

Application of potential harmonic expansion method to BEC: Thermodynamic properties of trapped ^{23}Na atoms

ANASUYA KUNDU¹, BARNALI CHAKRABARTI² and TAPAN KUMAR DAS¹

¹Department of Physics, University of Calcutta, 92 A.P.C. Road, Kolkata 700 009, India

²Department of Physics, K.N. College, Berhampore 742 101, India

E-mail: anasuya09@yahoo.co.uk; chakrabarti@rediffmail.com;

tkdas6@hotmail.com, tkdphy@caluniv.ac.in

MS received 3 June 2004; revised 15 September 2004; accepted 4 February 2005

Abstract. We adopt the potential harmonics expansion method for an *ab initio* solution of the many-body system in a Bose condensate containing interacting bosons. Unlike commonly adopted mean-field theories, our method is capable of handling two-body correlation properly. We disregard three- and higher-body correlations. This simplification is ideally suited to dilute Bose Einstein condensates, whose number density is required to be so small that the interparticle separation is much larger than the range of two-body interaction to avoid three- and higher-body collisions, leading to the formation of molecules and consequent instability of the condensate. In our method we can incorporate realistic finite range interactions. We calculate energies of low-lying states of a condensate containing ^{23}Na atoms and some thermodynamical properties of the condensate.

Keywords. Bose Einstein condensation; potential harmonics; two-body correlations in BEC.

PACS Nos 31.15.Ar; 31.15.Ja; 03.75.Fi

1. Introduction

Bose Einstein condensation (BEC) [1,2] in an ideal gas can be studied by quantum-statistical mechanics which offers a profound insight into this macroscopic quantum phenomena. Although BEC was first experimentally realized in 1995 on alkali atoms [3–5], experimental and theoretical research in this field started much earlier. At present, BEC is one of the most important topics in the frontline physics research, all over the world.

The phenomenon of BEC is based on the indistinguishability and wave nature of a collection of bosons (electrically neutral alkali atoms) [1]. Atoms in a gas may be regarded as quantum-mechanical wavepackets smeared over a distance λ_T (thermal de Broglie wavelength) $= \sqrt{2\pi\hbar^2/mk_B T}$, where T is the temperature, m is the

mass of the atom and k_B is the Boltzmann constant. The phenomenon of BEC sets in when the temperature is so low that λ_T is comparable to $n^{-1/3}$ (n is the number density of the magneto-optically trapped atoms), such that the de Broglie waves of the adjacent atoms overlap. As a result the entire system can be described by a single macroscopic wave function. At very low temperatures all the atoms occupy the lowest state in the trap, as they do not have enough energy to go to higher energy states. The transition from ordinary gaseous phase to BEC corresponds to a transition from a set of disordered atoms to coherent matter waves. For alkali atoms, the typical densities are 10^{13} cm^{-3} [5]. It is kept so low to avoid molecule formation (and consequent depletion of the condensate) through three- and higher-body collisions. The corresponding critical temperature below which BEC occurs is of the order of a few nK. This is achieved experimentally by laser cooling followed by evaporative cooling [1].

The theoretical study of BEC develops its full richness only after realistic interatomic interactions are included. Although the density of atoms is extremely low, two-body collisions and two-body correlations play important roles in the detailed properties of the condensate [1]. By treating the two-body interaction as a contact interaction, the many-body mean-field theory reduces to the non-linear Gross-Pitaevskii (GP) equation [1]. The numerical solution of GP equation is fairly easy and a lot of work has already been done [1,2] to study the static, dynamic and thermodynamic properties of the condensate. However, the corresponding wave function does not include any correlations produced by the interaction when two atoms are close to each other. In a mean-field approach the many-body wave function is taken as a product of single particle wave functions, which are obtained variationally. Clearly then the many-body wave function does not have any dependence on the relative separations of two or more particles. Thus the wave function lacks two- and higher-body correlations. Since the GP equation is based on mean field theories, it also lacks any correlation between particles. Only gross and average properties can be described by the mean-field approximation. Moreover, due to the non-linear nature of the GP equation standard quantum mechanics is not applicable without concession. So for a realistic study to get the finer details of the condensate, one has to go beyond the mean-field approximation and simple contact interactions. Thus it is desirable to solve the many-body linear Schrödinger equation directly. The Schrödinger equation for a system of $A = (N + 1)$ identical bosons interacting via two-body potential V has the form

$$\left[-\frac{\hbar^2}{2m} \sum_{i=1}^A \nabla_i^2 + \sum_{i=1}^A V_{\text{ext}}(\vec{x}_i) + \sum_{i < j=2}^A V(\vec{x}_i - \vec{x}_j) \right] \psi(\vec{x}) = E\psi(\vec{x}), \quad (1)$$

where m is the mass of each particle and $V_{\text{ext}} = \frac{1}{2}m\omega^2 x_i^2$ is the harmonic trapping field, ω being the frequency of the trap. The symbol \vec{x} is a short-hand notation for the set of position coordinates of A bosons. By eliminating the center of mass motion, the above equation can be transformed into a Schrödinger equation in $3N$ relative variables. The hyperspherical harmonics expansion (HHE) method [6] can be applied for the *ab initio* solution of the A -body Schrödinger equation. Introducing the Jacobi coordinates, the center of mass motion is automatically separated and the relative motion of an $(N + 1)$ -particle system is described in terms of N

