Potential harmonics expansion method for trapped interacting bosons: Inclusion of two-body correlation

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(Received 24 November 2003; published 1 December 2004)

We study a system of *A* identical interacting bosons trapped by an external field by solving *ab initio* the many-body Schrödinger equation. A complete solution by using, for example, the traditional hyperspherical harmonics (HH) basis develops serious practical problems due to the large degeneracy of HH basis. Symmetrization of the wave function, calculation of the matrix elements, etc., become an immensely formidable task as *A* increases. Instead of the HH basis, here we use a new basis, called "potential harmonics" (PH) basis, which is a subset of HH basis. We assume that the contribution to the orbital and grand orbital [in $3(A-1)$-dimensional space of the reduced motion] quantum numbers comes *only from the interacting pair*. This implies inclusion of two-body correlations only and disregard of all higher-body correlations. Such an assumption is ideally suited for the Bose-Einstein condensate (BEC), which is required, for experimental realization of BEC, to be extremely dilute. Hence three and higher-body collisions are almost totally absent. Unlike the $(3A-4)$ hyperspherical variables in HH basis, the PH basis involves only three *active* variables, corresponding to three quantum numbers—the orbital *l*, azimuthal *m*, and the grand orbital $2K+l$ quantum numbers for any arbitrary *A*. It drastically reduces the number of coupled equations and calculation of the potential matrix becomes tremendously simplified, as it involves integrals over *only three* variables for any *A*. One can easily incorporate realistic atom-atom interactions in a straightforward manner. We study the ground and excited state properties of the condensate for both attractive and repulsive interactions for various particle number. The ground state properties are compared with those calculated from the Gross-Pitaevskii equation. We notice that our many-body results converge towards the mean field results as the particle number increases.

I. INTRODUCTION

Although the phenomenon of Bose-Einstein condensation (BEC) was known for a long time [1–3], its experimental observation in trapped and supercooled (down to nanokelvin temperatures) alkali atoms in 1995 [4–6] renewed a great deal of interest, both experimental and theoretical, in the phenomemon. The importance of this topic is clearly demonstrated by the fact that two independent Nobel Prizes were awarded on BEC related works in quick succession in the recent past. The density of magneto-optically trapped atomic gas undergoing BEC is extremely low (to avoid recombination of atoms through three and higher body collisions) and the number of trapped atoms is typically of the order of a few hundred to a few million. This is extremely small compared to the Avogadro number. For such a small number of atoms an exact *ab initio* solution would have been ideally desirable. But an interacting system of $A=(N+1)$ particles has $3N$ relative degrees of freedom and an *ab initio* solution of the corresponding Schrödinger equation is practically impossible for $A > 3$. Hence the usual theoretical tools that have been used so far are the mean field models [7–10] and the Thomas-Fermi [8] approximation. The dilute atomic gas un-

dergoes BEC below a critical temperature (typically 10^{-9} K) when most of the atoms (bosons) go to the single particle ground state. Then the de Broglie wavelength associated with the atomic motion is much larger than the interaction length scale. Hence the resulting many body system emerges as essentially a single quantum system where all the atoms behave in a coherent manner [8,11]. At zero temperature, the effect of the excited states are absent and the condensate is described by a single equation involving the condensate wave function [8]. However this simple picture is no more true at a finite temperature due to the existence of interparticle interactions. The usual procedure is to start with the mean field approximation like the Hartree-Fock (HF) theory for the many body system [7–10]. This is an independent particle approach where each individual atom is assumed to move in a single particle orbit. These orbits are determined self consistently by allowing an atom in one orbital to be influenced by other atoms in other orbitals through two-body interaction. Assuming a contact interaction for the two-body potential, viz., $V(\vec{r}-\vec{r}') = g\,\delta(\vec{r}-\vec{r}')$, the many body equation reduces to the famous Gross-Pitaevskii (GP) equation [8]. At zero temperature, the effect of excited states are neglected and the condensate is described by the time independent GP equation

$$\left[-\frac{\nabla^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + g\,\phi^2(\vec{r})\right]\phi(\vec{r}) = \mu\phi(\vec{r}), \quad (1)$$

where $n(\vec{r}) = \phi^2(\vec{r})$ is the condensate density and μ is the chemical potential. For a first approach the contact interac-

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tion is justified since in the cold and dilute gas only binary collissions at low energies are relevant. These are characterized by the *s*-wave scattering length (a_{sc}), which is independent of the details of two-body potentials. The strength constant *g* of the contact interaction is related to the scattering length through [8]

$$g = \frac{4\pi\hbar^2 a_{sc}}{m}.$$ (2)

