11}$ o.u. for $^{87}$Rb atoms [26]. For a given value of $r_c$, $a_s$ is calculated by looking at the zero-energy solution of the two-body Schrödinger equation Eq. (2), where $V(r_{ij})$ is the van der Waals potential [26]. Its asymptotic form quickly attains $\eta(r_{ij}) \sim C(1 - a_{ij}/r_{ij})$ from which $a_s$ is calculated [26]. We choose the value of $r_c = 1.121054 \times 10^{-3}$ o.u. which corresponds to $a_s = 100$ Bohr = 0.0043 Bohr. It is to be noted that although $r_c$ is almost four times smaller than $a_s$, they are of same order. Smaller values of $r_c$ [corresponding to larger number of nodes in $\eta(r_{ij})$] has not been chosen to avoid the presence of many-body bound states and clustering. It is also to be noted that for hard sphere scattering, the effective range $r_e$ increases linearly with $a_s$, as $r_e = \frac{2}{3} a_s$, whereas for the van der Waals potential $r_e$ is determined from $a_s$ by

$$r_e = \frac{2}{3a_s} \frac{1}{\beta_0} \left( 1 + \left( 1 - x_c \left( \frac{a_s}{\beta_0} \right)^2 \right) \right),$$

where $\beta_0 = (mC_6/\hbar^2)^{1/4}$ and $x_c = [\Gamma(1/4)]^{2}/2\pi$. The calculated value of $r_e$ for our present work is $1.251 \times 10^{-3}$ o.u. which is comparable with but greater than the value of $r_c$, as expected.

As pointed earlier, the lowest eigenpotential $\omega_0(r)$ is treated as the many-body effective potential which describes the collective phenomena of dilute BEC. This is also in good agreement with experimental situation. As at the ultra-cold temperature all the individual atoms in the condensate lie within one single de-Broglie wavelength, the condensate is treated as a single lump of quantum staff. However before calculating the ground state energies, it is indeed required to check the convergence for $N = 10^7$ atoms. With the increase in the number of particles $N$, the effective interaction $N a_s$ increases, the condensate becomes more repulsive. The condensate density is pushed out as its average radius increases sharply. So higher $K_{max}$ may be needed for convergence of the ground state for larger particle number. In Fig. 1 we plot $\omega_0(r)$ as a function of $r$ for $K_{max} = 2, 4, 6, 8$ and 10 with $N = 10^7$ and observe very fast convergence. Although after $K_{max} = 4$, all the graphs appear to overlap completely as seen in the Fig. 1, still we noticed that the minimum of the effective potential decreases very slowly (which is not visible in the figure) as $K_{max}$ increases. This is consistent with the Rayleigh-Ritz principle. So, throughout our calculation we fix $K_{max} = 8$ and calculate the ground state energy per particle, which we present in Table I. We compare our many-body results with TF, GP and MGP results and for the compact presentation of different diluteness, we include the results for a wide range of $N a_s^3$, which basically determines the diluteness of the condensate. Comparison with MGP is needed for better justification as MGP includes the correction due to quantum fluctuation.

### TABLE I: Ground-state energy per particle (in o.u.) for $^{87}$Rb atoms. Results in TF approximation, solving the GP, MGP and the correlated many-body equations (CPHEL) are presented in unit of $(\hbar \omega_{ho})$.

| $N$ | $N a_s^3$ | TF | GP | MGP | CPHEL |
|-----|----------|----|----|-----|-------|
| $10^4$ | $10^{-4}$ | 1.90 | 2.42 | 2.43 | 2.43 |
| $10^4$ | $10^{-3}$ | 4.76 | 5.04 | 5.08 | 5.19 |
| $10^5$ | $10^{-2}$ | 11.96 | 12.10 | 12.25 | 12.67 |
| $10^6$ | $10^{-1}$ | 30.05 | 30.12 | 30.66 | 31.67 |
| $10^7$ | 1.0 | 75.49 | 75.52 | 77.48 | 79.48 |
| $10^8$ | 10.0 | 189.61 | 189.63 | 196.45 | 194.41 |

We calculate the GP energy by solving the standard...
FIG. 1: (color online) Plot of the effective potential \( \omega_0 \) (in o.u.) as a function of the hyperradius \( r \) (in o.u.) for different values of \( K_{\text{max}} \) for 10\(^7\) atoms in the trap. We have set the zero of the ordinate at the minimum \( \omega_{\text{min}} \) (= 79454262.3813 o.u.) of the effective potential \( \omega_0(r) \) for \( K_{\text{max}} = 10 \).