Jacobi vectors. Hyperspherical variables are then defined in terms of the Jacobi vectors and the wave function is expanded in the complete set of hyperspherical harmonics (HH), which are the eigenfunctions of the grand orbital operator, spanning the hyperangular space. The relative Schrödinger equation then reduces to a system of coupled differential equations. But with the increase in particle number, the most difficult computational aspect of this method is the calculation of coupling matrix elements (involving $(3N - 1)$ -dimensional integrals) and the solution of a large number of coupled differential equations. Moreover, due to large degeneracy of HH basis and slow convergence rate of this expansion, the wave function is not represented sufficiently accurately with a small number of harmonics. Several attempts have been made using the standard HHE method, but this was restricted to a system of three particles only [7]. On the other hand, in K-harmonic approximation [8], the HHE is restricted effectively to the first term only. The lowest harmonic is simply a constant. Although the average properties of the condensate is reproduced by a single collective coordinate (viz., the hyper-radius), restriction to lowest harmonics only basically excludes any correlation. Since there is no angle dependence, this approximation is not adoptable for a realistic interaction and can be applied for a hypercentral interaction only. Furthermore, with one collective variable (hyper-radius), only the gross features of the condensate can be described, leaving the finer details. Hyperspherical variables and adiabatic separation of hyperangular motion were used by Sørensen *et al* [9–11] to include the two-body correlation. But instead of treating the full N -body Schrödinger equation exactly, they separate the full Hamiltonian into hyper-radial and hyperangular parts (eq. (6) of ref. [9]) and solve the latter adiabatically. That is, they basically start with an adiabatic subset (where hyper-radial motion becomes decoupled from the hyperangular motion) instead of the full hyperspherical harmonics (HH) basis and study the hyperangular eigenvalue and wave function. The approximations made by Sørensen *et al* [9–11] are highly restricted to very short range interaction.

So from the above discussion it is clear, that an *ab initio* solution of the A -body Schrödinger equation for $A > 3$ is extremely difficult. However we utilize some of the special features of BEC to adopt an approximation to the HHE method, which is particularly suited to study BEC and at the same time remains quite manageable for a fairly large number of particles. Instead of the HH basis, we use a new basis, called ‘potential harmonics’ (PH) basis [12], which is a subset of the HH basis. In PH basis, we assume that the contributions to the orbital and grand orbital (in $3N$ -dimensional space of the relative motion) quantum numbers come only from the interacting pair. Hence the relative separation vector ($\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$) of the interacting pair (ij) appears as an argument of the many-body wave function. Thus two-body correlations are included. Since *any pair* of particles can interact, the total wave function can be decomposed in Faddeev-like components (ψ_{ij}). Each component depends on the corresponding relative vector. However the wave function will have no dependence on the relative separation of three or more particles. This implies inclusion of two-body correlations only. Such an assumption is ideally suited specially for the BEC, which is required to be extremely dilute for its experimental realization (so that three- and higher-body collisions leading to the possibility of molecule formation is excluded). Hence three and higher body collisions are absent and only two-body correlations are important. Out of many

degrees of freedom of the individual particles in BEC, only a few are physically relevant since the condensate can be treated as a single lump of quantum stuff. In PH, the contribution to the total orbital angular momentum as also the grand orbital quantum number comes only from the interacting pair. Any pair out of $A = (N + 1)$ atoms in the condensate can interact, while the rest of the particles in the condensate do not partake in any motion other than a collective one and are simply inert spectators. In HH, the hyperangles form a set of $(3N - 1)$ angular variables, which are constituted by $2N$ polar angles of the N Jacobi vectors and $(N - 1)$ angles defined in terms of the relative lengths of the Jacobi vectors. But in PH, there are only three active variables (length and polar angles of the relative separation vector of the interacting pair), corresponding to three quantum numbers – the orbital l , azimuthal m , and the grand orbital $(2K + l)$ quantum numbers for any arbitrary N . The number of coupled differential equations is then drastically reduced and calculation of potential matrix becomes tremendously simplified, as it needs integrals over only three variables. One can easily incorporate realistic atom–atom interactions in a straightforward manner. In our method the wave function is also properly symmetrized by using Faddeev-type decomposition and requiring each Faddeev component to be symmetric under the exchange of interacting pair.

Our roadmap in this communication is the following: In §2 we describe the theoretical framework of PH. Section 3 deals with the numerical results including the effects of finite range interactions on different thermodynamic properties of BEC formed by ^{23}Na atoms, both at $T = 0$ limit and at finite temperatures. Section 4 contains a summary and conclusions.