The GP equation has been used extensively to study the BEC [8,11]. Although most of the static, dynamic and thermodynamic properties are fairly well reproduced by the GP equation [8], the wave function does not include any correlation. Furthermore the assumption of a contact δ-interaction is too simple and does not represent the realistic situation. It has already been shown that the Dirac δ-function is not suitable as a replacement of the actual two-body interaction in exact theories in more than one dimension [12]. This is because the Hamiltonian then becomes unbound from below and the ground state energy diverges for an attractive zero range potential. Solutions are usually obtained in the metastable region (although such solutions are not rigorously correct for an attractive δ-function potential) and the condensate becomes unstable for *N* larger than a critical number, due to disappearance of the local minimum. This was shown by Bohn *et al.* in a hyperspherical calculation keeping the lowest (most dominant) harmonic [13]. A third disadvantage is the non-linearity of the GP equation, so that standard quantum mechanics is not applicable without concessional approximation. Thus one has to go beyond the mean field approximation and simple contact interactions.

Because of the limitations of the mean field theory and GP equation it is desirable to solve the many body *linear* Schrödinger equation directly. The Schrödinger equation for a system of $A=(N+1)$ identical bosons, each of mass *m*, confined by an external field V'_{trap} (acting on each individual boson) and interacting through a mutual two body interaction *V* is

$$\left[-\frac{\nabla^2}{2m}\sum_{i=1}^{A}\nabla_i^2 + \sum_{i=1}^{A}V'_{trap}(\vec{x}_i) + \sum_{i<j=2}^{A}V(\vec{x}_i-\vec{x}_j) \right]\Psi(\vec{x}) = E\Psi(\vec{x}),$$ (3)

where $\vec{x}$ refers to the set of particle coordinates $\{\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_A\}$ of *A* bosons. The center of mass (c.m.) motion can be eleminated resulting in a Schrödinger equation in $3N$ variables. A standard practice is the use of hyperspherical harmonics expansion (HHE) method, in which the wave function is expanded in the complete set of hyperspherical harmonics (HH) spanning the $(3N-1)$-dimensional hyperangular space [14]. Projection on a particular HH leads to a system of coupled differential equations (CDE). However there are several very serious difficulties associated with the solution of a fairly large number of particles. First the expansion basis of HH should be properly symmetrized and appropriate conserved quantum numbers properly taken care of. Secondly calculation of matrix elements of all the pairwise two-body potentials is an extremely formidable task. Finally,

due to very large degeneracy of the HH basis for a large number of particles, the number of CDE and the dimension of the potential matrix is too large to be handled by any computer [14]. On top of all these, the convergence rate of the HH expansion, especially for long-range interactions, is slow [15]. For these reasons the HHE method has been used fully for the three body system only [15–18]. On the other hand, as we discussed earlier, the condensate can be treated broadly as a "single lump of quantum stuff," since all the individual atoms in the condensate lie within one single de Broglie wavelength [8]. Thus it is reasonable to assume that the basic properties of the condensate in the lowest approximation, is described by a single collective coordinate. This led Bohn *et al.* [13] to go for the K-harmonic approximation, in which the HH expansion is restricted effectively to the first term only (which is independent of the hyperangles). Such a *drastic* approximation may be justified for a contact interaction only. Even in this case, for an attractive δ-function interaction, there are no *rigorously stable* solutions. Since the wave function becomes independent of the hyperangles and the hyperradius is invariant under any permutation of the particles, the wave function becomes totally symmetric, as required. The calculation of the potential matrix also simplifies immensely and the CDE reduces to a single differential equation [13]. The hyperradius emerges as the sought for collective coordinate. In spite of the great simplifications, there are serious criticisms of this approach: (1) The method cannot be applied to any realistic two-body interaction. (2) Even for a contact interaction, the method is not satisfactory for attractive δ-function interaction, for which no rigorous solution exists. (3) Only one collective variable is involved. Hence it can only describe the gross features of the condensate, without any finer details. Thus a more rigorous treatment is necessary. But as already mentioned a completely rigorous, essentially exact solution of the Schrödinger equation is possible for the three body system only. That has been done to get an idea of the initial trend as the particle number increases from three by Esry and Greene [12]. However that is far from the real situation in a condensate.

An alternative approach of exact numerical diagonalization of the many body Hamiltonian was adopted by Haugset and Haugerud [19] for a small number (≤ 30) of interacting (via contact interaction) bosons confined by a harmonic trap. However, this was restricted to *one and two dimensions only*. Moreover the process is extremely time consuming *even for two dimensional* condensates, with a nagging question of convergence of the chosen harmonic oscillator basis expansion. The rate of convergence is expected to be slower for a realistic two-body interaction and in three dimensional condensates. Although analytic expressions for the matrix elements are greatly simplified for a delta function interaction, all the problems associated with a contact interaction discussed above remain for the two dimensional condensate. However, there is no problem with the one dimensional condensate, as one dimensional delta function is not pathological.