GP energy functional

\[
E_{\text{GP}}[\Psi] = \int d\vec{r} \left[ \frac{\hbar^2}{2m} |\nabla \Psi|^2 + \frac{1}{2} m \omega_0^2 r^2 |\Psi|^2 + \frac{2\pi \hbar^2 a_s}{m} |\Psi|^4 \right].
\]  

and the MGP energy is calculated by solving

\[
E_{\text{MGP}}[\Psi] = \int d\vec{r} \left[ \frac{\hbar^2}{2m} |\nabla \Psi|^2 + \frac{1}{2} m \omega_0^2 r^2 |\Psi|^2 + \frac{2\pi \hbar^2 a_s}{m} |\Psi|^4 \left( 1 + \frac{128a_s^3}{15\sqrt{\pi}} |\Psi| \right) \right].
\]  

The additional term in Eq. (16) basically adds the quantum correction to the mean-field effective potential whereas the TF energy is calculated by using the simple analytic expression [8]. All the results are presented in Table I. We observe that our many-body ground state energy is very close to the GP and MGP results when the condensate is extremely dilute. However deviation starts to develop gradually with increase in \( na_s^3 \). We noticed that for higher density, compared to the GP results, MGP results are closer to the many-body results. It is expected as MGP equation includes some effects due to correlations. It is still independent of the shape of the interatomic interaction. The additional shape-dependent correction may improve the situation. The use of realistic finite range shape-dependent potential and inclusion of all possible two-body correlations in an exact way are additional desirable features in our approach. Note that TF results are always lower than both the GP and many-body results as the kinetic energy term is completely ignored in the TF limit. We calculate the correlation energy \( \Delta E_{\text{corr}} = (E_{\text{many-body}} - E_{\text{GP}})/E_{\text{many-body}} \) [27] as a measure of the deviation of mean-field GP result from our many-body results and observed their crucial dependence on the long attractive tail of the van der Waals interaction. However for particle number \( N \sim 10^7 - 10^8 \), it is also required to calculate the correlation energy with respect to TF results as at such large particle number limit the system is more classical. We present our results in Fig. 2 and observe that \( \Delta E_{\text{corr}}^{\text{TF}} \) and \( \Delta E_{\text{corr}}^{\text{GP}} \) merge together at very large particle number limit. It reaffirms that the ground state properties of dilute BEC in the truly thermodynamic limit should be correctly described by TF equation.

IV. VALIDITY OF SHAPE INDEPENDENT APPROXIMATION

Before closing the discussion regarding the ground state energies it is indeed required to present detailed study of ground state energies over a wide range of \( C_6 \) parameter. Although some interesting papers [11–15] already discuss the issue, however none of them consider the wide range of particle number and use the realistic interatomic interaction. Considering few tens of atoms in the trap, it is shown that the many-body results are closer to the mean-field results when the number of particles in the trap increases. It is intuitively true as the system becomes more classical. In fact, for such truly finite number of atoms (few tens) and in the extremely dilute condition the shape independent approximation (SIA) is valid. However our present calculation starts with just few atoms and goes up to order of millions of atoms in the trap. Increasing \( C_6 \) gradually, while keeping \( a_s \) fixed, we find that for few hundred of atoms the SIA is valid, however for large \( N \), the condensate gradually becomes more attractive and SIA starts to be invalid. In Table II, we present ground state energy \( E_0 \) obtained from our many-body calculation for various \( C_6 \) parameters and compare with GP results. It is seen that the SIA
is valid till \( N \sim \) few hundreds. The many-body results are independent of the choice of \( C_6 \) parameters in this particle number range. Basically making \( C_6 \) larger, the many-body effective potential becomes more attractive and the effect is significant for larger \( N \) as the many-body effective potential increases with \( \frac{N(N-1)}{2} \) van der Waals pairs. It causes decrease in \( \ell \) as shown in Table II. Chosen values of \( C_6 \) in o.u. are presented in the top line of columns 2 – 6. The third column corresponds to the actual value of \( C_6 \) for Rb atoms. Whereas for the positive scattering length, the condensate is repulsive, mean field results using only \( \delta \)-interaction also give rise to the effective repulsion. However the condensate is always stable due to external confinement. Using the realistic interatomic interaction with an attractive tail in the many-body calculation and the inclusion of two-body correlation decreases the energy. This decrease is appreciable for large \( N \), when the net interaction due to all the pairs is appreciable. It is also to be noted that the difference of the many-body results for the correct \( C_6 \) (third column) and the GP (last column) is small for small \( N \) and increases gradually with \( N \). This is due to the effect of correlations included in the many-body treatment, which increases with \( N \).