2. Theoretical framework

A system of $A = (N + 1)$ mutually interacting identical bosons, each of mass m , trapped in an external field approximated by a spherically symmetric harmonic oscillator potential of angular frequency ω is described by eq. (1). We decompose the wave function as the sum of pair-wise Faddeev-like components [12]

$$\psi(\vec{x}) = \sum_{ij>i}^{N+1} \psi_{ij}(\vec{x}). \quad (2)$$

If we now require $\psi_{ij}(\vec{x})$ to be dependent explicitly on \vec{r}_{ij} , all two-body correlation in $\psi(\vec{x})$ are included. The Schrödinger equation for ψ_{ij} becomes

$$(T_k + V_{\text{trap}} - E)\psi_{ij}(\vec{x}) = -V(\vec{r}_{ij}) \sum_{k,l>k} \psi_{kl}(\vec{x}), \quad (3)$$

where T_k is the total kinetic energy operator, V_{trap} is the trapping potential $\sum_{i=1}^A \frac{1}{2}m\omega^2 x_i^2$, and $V(\vec{r}_{ij})$ is the two-body potential between (ij) pair. Applying $\sum_{ij>i}$ on both sides of (3), one gets eq. (1). We introduce the center of mass coordinate \vec{R}

$$\vec{R} = \frac{1}{N+1} \sum_{i=1}^{N+1} \vec{x}_i \quad (4)$$

and N Jacobi coordinates

$$\vec{\zeta}_i = \sqrt{\frac{2i}{i+1}} \left(\vec{x}_{i+1} - \frac{1}{i} \sum_{j=1}^i \vec{x}_j \right) \quad (i = 1, \dots, N). \quad (5)$$

The normalization of $\vec{\zeta}_i$ is chosen in such a way that the Laplace operator becomes

$$\frac{1}{2} \sum_{i=1}^{N+1} \nabla_i^2 = \frac{1}{2A} \nabla_R^2 + \sum_{i=1}^N \nabla_{\zeta_i}^2. \quad (6)$$

After the removal of the center of mass motion from eq. (1), the relative motion of the system is governed by

$$\left[-\frac{\hbar^2}{m} \sum_{i=1}^N \nabla_{\zeta_i}^2 + \sum_{i=1}^N \frac{1}{2} m \omega^2 \zeta_i^2 + V_{\text{int}}(\vec{\zeta}_1, \dots, \vec{\zeta}_N) - E \right] \psi(\vec{\zeta}_1, \dots, \vec{\zeta}_N) = 0, \quad (7)$$

where $V_{\text{int}} = \sum_{ij>i}^{N+1} V(r_{ij})$, expressed in terms of the Jacobi coordinates.

The hyper-radius r , symmetric under any permutation of the particle labels, is defined as

$$r = \left[\sum_{i=1}^N \zeta_i^2 \right]^{1/2} = \left[\frac{2}{N+1} \sum_{i,j>i} r_{ij}^2 \right]^{1/2}. \quad (8)$$

The hyperspherical coordinates are constituted by the hyper-radius r and a set Ω_N of $(3N-1)$ angular coordinates. We choose the labelling of particles such that \vec{r}_{ij} is $\vec{\zeta}_N$. Then the angular coordinates ϕ , θ and φ are such that (θ, φ) are two spherical polar angles (ω_{ij}) of \vec{r}_{ij} and ϕ is defined by $r_{ij} = r \cos \phi$. The set Ω_{N-1} of the remaining angular coordinates is associated with coordinates $\vec{\zeta}_1, \dots, \vec{\zeta}_{N-1}$ and we define the hyper-radius in $3(N-1)$ -dimensional space by

$$\rho_{ij} = \left[\sum_{i=1}^{N-1} \zeta_i^2 \right]^{1/2} \quad (9)$$

which is related to r_{ij} by

$$\rho_{ij}^2 + r_{ij}^2 = r^2 \quad (10)$$

i.e. $\rho_{ij} = r \sin \phi$. Our hyperspherical coordinates become

$$(r, \Omega_N) \equiv (r, \phi, \theta, \varphi, \Omega_{N-1}); \quad \omega_{ij} \equiv (\theta, \varphi). \quad (11)$$

The Laplace operator is

$$\nabla^2 \equiv \sum_{i=1}^N \nabla_{\vec{\zeta}_i}^2 = \frac{\partial^2}{\partial r^2} + \frac{3A-4}{r} \frac{\partial}{\partial r} + \frac{L^2(\Omega_N)}{r^2}, \quad A = N+1, \quad (12)$$

where $L^2(\Omega_N)$ is the grand orbital operator in $D = 3N$ -dimensional space. The eigenfunctions of $L^2(\Omega_N)$ subject to the conditions stated below are the so-called ‘potential harmonics’ (PH) [12]. The eigenvalue equation satisfied by $L^2(\Omega_N)$ corresponding to the PH subset of eigenfunctions is

$$[L^2(\Omega_N) + \mathcal{L}(\mathcal{L} + D - 2)] \mathcal{P}_{2K+l}^{l,m}(\Omega_{ij}) = 0, \quad \mathcal{L} = 2K + l. \quad (13)$$