From the above discussion it is clear that an exact treatment of the many body system in three dimensions is not possible beyond the three body system. On the other hand,

the single quantum nature of the entire condensate suggests that out of the thousands to millions of degrees of freedom of the individual particles *only a few* are physically relevant. This is due to the fact that the condensate is possible only at extremely low temperatures (low energy of the individual particles) and extremely low densities. Under these conditions *only two body collisions* are relevant. Three and higher body collisions are *extremely* rare and correlations beyond two body correlations in the condensate wave function are completely negligible up to a very high degree of precision. Indeed in an experimental situation this is ensured by keeping the density extremely low, so that there are no recombination via three and higher body collisions [8]. The mean field approach ignores all correlations including two-body correlations. Importance of two-body correlations in BEC has been emphasized by several authors [20,21]. Thus physically relevant quantities are contributed by two-body collisions, while the rest of the particles in the condensate do not partate in any motion other than a collective one and are simply inert spectators. The emerging picture then suggests that most of the degrees of freedom of these spectators can be frozen, while a single pair interacts. This reduces the physically important degrees of freedom of the condensate to just four—a global length scale (hyperradius) of the entire condensate, and the three degrees of freedom of the relative vector $\vec{r}_{ij}=\vec{x}_i-\vec{x}_j$ of the interacting pair. However one has to concede that *any* pair out of the $A=(N+1)$ atoms in the condensate can interact. These are also consistent with the intuitive "single quantum stuff" concept of the condensate.

Among the various possible theoretical approaches to handle the many body system, the HHE method appears to be the most lucrative one, as it readily provides the hyperradius as the most important collective variable. A theoretical formalism, arising out of the HHE method, was adopted by Fabre de la Ripelle [22] in 1986. Although the primary concern there was an application to the nuclear systems consisting of fermions, it was noted that the formalism is applicable to a system of identical bosons also [23]. To incorporate the importance of the interacting pair and two-body correlations, he introduced the potential harmonics (PH) expansion basis [23], rather than the general HH basis, thereby reducing the expansion basis to a great extent. Potential harmonics is a subset of HH, where all correlations higher than two-body ones are disregarded. In PH, the contribution to the total orbital angular momentum as also the grand orbital quantum number comes *only* from the interacting pair. Here all the $(A-2)$ spectators are assumed to be described by the HH of the lowest (zero) order. We adopt this procedure since this approximation is quite justified in our situation due to the diluteness of BEC, where two-body correlation is the most important and all higher-body correlations can be safely ignored. Using Faddeev like decomposition of the total wave function, and then expanding each such component in an appropriate set of PH, the number of CDE can be reduced drastically. Since the PH involves only four active degrees of freedom, calculation of potential matrix elements is simplified tremendously as compared to that in HH basis. Use of realistic two-body interactions and calculation of their matrix elements are quite straight forward. Requiring the Faddeev component for the (ij) interacting pair to be symmetric under

(ij)-pair exchange, the total wave function becomes automatically totally symmetric. Thus the symmetrization of the wave function is also handled properly.

Thus a truly many body equation is reduced to a tractable mathematical form. The assumptions leading to this are especially appropriate for the BEC. Hence we adopt the PH basis as our starting point. This is theoretically applicable to a system containing any number of particles, but we will see in Sec. III, that numerical difficulties arise as the number of particles increases beyond a certain number. In this paper we report some of the basic properties of the condensate for various particle numbers and compare them with previous calculations.