TABLE II: Ground-state energies per particle calculated by CPHEL in o.u. for different values of \( C_6 \) for 3 \( \leq N \leq 10^7 \) atoms in Rb condensate. All values of \( C_6 \) (given in o.u. in the top line of columns 2 – 6) correspond to the same scattering length \( a_s = 100 \) Bohr. GP results are presented for comparison.

| \( N \) | \( 5 \times 10^{-12} \) | \( 6.489 \times 10^{-11} \) | \( 7 \times 10^{-11} \) | \( 8 \times 10^{-11} \) | \( 9 \times 10^{-11} \) | GP |
|---|---|---|---|---|---|---|
| 3 | 1.512 | 1.512 | 1.512 | 1.512 | 1.511 |
| 5 | 1.5191 | 1.519 | 1.519 | 1.519 | 1.514 |
| 10 | 1.522 | 1.522 | 1.522 | 1.522 | 1.522 | 1.517 |
| 20 | 1.548 | 1.547 | 1.547 | 1.547 | 1.533 |
| 100 | 1.678 | 1.677 | 1.677 | 1.676 | 1.652 |
| \( 10^3 \) | 2.435 | 2.434 | 2.432 | 2.432 | 2.430 | 2.424 |
| \( 10^4 \) | 5.199 | 5.198 | 5.194 | 5.188 | 5.182 | 5.08 |
| \( 10^5 \) | 12.70 | 12.68 | 12.66 | 12.64 | 12.62 | 12.10 |
| \( 10^6 \) | 31.75 | 31.68 | 31.64 | 31.60 | 31.56 | 30.12 |
| \( 10^7 \) | 79.80 | 79.56 | 79.42 | 79.31 | 79.22 | 75.52 |

Next we compare the one-body density for various \( C_6 \) parameters and for wide range of particle numbers.

Although we have reported some results on one-body density for smaller particle number and have observed an appreciable effect of finite size, in the present work we are interested in effectively thermodynamic limit. The one-body density is a key quantity as it contains information regarding one-particle aspect of the condensate and can be indirectly measured in the interferometry experiments. We define it as the probability density of finding a particle at a distance \( r_k \) from the centre of mass of the condensate [28]

\[
R_1(r_k) = \int r \left| \Psi \right|^2 dr
\]  

where \( \Psi \) is the full many-body wave function and the integral over hypervolume \( r' \) excludes the variable \( r_k \).

In Fig. 3 we present the calculated one-body density for \( N = 10 \) atoms in the trap and compare with GP results. The calculated one-body density for various \( C_6 \) parameters perfectly match with the GP results as SIA needs to be valid and also confirms our previous observations. In Fig. 4 [ panel (a)] we plot the same for \( N = 10^4 \) atoms in the trap and for \( N = 10^5 \) atoms in panel (b) of Fig. 4 and compared with the GP results. The density profiles calculated from the GP equation has the same qualitative features, however disagreement remains in the peak value of the density distribution as well as in the extension of the density profile. To show how the disagreements between the many-body results and the GP results depend on the \( C_6 \) parameters, we plot the enlarged profile of one-body density near the peak [panel(c) for \( N = 10^4 \) and panel(d) for \( N = 10^5 \)] and near the tail part [panel(e) for \( N = 10^4 \) and panel(f) for \( N = 10^5 \)]. The actual two-body attraction is determined by the integration \( 4\pi \int _{r_c} ^\infty V(r)\eta(r)^2 dr \). A many-body calculation which uses the van der Waals potential having a long attractive tail \( -\frac{C_6}{r^6} \), the net effective interaction is more attractive than GP. Being more repulsive, GP lowers the central density and expands the density distribution. Increasing \( C_6 \) gradually, the central peak shifts upwards, as the effective interaction becomes more attractive and particles are pulled inwards. This effect is shown in the enlarged peak and tail parts. For larger \( N \), the effect due to all the pairs becomes prominent as the many-body effective potential becomes less repulsive.