The potential harmonics ($\mathcal{P}_{2K+l}^{l,m}(\Omega_{ij})$) for the (ij) pair, where $\vec{r}_{ij} = \vec{\zeta}_N$ are subjected to the condition that they are invariant under rotations in the $(D - 3)$ -dimensional space spanned by $\vec{\zeta}_1, \dots, \vec{\zeta}_{N-1}$ (i.e., all Jacobi vectors, excepting $\vec{\zeta}_N$, the one proportional to the interacting pair (ij)). Consequently the contribution to the grand orbital quantum number comes only from the interacting pair. Then the PH corresponding to the pair (ij) is given by

$$\mathcal{P}_{2K+l}^{l,m}(\Omega_{ij}) = Y_l^m(\omega_{ij}) \ ^{(N)}P_{2K+l}^{l,0}(\phi) \mathcal{Y}_0(D-3), \quad (14)$$

where $\ ^{(N)}P_{2K+l}^{l,0}(\phi)$ is a function related to the Jacobi polynomial [13] and $\mathcal{Y}_0(D-3)$ is the HH of order zero in $3(N-1)$ -dimensional space. This subset of the full HH basis is called the ‘potential harmonics basis’, because if we wish to expand the interacting pair potential $V(\vec{r}_{ij})$, which is a function of ϕ, θ and φ only (for a given r) in the HH basis, we just need the PH basis. Expanding $\psi_{ij}(\vec{r}_{ij}, r)$ in the PH basis appropriate for the pair (ij) , we have $L^2(\Omega_{N-1})\psi_{ij}(\vec{r}_{ij}, r) = 0$ for any N . As a result, in this new basis the relevant set of quantum numbers is reduced to only three – orbital l , azimuthal m and grand orbital $2K + l$ for any N , instead of $(3N - 1)$ quantum numbers corresponding to $(3N - 1)$ hyperspherical variables in the general HH basis. Thus the (ij) Faddeev component, $\psi_{ij}(\vec{r}_{ij}, r)$, will be a function of \vec{r}_{ij} and r only and satisfies eq. (3). We expand ψ_{ij} in the complete set of potential harmonics

$$\psi_{ij} = r^{-(D-1)/2} \sum_K \mathcal{P}_{2K+l}^{l,m}(\Omega_{ij}) u_K^l(r). \quad (15)$$

From eq. (14) we see that the PH $\mathcal{P}_{2K+l}^{l,m}(\Omega_{ij})$ is a function of ω_{ij} and ϕ . Hence it is a function of \vec{r}_{ij} and r . Thus $\psi(\vec{x})$ given by eq. (2) includes all two-body correlations. As this ψ does not depend on the relative separations of more than two particles, it does not have correlations higher than two-body ones. Substituting in (3) and taking projection on a particular PH, a set of coupled differential equations (CDE) [12] is obtained, which can be put in a symmetric form as

$$\left[-\frac{\hbar^2}{m} \frac{d^2}{dr^2} + V_{\text{trap}} + \frac{\hbar^2}{mr^2} \{ \mathcal{L}(\mathcal{L} + 1) + 4K(K + \alpha + \beta + 1) \} - E \right] U_{Kl}(r) + \sum_{K'} \bar{V}_{KK'}(r) U_{K'l}(r) = 0, \quad (16)$$

where $\mathcal{L} = l + \frac{3A-6}{2}$, $\alpha = \frac{3A-8}{2}$, $\beta = l + \frac{1}{2}$ and symmetrized potential matrix $\bar{V}_{KK'}$ is given by

$$\bar{V}_{KK'}(r) = f_{Kl}V_{KK'}(r)f_{K'l}(h_K^{\alpha\beta}h_{K'}^{\alpha\beta})^{-1/2}, \quad (17)$$

while $U_{Kl}(r)$ is given by

$$U_{Kl}(r) = f_{Kl}(h_K^{\alpha\beta})^{1/2}u_K^l(r). \quad (18)$$

Here f_{Kl} is given in ref. [12], $h_K^{\alpha\beta}$ is the norm of the Jacobi polynomial [13] and

$$V_{KK'}(r) = \int_{-1}^{+1} P_K^{\alpha\beta}(z)V\left(r\sqrt{\frac{1+z}{2}}\right)P_{K'}^{\alpha\beta}(z)w_l(z)dz, \quad (19)$$

where $w_l(z) = (1-z)^\alpha(1+z)^\beta$ is the weight function of the Jacobi polynomials [13].

3. Numerical method and results

For our calculations we fix $l = 0$ and truncate the PH basis to a maximum value of K ($=K_{\max}$), requiring proper convergence. The set of CDEs (eq. (16)) is solved by hyperspherical adiabatic approximation (HAA) [14]. We assume that the hyper-radial motion is slow compared to the hyperangular motion and solve the latter adiabatically for a fixed value of r . This is done by diagonalizing the potential matrix together with the hypercentrifugal and trapping terms of eq. (16) for a fixed value of r and choosing the lowest eigenvalue, $\omega_0(r)$, as the ‘effective potential’ for the hyper-radial motion [14]. Thus the adiabatically separated hyper-radial equation becomes

$$\left[-\frac{\hbar^2}{m} \frac{d^2}{dr^2} + \omega_0(r) + \sum_{K=0}^{K_{\max}} \left| \frac{d\chi_{K0}(r)}{dr} \right|^2 - E \right] \zeta_0(r) = 0, \quad (20)$$

subject to appropriate boundary conditions. The hyper-radius r behaves as the most important collective coordinate describing the collective motion of the condensate. The third term on the left-hand side of eq. (20) is the overbinding correction term where $\chi_{K0}(r)$ is the K th component of the eigenvector corresponding to the eigenvalue $\omega_0(r)$. Equation (20) is called the uncoupled adiabatic approximation (UAA) while dropping the overbinding correction term one has the extreme adiabatic approximation (EAA).