Sorensen *et al.* [20,21] have followed a method which is similar in spirit to the present work, although it differs in details. They expand the wave function in the adiabatic subset $\Phi_n(\rho,\Omega)$ of the *full* $(N-1)$-body Hamiltonian (in c.m. frame). Later this is decomposed in Faddeev-like components ϕ_{ij}. This leads to an integro-differential equation (IDE) for ϕ ($=\phi_{ij}$, which is the same for *all ij*-pairs due to boson symmetry) involving *five* dimensional integrals and the full $(3N-4)$-dimensional hyperangular differential operator $\hat{\Lambda}^2$. All $(3N-5)$ angle derivatives other than $\alpha=\alpha_{12}$ (where $r_{ij}=\sqrt{2}\rho\sin\alpha_{ij}$ is the relative separation of the (ij)-pair and ρ is the hyperradius of the full system), are disregarded, leaving only one angle variable. Assumption of a *very short ranged* two-body potential reduces the five dimensional integrals to two dimensional ones. In this limit simple expressions are obtained for the integrals in IDE. On the other hand, we write the complete $3N$-dimensional Schrödinger equation of the relative motion of a $(N+1)$ boson system in terms of Faddeev like components $\Phi(\vec{r}_{ij},r)$, subject to the approximation that $\Phi(\vec{r}_{ij},r)$ corresponds to zero eigenvalue of the hyperangular momentum operator (see later) for the $(N-1)$ remaining relative vectors of the spectators, while (ij)-pair interacts. These are then expanded in the potential harmonics (PH) basis. The assumptions in our method are clearly justified in terms of the physics of the chosen system, which have been stated earlier. While the use of PH basis in nuclei (as originally used by Fabre in [22,23]) is questionable due to high spatial density of nucleons in a nucleus, its application in BEC is ideally suited (the number of atoms in the condensate is $\leq 10^6$ in a space of macroscopic linear dimensions of order 10^{-2} cm, which is immensely smaller than the Avogadro number). As a consequence, the total orbital (l) and grand orbital (K) angular momenta of the system are contributed by the interacting pair alone. Apart from this well justified fundamental approximation, we need no other approximation. Although for the first calculation, we have restricted ourselves to $l=0$ and a *central* two-body interaction, both these can be relaxed resulting in a somewhat more complicated equation. Finally the system of coupled differential equations in one variable (hyperradius, r) can be solved numerically, *without additional approximation* [as done in Ref. [15] and compared with adiabatic approximation (AA) in Ref. [28]] using, e.g., renormalized Numerov method. Once again, as a preliminary calculation, we use AA to solve the CDE. Our use of AA in solving the CDE is not an indispensable one; it is done only to reduce the numerical

calculation. But in the approach of Sorensen *et al.*, adiabatic subset is the starting point to separate the hyperangular and hyperradial motions. Furthermore our method can handle any two-body potential (central or not, short ranged or not); for noncentral potential, calculation of matrix elements will involve integrals over two polar angles in addition. The approach of Refs. [20,21] requries a very short ranged, central potential to reduce the equation to a manageable form. The present method has no such restriction.

The paper is organized as follows. In Sec. II, we present our choice of Jacobi coordinates and express the kinetic energy in the chosen set of hyperspherical variables. In the same section, we introduce the concept of potential harmonics basis and obtain the set of coupled differential equations resulting from the many-body Schrödinger equation. The numerical method for solving the CDE and results of our calculation are presented in Sec. III. There we compare our results for different numbers of particles with those of earlier calculations. Finally in Sec. IV we draw our conclusions. Some of the detailed expressions have been given in the Appendix.

II. THEORY

A. Choice of Jacobi coordinates

We consider a system of $A=(N+1)$ identical bosons, each of mass m and confined magnetically in a trap which is approximated by a spherically symmetric harmonic oscillator potential with frequency ω. We assume that the atomic cloud is at zero temperature. The full many body Hamiltonian is given by

$$\left[-\frac{\nabla^2}{2m} \sum_{i=1}^{N+1} \nabla_i^2 + \sum_{i=1}^{N+1} \frac{1}{2} m\omega^2 x_i^2 + \sum_{ij>i}^{N+1} V(\vec{x}_i - \vec{x}_j) \right] \Psi(\vec{x})$$
$$= E' \Psi(\vec{x}), \qquad (4)$$

where $\vec{x}$ refers to the set of particle coordinates $\{\vec{x}_1, \vec{x}_2, \dots, \vec{x}_{N+1}\}$ of $(N+1)$ bosons and E' is the total energy. We decompose the total wave function $\Psi(\vec{x})$ as the sum of pairwise partial waves

$$\Psi(\vec{x}) = \sum_{ij>i}^{N+1} \psi_{ij}(\vec{x}). \qquad (5)$$

The Schrödinger equation for ψ_{ij} can be written as

$$(T + V'_{trap} - E')\psi_{ij}(\vec{x}) = -V(r_{ij}) \sum_{kl>k}^{N+1} \psi_{kl}(\vec{x}), \qquad (6)$$

where T is the total kinetic energy operator, V'_{trap} is the confining potential, $V'_{trap} = \sum_{i=1}^{N+1} \frac{1}{2} m\omega^2 x_i^2$ and $V(r_{ij})$ is the pairwise local central two-body interaction between ith and jth particles, $\vec{r}_{ij} = \vec{x}_i - \vec{x}_j$. Applying the operator $\sum_{ij>i}^{N+1}$ on both sides of Eq. (6), and using Eq. (5), we get back Eq. (4). Now instead of $(N+1)$ particle coordinates $\vec{x}_i$, the system can alternatively be described by the center of mass coordinate $\vec{R}$

$$\vec{R} = \frac{1}{N+1} \sum_{i=1}^{N+1} \vec{x}_i \qquad (7)$$

and N Jacobi coordinates defined as

$$\vec{\zeta}_i = \sqrt{\frac{2i}{i+1}} \left(\vec{x}_{i+1} - \frac{1}{i} \sum_{j=1}^{i} \vec{x}_j \right), \quad i = 1, \dots, N. \qquad (8)$$