FIG. 3: (color online) Plot of one-body density distribution for \( N = 10^8 \) Rb atoms in the condensate for various \( C_6 \) values corresponding to same \( a_s = 100 \) Bohr. Corresponding GP result is also presented for comparison.
 corresponding to same condensate in the hyperradial space takes place in the mean-field theory. Investigation and checking the many-body effects beyond nature in the macroscopic dynamics. It needs careful in-
cial collective excitations, including the transition from
which is the hydrodynamic
cially interested in examining collective features of the
es. In the present work we study both low- and high-
lies. For quite large number of bosons. We are spe-
citations provide valuable information about the interac-

\[ E_{n\ell} = E_{n\ell} \text{(fourth breathing mode)} \]

\[ E_{M1} = E_{10} - E_{00} \]

\[ E_{M2} = E_{20} - E_{00} \]

\[ E_{M3} = E_{30} - E_{00} \]

\[ E_{M4} = E_{40} - E_{00} \]

\[ \omega(n, \ell) = \omega_{ho}(2n^2 + 2n\ell + 3n + \ell)^{1/2}. \]  

where \( \ell \) and \( n \) are the angular momentum quantum number and number of nodes in the radial solution respectively. For quite large \( N \), when the dimensionless parameter \( \frac{\Delta E}{E_{ho}} \) is large, the kinetic energy term in the ground state GP equation becomes negligibly small compared to mean-field term and one gets the TF approximation [8]. In the same limit the eigen frequencies are

FIG. 5: (color online) Plot of different breathing mode frequencies as a function of \( \log N \).

effective potential \( \omega_0(r) \). Ground state in this well gives the ground state energy \( E_{00} \) of the condensate corresponding to \( a_0 = 100 \) Bohr are plotted for (a) \( N = 10000 \) and (b) \( N = 100000 \). For comparison corresponding GP results are also plotted. To highlight the effect of shape dependence of the interacting potential we present the enlarged view of the peak portions of the curves in panel (c) (for \( N = 10000 \)) and (d) (for \( N = 100000 \)) and the corresponding tail portions in the panel (e) and panel (f) respectively.

V. COLLECTIVE EXCITATIONS AT LOW AND HIGH ENERGIES

It is already pointed out that low-energy collective ex-

cations provide valuable information about the interaction, while the high-lying excitations are of single particle nature and are useful for the study of statistical properties. In the present work we study both low- and high-lying collective excitations, including the transition from collective to single particle nature as excitation energy increases, for quite large number of bosons. We are spe-
cially interested in examining collective features of the high-lying excitations as envisaged in the hydrodynamic mod-

In our present picture, the collective motion of the condensate in the hyperradial space takes place in the
calculated using the hydrodynamic equation of superfluidity (Eq. (18)). So the comparison of the many-body results to the HD prediction is well justified. Note that the HD equation (Eq. (18)) depends only on \( n \) and \( \ell \) and not explicitly on \( N \), thus the effect of finite size correction does not appear here and the many-body results should coincide with HD results in the true thermodynamic limit whereas small deviation may exist for finite size system. In Fig. 5, all the breathing mode frequencies saturate at large \( N \) limit. The asymptotic values for several breathing modes are presented in Table III and compared with the HD results. It is seen that the HD prediction is very accurate for the description of the lowest excitation of large systems. However we observe gradually increasing deviations as we go to higher modes. This is expected because the HD model is based on the assumption of collisionless hydrodynamics of a superfluid at zero temperature which is valid only for the low-lying states and for higher-lying states, the single particle nature gradually dominates over the collective behavior [8]. The slow but smooth increase in \( \omega_{Mn} \) with increase in \( N \) is visible in all four panels of Fig. 5, which basically manifests the finite size effect.