The choice of a delta-function interaction in the GP equation is an approximation, which is usually justified by stating that the average interparticle spacing is much larger than a_{sc} , the s -wave scattering length. But it diverges at $r_{ij} = 0$, and so this interaction is pathological in a two- or three-dimensional condensate and cannot be a realistic one. The Hamiltonian becomes unbound from below for an attractive delta interaction and the total energy diverges, leading to the breakdown of a rigorous quantum mechanical solution. This is usually described as the ‘collapse of the condensate’. For A less than a critical number (A_c), there is a metastable

region in $\omega_0(r)$ corresponding to a local minimum. For $A > A_c$, the local minimum disappears as there is no solution [8]. However even for $A < A_c$ (for which a solution restricted to the metastable region is called a ‘metastable condensate’), there are no rigorous quantum mechanically acceptable solution if the singular point ($r_{ij} = 0$) is included in the domain of hyper-radial variable. Again the use of realistic potentials in self-consistent mean-field calculation [7] gives wrong results as the wave function does not include correlations. To include the correlations one has to go beyond mean-field theories and the choice of realistic potential is crucial. We need a more physically meaningful realistic interaction which should not be pathological as $r_{ij} \rightarrow 0$. Then hypercentrifugal repulsion (which is non-vanishing even for $l = 0$) will prevent the particles to come too close to each other. We choose a Gaussian potential of strength V_0 and range r_0 of the form

$$V(r_{ij}) = V_0 e^{-r_{ij}^2/r_0^2}. \quad (21)$$

Depending on the sign of V_0 , we have either attractive or repulsive potential. The strength of the interaction is measured by

$$a_B = \frac{m}{2\pi\hbar^2} \int d^3r V(\vec{r}) \quad (22)$$

which is the Born approximation of the scattering length a_{sc} . This is approximately equal to the s -wave scattering length (a_{sc}), $a_B \simeq a_{sc}$ when $V_0 r_0^2 \ll \hbar^2/m$ is satisfied. For purely repulsive potential ($V_0 > 0$), a_{sc} is positive, but for $V_0 < 0$, a_{sc} initially becomes negative, then decreases and goes through infinite discontinuities from $-\infty$ to $+\infty$ at particular values of V_0 . In the case of ^{23}Na atoms V_0 is positive, i.e. two-body potential is repulsive since the experimental a_{sc} is positive.

For ^{23}Na atoms, we take the experimental value of scattering length $a_{sc} = 4.9$ nm of the MIT experiment [15]. We take $\nu = 150$ Hz, which is the trapping frequency used to achieve BEC of ^{23}Na atoms [16]. Throughout our calculation we use oscillator units (o.u.) in which energies and lengths are expressed in terms of the oscillator energy ($\hbar\omega$) and oscillator length ($\sqrt{\hbar/m\omega}$) respectively. The value of r_0 is chosen to be 0.05 o.u. which is less than the characteristic length of the condensate. We have verified by actual calculation that the results are stable against a variation of r_0 , when corresponding V_0 is obtained from eqs (21) and (22). For $a_{sc} = 4.9$ nm and $r_0 = 0.05$ o.u., the value of V_0 turns out to be 25.8331 o.u.

The repulsive interaction will push the condensate against the walls of the trap and the condensate energies will be higher than the non-interacting case. In earlier calculations [17,18] it has been observed that the condensate energy converges very rapidly as K_{\max} increases for smaller number of particles. With increase of K_{\max} , the condensate energy decreases. This is consistent with the Rayleigh–Ritz principle. It was found that $K_{\max} = 4$ is sufficient for our purpose, which is adopted in the present work also.

As in our previous work, we face numerical difficulty for $A > 35$. With increase in particle number, the Jacobi polynomial $P_n^{\alpha,\beta}(z)$ and its weight function $w_l(z)$ vary extremely rapidly in the interval $[-1,1]$ as α ($\alpha = \frac{3A-8}{2}$) increases rapidly with A . So the numerical integration of the potential matrix becomes very difficult. Hence instead of carrying out the numerical integration from $z = -1$ to $z = 1$

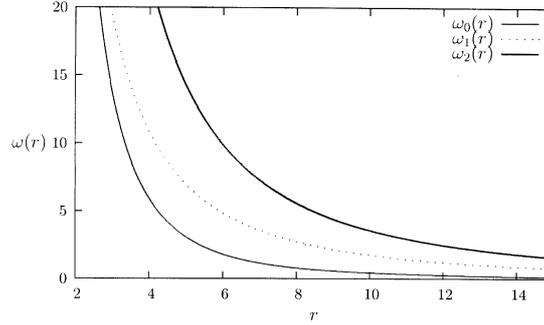


Figure 1. Three lowest hyperangular eigenpotentials, in oscillator units (o.u.) of energy, corresponding to the interaction energy as a function of r (in o.u.) for 30 bosons (^{23}Na atoms with $a_{\text{sc}} = 4.9$ nm) in a harmonic trap of frequency $\nu = 150$ Hz.