The chosen normalization of $\vec{\zeta}_i$ facilitates writing the Laplace operator in the form

$$\frac{1}{2} \sum_{i=1}^{N+1} \nabla_i^2 = \frac{1}{2A} \nabla_R^2 + \sum_{i=1}^{N} \nabla_{\zeta_i}^2 \qquad (9)$$

Then the relative motion [after removal of center of mass motion from Eq. (4)] is described by [14,23]

$$\left[-\frac{\hbar^2}{m} \sum_{i=1}^{N} \nabla_{\zeta_i}^2 + V_{trap} + V_{int}(\vec{\zeta}_1, ..., \vec{\zeta}_N) - E \right] \psi(\vec{\zeta}_1, \dots, \vec{\zeta}_N) = 0, \qquad (10)$$

where $V_{trap} = \sum_{i=1}^{N} \frac{1}{2} m\omega^2 \zeta_i^2$ and V_{int} is the sum of all pairwise interactions, $V_{int} = \sum_{ij>i}^{N+1} V(r_{ij})$ expressed in the relative coordinates. Here E is the energy of the relative motion, i.e., E' minus energy of c.m. motion. The hyperradius r is defined as [22]

$$r = \left[\sum_{i=1}^{N} \zeta_i^2 \right]^{1/2} = \left[\frac{2}{N+1} \sum_{i,j>i} r_{ij}^2 \right]^{1/2}, \qquad (11)$$

which is invariant under permutations of the particle indices as also three dimensional rotations. The hyperspherical coordinates are constituted by the hyperradius r and remaining $(3N-1)$ hyperangles, denoted collectively by Ω_N in $D=3N$ dimensional space. Note that the choice of Jacobi coordinates Eq. (8), is not unique, since the labeling of the particle indices and consequently that of the Jacobi coordinates are arbitrary. We choose a particular set by specifying the relative separation of the interacting pair, $\vec{r}_{ij}$ as $\vec{\zeta}_N$ and (ϑ, φ) are the two spherical polar coordinates associated with $\vec{r}_{ij}$. The relative length is defined in terms of ϕ through $r_{ij} = r \cos \phi$. For the rest of $(N-1)$ Jacobi coordinates, we define the hyperradius ρ_{ij} in the $3(N-1)$-dimensional space by

$$\rho_{ij} = \left[\sum_{k=1}^{N-1} \zeta_k^2 \right]^{1/2}, \qquad (12)$$

which is related with $\vec{\zeta}_N = \vec{r}_{ij}$ by

$$\rho_{ij}^2 + r_{ij}^2 = r^2, \quad \rho_{ij} = r \sin \phi \cdot \qquad (13)$$

Then our hyperspherical coordinates become

$$(r, \Omega_N) = (r, \phi, \vartheta, \varphi, \Omega_{N-1}) \cdot \qquad (14)$$

Here Ω_{N-1} involves $2(N-1)$ spherical polar angles associated with each of $(N-1)$ Jacobi vectors $\{\vec{\zeta}_1, \vec{\zeta}_2, \dots, \vec{\zeta}_{N-1}\}$ and $(N-2)$ angles (expressing relative lengths), i.e., a total of $(3N-4)$ variables. In this choice of hyperspherical coordinates, the Laplace operator takes the form [22]

$$\nabla^2 \equiv \sum_{i=1}^{N} \nabla^2_{\zeta_i} = \frac{\partial^2}{\partial r^2} + \frac{3A-4}{r}\frac{\partial}{\partial r} + \frac{L^2(\Omega_N)}{r^2}, \quad A = N+1.$$

(15)

$L^2(\Omega_N)$ is the grand orbital operator in $3N$-dimensional space which is obtained from a recurrence formula [22] and has the form

$$L^2(\Omega_N) = 4(1-z^2)\frac{\partial^2}{\partial z^2} + 6[2-N(1+z)]\frac{\partial}{\partial z} + 2\frac{l^2(\omega_{ij})}{1+z}$$

$$+ 2\frac{L^2(\Omega_{N-1})}{1-z},$$

(16)

where $z=\cos 2\phi$, ω_{ij} represents the two polar angles (ϑ, φ) associated with $\vec{r}_{ij}$ and $L^2(\Omega_{N-1})$ is the grand orbital operator in $3(N-1)$ dimensional space.