To better understand the transition from collective to single particle picture we thoroughly investigate the evolution of excitation energies of both the surface mode \((n = 0)\) and higher mode \((n = 1)\) as a function of angular momentum \( \ell \). In general for high excitation energies \((\ell > \ell_M)\) the results should follow the predictions of the non-interacting harmonic oscillator (HO) model \( \omega(n, \ell) = \omega_{ho}(2n + \ell) \). Thus for the surface modes \((n = 0)\), the HO model results to \( \omega = \ell \omega_{ho} \) or \( \frac{\omega}{\ell} = \omega_{ho} \). The surface excitations \((n = 0)\) are specially important as the effects of interaction are particularly important for such modes. The quantity \( \frac{\omega}{\ell} \) is also a very important quantity, as according to Landau’s criterion for superfluidity, it provides the rotational frequency at which the \( \ell \)-th surface excitation becomes unstable. In Fig. 6 we plot our many-body results for \( n = 0 \) and \( n = 1 \). Both for \( n = 0 \) and \( n = 1 \), we observe that our many-body results nicely saturates close to 1 as predicted by the HO model, whereas the HD predictions asymptotically goes to zero for large \( \ell \). For \( n = 1 \), we observe that initially for smaller values of \( \ell \), the many-body results tend to follow the HD predictions, however deviation starts soon.

Unlike the Bogoliubov results reported in Ref. [9], we fail to get any local minima of \( \frac{\omega}{\ell} \) in our many-body results.

![Plot of surface mode and higher excitation frequencies](image.png)

So the study of critical rotational frequency and the instability of surface excitation is beyond the capacity of our present calculation.

### VI. SUMMARY AND CONCLUSION

We have calculated the low and high lying excitation frequencies for very large number of trapped bosons which is close to the real experimental situation. We utilize the two-body correlated basis function and use van der Waals interaction as an interatomic interaction. Thus our many-body method prescribed in the present manuscript can reveal the realistic features of the trapped bosons. The most convenient and widely used tool in this direction is the mean-field GP equation which basically ignores interatomic correlation and uses the simple contact interaction. In that respect our many-body approach is few steps ahead of the mean-field results as by keeping all possible two-body correlations one can expect to get beyond-mean-field effects. On the other hand the diffusion Monte-Carlo (DMC) is the exact many-body technique. However due to computational difficulty it can handle only up to few hundreds of bosons in the trap which is far from the real experimental situation, whereas our many-body method keeps only two-body correlations and can handle as large as \( 10^7 - 10^8 \) atoms in the trap. The effect of only two-body correlation is relevant as the higher-body correlations are almost negligible for dilute BEC.

In the first part of our calculation we apply the many-body approach for the calculation of ground state energy. Calculation of correlation energy with respect to GP and TF results nicely demonstrate that the BEC looses its many-body effects and becomes more classical at truly large particle limit. This can be understood from the fact that for large effective repulsion (large
with \( a_s > 0 \), particles are far apart from each other and the effect of interaction becomes small. The TF approximation can well describe the situation. Our present calculation also deals with the wide range of particles and present an exhaustive study of the validity of shape independent approximation. However our another fundamental motivation of the present work is to study the collective and single particle excitations. We calculate several excited modes of breathing mode frequencies and compare with the HD model. We observe that the asymptotic value \((N \rightarrow \infty)\) of the lowest breathing mode (monopole frequency) exactly matches with the HD prediction. Whereas the higher breathing modes \((\omega_{\mu n}, n = 2, 3, 4)\) have the same qualitative nature as \(\omega_{M_1}\), the asymptotic values are bit higher than that of HD prediction. For smaller \(N\), the finite size effects exist and the breathing modes show slow and smooth increase until it approaches the asymptotic value \((N \rightarrow \infty)\). We conclude that the low-lying collective excitations are well described by the HD model at \(N \rightarrow \infty\) limit. We also calculate \(\ell \neq 0\) surface modes with \(\ell \rightarrow \infty\) for \(N \sim 10^7\). Our many-body results nicely reproduce the asymptotic value of non-interacting limit. The HD prediction completely fails which predicts the asymptotic value goes to zero. This is expected, since for strong effective repulsion (large \(\frac{N a_s}{ho}\)) the bosons tend to be non-interacting giving rise to single particle nature. Thus our prescribed many-body approach is a nice tool for the description of large number of interacting bosons, and can easily mimic the real experimental situation going from collective to single particle nature. Our present calculation is an exhaustive study of both the static and dynamic behavior of trapped bosons.