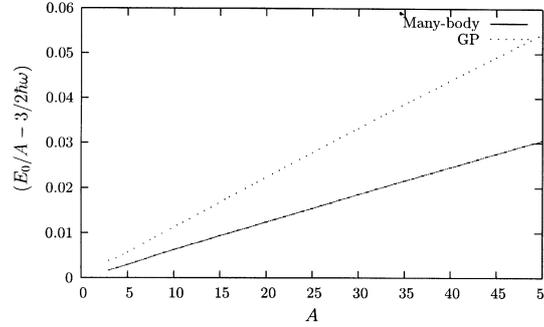


Figure 2. Condensate ground state energy (in o.u.) for a condensate of ^{23}Na atoms with $a_{\text{sc}} = 4.9$ nm and $\nu = 150$ Hz, for different values of A .

of the interval $[-1,1]$ in a single step, we have searched for the nodes of Jacobi polynomial, $P_n^{\alpha\beta}(z)$, and integrated between consecutive zeroes of $P_n^{\alpha\beta}(z)$ using an appropriate numerical quadrature. We have achieved a much better result this time and could go up to $A = 50$.

In figure 1 we have presented the general features of three lowest hyperangular eigenpotentials as a function of hyper-radius r for 30 bosons. In eq. (16), the effective potential consists of three terms: the hypercentrifugal repulsion which is repulsive and diverges as $r \rightarrow 0$, the interaction term and also the harmonic trapping potential which diverges as r^2 at large r limit. Figure 1 shows only the interaction energy as a function of hyper-radius where the condensate has the energy 0.57447 o.u. It is clear from figure 1 that the upper two eigenpotentials lie much above the lowest eigenpotential and its effect on the condensate energy is almost negligible. Thus the choice of uncoupled adiabatic approximation keeping only the lowest eigenpotential is justified in our calculation. This is also reflected in the very fast convergence as K_{max} increases, in our method. In figure 2 we present the condensate ground state energy ($\frac{E_0}{A} - \frac{3}{2}\hbar\omega$) against the particle number (A). In the same figure we also present the GP results. This figure shows the deviation of

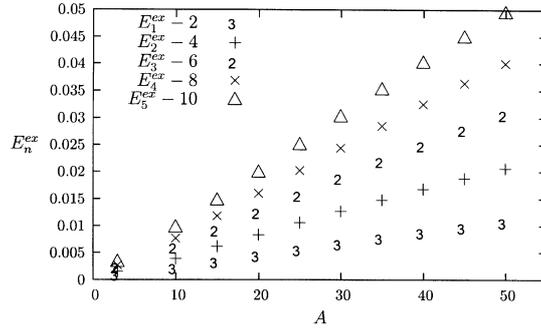


Figure 3. The low-lying excitation frequencies (in o.u.) for various A , for the same parameters as in figure 2.

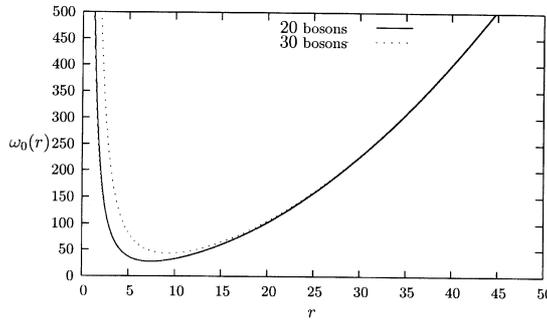
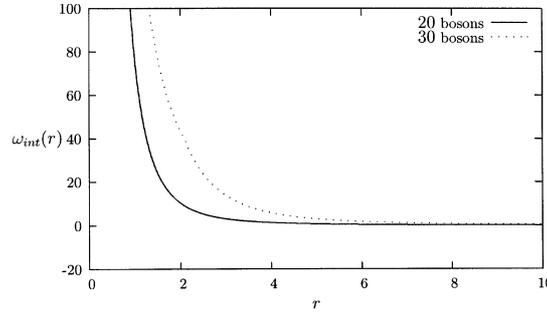


Figure 4. Total effective potentials $\omega_0(r)$ (in o.u.) as a function of r (in o.u.), for 20 and 30 bosons in the same trap as in figure 2.

the condensate from the non-interacting ideal gas, for which the plotted quantity would have been zero. We present the GP results just to see the effect of two-body correlation in our calculation. As GP does not include any correlation, direct comparison of correlation dependent quantities with the GP results is really not meaningful. GP uses zero range contact interaction as $V_\delta(\vec{r}) = \frac{4\pi\hbar^2 a_{sc}}{m} \delta(\vec{r})$, while our chosen potential is a finite range Gaussian $V(r) = V_0 e^{-r^2/r_0^2}$. It is easy to see that Gaussian interaction tends to $V_\delta(\vec{r})$ as $r_0 \rightarrow 0$. Mathematically $r_0 \rightarrow 0$ can be easily approached with appropriate change in V_0 to get the correct scattering length. But calculation of the potential matrix with very small r_0 is extremely CPU time consuming. Hence we keep $r_0 = 0.05$ o.u. as mentioned earlier. The low-lying excitation frequencies of the radial breathing modes up to 50 particles are presented in figure 3. Energies of ground and excited states increase gradually with particle number. The numerical values for four lowest lying states have been presented in table 1. This increase is also justified from figures 4 and 5. In figure 4 we show the total effective eigenpotential (including trapping potential and the two-body interactions) for 20 and 30 bosons in the same trap. Next we define the lowest eigenpotential corresponding only to the interaction energy, ($\omega_{\text{int}}(r)$), i.e. excluding trapping potential. In figure 5, we present a plot of $\omega_{\text{int}}(r)$ against r for the same number of bosons. We see that both $\omega_0(r)$ and $\omega_{\text{int}}(r)$ become more repulsive

Table 1. Energies of ground (E_g) and first three excited states for different particle numbers (A) of ^{23}Na atoms.