B. Potential basis and potential multipoles

To expand a function $V(r_{ij})$ in hyperspherical harmonics (HH) we use the above definition of Jacobi coordinates. It is easy to see that HH basis which is complete for the expansion of $V(r_{ij})$ does not contain any function of the coordinate $\vec{\zeta}_i$ with $i < N$ and is given by [23]

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

(17)

where $^{(N)}P^{l,0}_{2K+l}$ is a function involving the Jacobi polynomial and is needed in the general expression of the hyperspherical harmonics (see Appendix) of grand orbital $2K+l$ and orbital angular momemtum l. The quantity $\mathcal{Y}_0(D-3)$ is the HH of order zero (i.e. grand orbital quantum number is zero) in $3(N-1)$ dimensional space, $\mathcal{Y}_0(D-3)=[\Gamma((D-3)/2)/2\pi^{(D-3)/2}]^{1/2}$. This new basis set which is a subset constituted by HH of order $(2K+l)$ are called "potential harmonics" (PH). These are the eigenfunctions of $L^2(\Omega_N)$, when the eigenvalue of $L^2(\Omega_{N-1})$ is 0 and satisfies the eigenvalue equation:

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

(18)

The relation $L^2(\Omega_{N-1})\psi_{ij}(\vec{x})=0$ implies that we are considering only those states which are invariant under all generalized rotations in $3(N-1)$-dimensional space. Naturally the contribution to the grand orbital quantum number comes only from the interacting pair. This corresponds effectively to two-body correlations only in the wave function. Due to diluteness of atomic BEC, the effect of higher body correlations can be ignored as the probability for three or more particles to come close at the same time is extremely small. This reduces the number of quantum numbers in the new basis [all the quantum numbers specifying the eigenfunctions of $L^2(\Omega_{N-1})$ are zero]. It contains only three quantum numbers; 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. The normalization condition is given by

$$\int \mathcal{P}^{l,m}_{2K+l}{}^*(\Omega_{ij})\mathcal{P}^{l'm'}_{2K'+l'}(\Omega_{ij})d\Omega_{ij} = \delta_{KK'}\delta_{ll'}\delta_{mm'}.$$

(19)

Then the PH expansion of the potential is

$$V(r_{ij}) = \sum_{K,l,m} A^m_l(i,j)\mathcal{P}^{l,m}_{2K+l}(\Omega_{ij})V^{(D,l)}_K(r).$$

(20)

$A^m_l(i,j)$ is an operator which is independent of r_{ij}, but may act on other variables like spin variables. The quantity $V^{(D,l)}_K(r)$ are the "potential multipoles" and for a central potential, it is given by [23]

$$V^{(D,l)}_K(r) = \langle \mathcal{P}^{l,m}_{2K+l}(\Omega_{ij})|V(r_{ij})\rangle$$

$$= |\mathcal{Y}_0(D-3)|^{-1}\int_0^{\pi/2} {}^{(N)}P^{l,0}_{2K+l}(\phi)V_l(r\cos\phi)$$

$$\times(\sin\phi)^{D-4}(\cos\phi)^2 d\phi,$$

(21)

where the functions $^{(N)}P^{l,0}_{2K+l}(\phi)$ are defined in the Appendix. Starting from the multipoles calculated either for the $D=5$ or $D=6$ (depending whether D is odd or even) and using simple recurrence formulas potential multipoles for any D can be calculated [23].

C. Coupled differential equations

Splitting Eq. (10) in the manner of Eq. (6) for the (ij)-interacting pair and using Eqs. (14)–(16), subject to the restriction that the eigenvalue of $L^2(\Omega_{N-1})$ is zero, we see that the (ij) Faddeev component will be a function of $\vec{r}_{ij}$ and r only and satisfies [23]

$$(T + V_{trap} - E)\Phi(\vec{r}_{ij},r) = -V(r_{ij})\sum_{k,l>k}\Phi(\vec{r}_{kl},r),$$

(22)

where $\Phi(\vec{r}_{ij},r)$ differs from the general solution ψ_{ij} by the fact that it corresponds to eigenvalue zero of the operator $L^2(\Omega_{N-1})$. Next expand the wave function $\Phi(\vec{r}_{ij},r)$ in the complete set of potential harmonics (when l is a good quantum number) as

$$\Phi(\vec{r}_{ij},r) = r^{-(D-1)/2}\sum_{K'}\mathcal{P}^{lm}_{2K'+l}(\Omega_{ij})u^l_{K'}(r).$$