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[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science 269, 198 (1995).
[2] C. C. Bradley et al., Phys. Rev. Lett. 75, 1687 (1995).
[3] K. K. Davis et al., Phys. Rev. Lett. 75, 3969 (1995).
[4] D. S. Jin, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 77, 420 (1996).
[5] S. Stringari, Phys. Rev. Lett. 77, 2360 (1996).
[6] F. Dalfovo, S. Stringari, Phys. Rev. A 53, 2477 (1996).
[7] H. Hu, G. Xianlong, and X. J. Liu, Phys Rev A 90, 013622 (2014).
[8] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 71, 463 (1999)
[9] F. Dalfovo, S. Giorgini, M. Guilleumau, L. Pitaevskii, and S. Stringari, Phys. Rev. A 56, 3840 (1997).
[10] V. V. Goldman, I. F. Silvera, and A. Leggett, Phys. Rev. B 24, 2870 (1981).
[11] B. Chakrabarti and T. K. Das, Phys. Rev. A 78, 063608 (2008).
[12] B. D. Esry, Phys. Rev. A 55, 1147 (1997).
[13] T. Haugset and H. Haugerud, Phys. Rev. A 57, 3809 (1998).
[14] B. D. Esry and C. H. Greene, Phys. Rev. A 60, 1451 (1999).
[15] D. Blume and C. H. Greene, Phys. Rev. A 63, 063601 (2001).
[16] M. Fabre de la Ripelle, Ann. Phys. (N.Y.) 147, 281 (1983).
[17] B. Chakrabarti, and T. K. Das, Phys. Rev. A 81, 015601 (2010).; A. Biswas, T. K. Das, L. Salasnich, and B. Chakrabarti, Phys. Rev. A 82, 043607 (2010); S. Goswami, T. K. Das, and A. Biswas, Phys. Rev. A 84, 053617 (2011); S. Bhattacharyya, T. K. Das, and B. Chakrabarti, Phys. Rev. A 88, 053614 (2013); S. K. Halder, B. Chakrabarti, T. K. Das, and A. Biswas, Phys. Rev. A 88, 033602 (2013).
[18] T. K. Das, and B. Chakrabarti, Phys. Rev. A 70, 063601 (2004)
[19] T. K. Das, S. Canuto, A. Kundu, and B. Chakrabarti, Phys. Rev. A 75, 042705 (2007)
[20] T. K. Das, A. Kundu, S. Canuto, and B. Chakrabarti, Phys. Lett. A 373, 258-261 (2009).
[21] J. L. Ballot, and M. Fabre de la Ripelle, Ann. Phys. (N.Y.) 127, 62 (1980).
[22] T. K. Das, H. T. Coelho, and M. Fabre de la Ripelle, Phys. Rev. C 26, 2281 (1982).
[23] M. Abramowitz, and I. A. Stegun, Handbook of mathematical functions, National Institute of Standards and Technology, USA, (1964)
[24] T. K. Das, S. Canuto, A. Kundu and B. Chakrabarti, Phys. Rev. A 75, 042705 (2007).
[25] S. A. Sofianos, T. K. Das, B. Chakrabarti, M. L. Lekala, R. M. Adam, and G. J. Rampho, Phys. Rev. A 87, 013608 (2013).
[26] C. J. Pethick and H. Smith, Bose-Einstein condensation in dilute gases (Cambridge University Press, Cambridge, England, 2001).
[27] M. L. Lekala, B. Chakrabarti, G. J. Rampho, T. K. Das, S. A. Sofianos, and R. M. Adam, Phys. Rev. A 89, 023624 (2014).
[28] A. Biswas, B. Chakrabarti and T. K. Das, J. Chem Phys. 133, 104502 (2010).