A	E_g	First	Second	Third
5	7.517997	9.519583	11.520950	13.522218
10	15.068533	17.070794	19.072914	21.074982
15	22.649272	24.652682	26.655866	28.658922
20	30.260663	32.265206	34.269473	36.273559
25	37.902478	39.908128	41.913473	43.918596
30	45.574470	47.581199	49.587602	51.593754
35	53.276361	55.284138	57.291573	59.298737
40	61.007825	63.016613	65.025050	67.033199
45	68.768448	70.778207	72.787606	74.796704
50	76.557665	78.568340	80.578649	82.589751


Figure 5. Comparison of lowest eigenpotentials (in o.u.) corresponding to interaction energy only ($\omega_{\text{int}}(r)$) as a function of r (in o.u.) for 20 and 30 bosons in the same trap as in figure 2.

as one goes from 20 to 30 bosons. Naturally the condensate energy will increase with particle number. The chemical potential (μ) in o.u. at $T = 0$ is plotted against the particle number in figure 6. We may recall the definition [18] of μ as the energy required to add the $(A + 1)$ th particle to a system containing A particles or as the energy required to separate one particle from the system, i.e. $\mu|_{T=0} = \left(\frac{\partial E}{\partial N}\right)_V$. So we calculate μ at $T = 0$ as the difference between the ground state energy of $(A + 1)$ particle system and that of A particle system. We present the GP results also in the same figure. To study $T \neq 0$ thermodynamic property we use canonical ensemble, since our calculation is for a finite (and not too large) number of particles. We have calculated the average energy starting from the canonical partition function $z(N, V, T) = \sum_i \exp(-\beta E_i)$ where $\beta = 1/k_B T$ and E_i is the energy of the i th state of the condensate. The average energy is given by $\bar{E} = \sum_i E_i \frac{\exp(-\beta E_i)}{z}$. In figure 7 we have plotted the energy per particle for 50 ^{23}Na atoms in the condensate against temperature, where the upper cut-off energy (in the calculation of the partition function) $E_{\text{cut off}} = 93.082256$ o.u. We have checked the convergence of the partition function in this limit. The average energy is higher than the non-interacting classical limit. Another thermodynamic property of the system, viz., specific heat

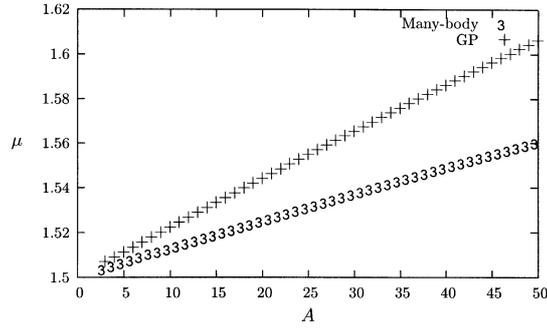


Figure 6. Chemical potential (μ) in o.u. at $T = 0$ for various numbers (A) of interacting bosons in the same trap as in figure 2.

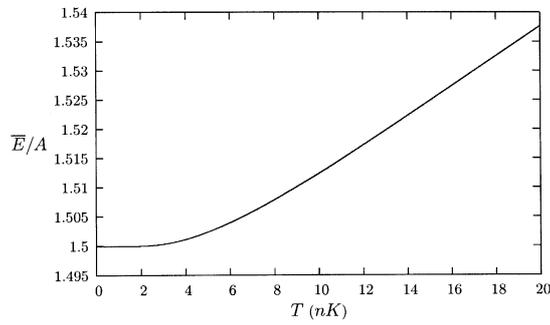


Figure 7. Average energy per atom (in o.u.) as a function of T for 50 interacting bosons in the same trap as in figure 2.

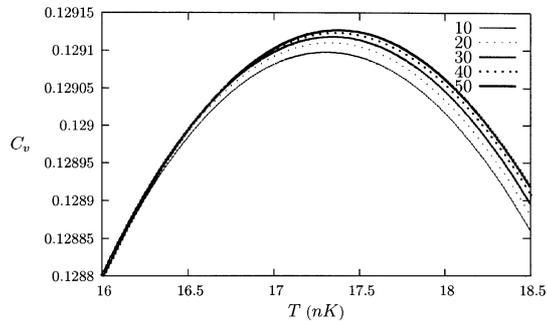


Figure 8. Specific heat (in o.u.) as a function of temperature for different number of interacting bosons in the same trap as in figure 2.