(23)

Substitution of Eq. (23) in Eq. (22) and projection on the same basis, leads to the set of coupled differential equations [23]

$$\left[-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{\hbar^2}{m}\frac{\mathcal{L}_K(\mathcal{L}_K+1)}{r^2} + V_{trap}(r) - E\right]u^l_K(r)$$

$$+ \sum_{K'}f^2_{K'l}V_{KK'}(r)u^l_{K'}(r) = 0,$$

(24)

where

$$\mathcal{L}_K = 2K+l+\frac{D-3}{2},$$

$$f^2_{Kl} = \sum_{k,l>k}\langle\mathcal{P}^{lm}_{2K+l}(\Omega_{ij})|\mathcal{P}^{lm}_{2K+l}(\Omega_{kl})\rangle.$$

(25)

The potential matrix is given by

$$V_{KK'}(r) = \int \mathcal{P}_{2K+l}^{lm*}(\Omega_{ij}) V(r_{ij}) \mathcal{P}_{2K'+l}^{lm}(\Omega_{ij}) d\Omega_N. \quad (26)$$

So instead of $(3N-1)$ angle variables in HHE method, in potential harmonics expansion method (PHEM) the integral involves only 3 angle variables. It greatly simplifies the calculation of the matrix element for any N.

The quantity f_{kl}^2 of Eqs. (24) and (25) is given by [23]

$$f_{Kl}^2 = 1 + \left[2(A-2)\left(-\frac{1}{2}\right)^l P_K^{\alpha\beta}\left(-\frac{1}{2}\right) + \frac{(A-2)(A-3)}{2} P_K^{\alpha\beta}(-1)\delta_{l,0} \right] \Big/ P_K^{\alpha\beta}(1), \quad (27)$$

where $\alpha = (3A-8)/2$ and $\beta = l + \frac{1}{2}$ and $P_K^{\alpha\beta}(x)$ is the Jacobi polynomial. Multiplying Eq. (24) by appropriate constant factors, it can be put in a symmetric form:

$$\left[-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{\hbar^2}{mr^2}\{\mathcal{L}(\mathcal{L}+1) + 4K(K+\alpha+\beta+1)\} + V_{trap}(r) - E \right] U_{Kl}(r) + \sum_{K'} \bar{V}_{KK'}(r) U_{K'l}(r) = 0, \quad (28)$$

where $\mathcal{L} = l + (3A-6)/2$, the symmetrized potential matrix $\bar{V}_{KK'}$ has the form

$$\bar{V}_{KK'}(r) = f_{Kl} V_{KK'}(r) f_{K'l}(h_K^{\alpha\beta} h_{K'}^{\alpha\beta})^{-1/2} \quad (29)$$

and

$$U_{Kl}(r) = f_{Kl}(h_K^{\alpha\beta})^{1/2} u_K^l(r). \quad (30)$$

Here $h_K^{\alpha\beta}$ is the norm of the Jacobi polynomial $P_K^{\alpha\beta}(x)$ [24]. The potential matrix element is obtained from Eq. (26), using Eqs. (17) and (A4) of the Appendix, in the form

$$V_{KK'}(r) = \int_{-1}^{+1} P_K^{\alpha\beta}(z) V\left(r\sqrt{\frac{1+z}{2}}\right) P_{K'}^{\alpha\beta}(z) w_l(z) dz, \quad (31)$$

where $w_l(z) = (1-z)^\alpha(1+z)^\beta$ is the weight function of the Jacobi polynomials [24]. For Gaussian interaction with $A=3$, the integral can be obtained analytically [25], from where one can directly check the numerical accuracy.

III. NUMERICAL METHOD AND RESULTS

A. Numerical method

For a chosen number of particles (A) and a chosen interaction potential $[V(r_{ij})]$, we calculate the potential matrix for a fixed value of hyperradius (r) from Eqs. (29) and (31) using a multipoint Gauss-Jacobi quadrature. For the present calculation we select $l=0$ and truncate the PH expansion basis of Eq. (23) to a maximum K value $(=K_{max})$. In order to simplify the solution of the set of coupled differential equations, Eq. (28), we adopt the hyperspherical adiabatic approximation (HAA) [16,26]. In this approximation it is assumed that the hyperradial motion is slow compared to the hyperangular motions. Hence the latter can be solved adia-

batically for a fixed value of r to get an effective potential as a parametric function of r [16]. This is done by diagonalizing the potential matrix together with the diagonal hypercentrifugal repulsion and the trapping potential for each value of r:

$$\sum_{K'=1}^{K_{max}} M_{KK'}(r) \chi_{K'\lambda}(r) = \omega_\lambda(r) \chi_{K\lambda}(r), \quad (32)$$

where

$$M_{KK'}(r) = \bar{V}_{KK'}(r) + \left[\frac{\hbar^2}{mr^2}\{\mathcal{L}(\mathcal{L}+1) + 4K(K+\alpha+\beta+1)\} + V_{trap}(r) \right]\delta_{KK'}. \quad (33)$$