(C_v) is calculated for $T > 0$ by differentiating \bar{E} with respect to T . Figure 8 shows the specific heat against temperature (in degree nK) for $A = 10, 20, 30, 40$ and 50 particles, where $E_{\text{cut off}} = 31.573102, 46.770149, 62.089381, 77.528071, 93.082256$ o.u. respectively. To bring out the detailed feature of C_v as a function of T we have used a fine mesh for temperature near the point where the maximum of C_v occurs.

The C_v vs. T curve usually shows a sharp change at the critical temperature (T_c) for large values of A . In fact for $A \rightarrow \infty$, there is a discontinuous change [19]. Our curves for C_v are smooth (i.e. showing no discontinuity) as we have restricted ourselves to smaller values of A . With such small number of particles no phase transition occurs. So we cannot define the critical temperature in such small A limit. However we define [18] the condensation temperature to be the temperature at which C_v attains a maximum. In our calculation, the condensation temperatures are $T = 17.307, 17.327, 17.344, 17.364$ and 17.380 degree nK for $A = 10, 20, 30, 40$ and 50 particles respectively. The increase in the condensation temperature with increase in number of bosons is also intuitively correct.

4. Summary and conclusion

In this communication we have studied a finite number (3–50) of mutually interacting bosons (neutral ^{23}Na atoms) confined in a harmonic trapping field. We have solved the many-body Schrödinger equation by using potential harmonic basis (a subset of HH basis), where two-body correlations are properly taken into account and higher order correlations are ignored. This is justified because BEC is possible only at extremely low densities where three- and higher-body collisions are absent (so that there is no recombination and molecule formation, which depletes the condensate). Thus while a single pair interacts, most of the degrees of freedom of the remaining spectators can be frozen, resulting in only three active variables, corresponding to three quantum numbers for the potential harmonics. We have presented the ground and excited state properties of the condensate for the repulsive interaction represented by positive scattering length of ^{23}Na atoms. Several thermodynamic properties have been investigated in the $T = 0$ limit and also at finite temperatures. At present, we are trying to develop a method (using recurrence relations of Jacobi polynomials and other numerical tricks) to handle larger number of interacting bosons. We conclude that the use of potential harmonics expansion method is an appropriate and promising theoretical approach to investigate Bose Einstein condensation from first principles. This approach can handle finite range realistic two-body interactions and treats the all important two-body correlations properly. At present there are numerical difficulties when the particle number exceeds fifty. We are trying to overcome this difficulty.

Acknowledgements

Financial assistance from the Department of Science and Technology (DST), Government of India supporting the research project (SP/S2/M-01/2001) is thankfully acknowledged. One of the authors (AK) acknowledges a Junior Research Fellowship (JRF) from the DST, India.

References

- [1] F Dalfovo, S Giorgini and L P Pitaevskii, *Rev. Mod. Phys.* **71**, 463 (1999)
- [2] A J Leggett, *Rev. Mod. Phys.* **73**, 307 (2001)

- [3] C C Bradley, C A Sackett, J J Tollett and R G Hulet, *Phys. Rev.* **75**, 1687 (1995)
- [4] M H Anderson, J R Ensher, M R Matthews, C E Wiemann and E A Cornell, *Science* **269**, 198 (1995)
- [5] C J Pethik and H Smith, *Bose–Einstein condensation in dilute gases* (Cambridge University Press, Cambridge, 2001)
- [6] J L Ballot and M Fabre de la Ripelle, *Ann. Phys. (N.Y.)* **127**, 62 (1980)
- [7] B D Esry and C H Greene, *Phys. Rev.* **A60**, 1451 (1999)
- [8] J L Bohn, B D Esry and C H Greene, *Phys. Rev.* **A58**, 584 (1998)
- [9] O Sørensen, D V Fedorov, A S Jensen and E Nielsen, *Phys. Rev.* **A65**, 051601 (R) (2002)
- [10] O Sørensen, D V Fedorov and A S Jensen, *Phys. Rev.* **A66**, 032507 (2002)
- [11] O Sørensen, D V Fedorov and A S Jensen, *Phys. Rev. Lett.* **89**, 173002 (2002)
- [12] M Fabre de la Ripelle, *Ann. Phys. (N.Y.)* **147**, 281 (1983)
M Fabre de la Ripelle, *Few-Body Systems* **1**, 181 (1986)
- [13] M Abramowitz and I A Stegun, *Handbook of mathematical functions* (Dover Publications, New York, 1972), p. 773
- [14] T K Das, H T Coelho and M Fabre de la Ripelle, *Phys. Rev.* **C26**, 2281 (1982)
J L Ballot, M Fabre de la Ripelle and J S Levinger, *Phys. Rev.* **C26**, 2301 (1982)
- [15] K B Davis, M Mewes, M A Joffe, M R Andrews and W Ketterle, *Phys. Rev. Lett.* **74**, 5202 (1995)
- [16] K Goral, K Rzazewski and T Pfau, *Phys. Rev.* **A61**, 051601 (2000)
- [17] T K Das and B Chakrabarti, *Phys. Rev.* **A70**, 063601 (2004)
- [18] B Chakrabarti, A Kundu and T K Das, *J. Phys. B* (2004) (accepted)
- [19] R Napolitano, J De Luca, V S Bagnato and G C Marques, *Phys. Rev.* **A55**, 053954 (1997)