The lowest eigenvalue gives the "lowest eigenpotential," $\omega_0(r)$. As we discussed in the Introduction, the hyperradius behaves as the most important collective coordinate and $\omega_0(r)$ is the potential in which the condensate moves as a "single quantum stuff," except for attractive two-body interactions and $A > A_{cr}$ (see later). Another collective coordinate is the hyperangle ϕ appearing in the wave function through Eqs. (23) and (17), which describes the deviations of the condensate from hyperspherically symmetric distribution.

In the HAA approach, an approximate solution of Eq. (28) is obtained by solving a single uncoupled differential equation [16]

$$\left[-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \omega_0(r) + \sum_{K=0}^{K_{max}} \left| \frac{d\chi_{K0}(r)}{dr} \right|^2 - E \right] \zeta_0(r) = 0. \quad (34)$$

The solution of Eq. (34) subject to appropriate boundary conditions on $\zeta_0(r)$ gives the energy E, which is an upper bound for the eigenenergy of Eq. (28) . The partial waves of Eq. (28) are given in HAA by [16]

$$U_{Kl}(r) \simeq \zeta_0(r)\chi_{K0}(r). \quad (35)$$

This approximation is usually called uncoupled adiabatic approximation (UAA) in the literature [16,26]; disregarding the third term on the left side of Eq. (34) one gets the so-called extreme adiabatic approximation (EAA). It has been shown that the HAA is in very good agreement (having less than 1% error) with the exact solution of the CDE for both atomic [27–29] and nuclear [30,31] cases. Since this is adequate for this preliminary application of this new method, we adopt the HAA, instead of solving the full set of CDE by exact numerical algorithm like the renormalized Numerov method [32,33].

B. Choice of two body interaction potential

In this paper we compare our results with those of the GP equation as also with other calculations using a contact δ-interaction. But a δ-function interaction is not a physical one since it diverges at $r_{ij}=0$ and nothing (e.g., centrifugal repulsion) can prevent its overwhelming effect. As a result, the Hamiltonian becomes unbound from below for an attractive δ interaction. This is manifest in the effective potential
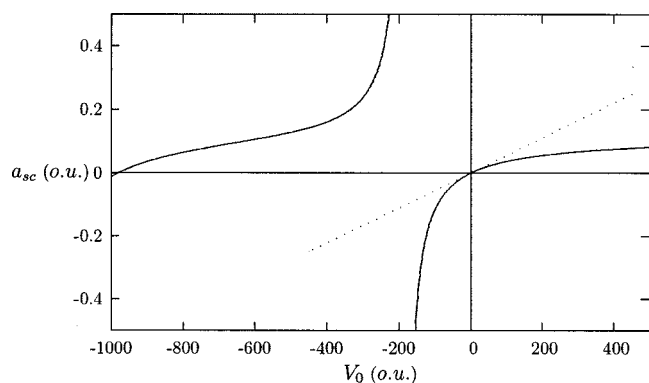
FIG. 1. Plot of calculated a_{sc} as a function of V_0 for r_0 =0.0855 o.u. The dotted line corresponds to the Born approximation ($a_{sc}^{(B)}$).

$\omega_0(r)$, which for a particle number (A) less than a critical value (A_{cr}) produces a local minimum at a finite value of r (giving rise to a metastable solution), but $\omega_0(r) \rightarrow -\infty$ as $r \rightarrow 0$ for any number of particles (see following subsection, as also Ref. 12). Thus there are no rigorously acceptable and stable solution for any A, since the attractive essential singularity at $r=0$ will pull the system to $r \rightarrow 0$ and the corresponding wave function will diverge at $r=0$. Although the δ-function is particularly convenient for analytic calculations, it is desirable to choose an interaction which would either remain finite or at worst introduce a removable singularity as $r_{ij} \rightarrow 0$ for attractive cases. Then the hypercentrifugal repulsion in Eq. (28) (which is nonvanishing even for l =0, $K=0$ and increases rapidly as A increases) will not allow the interacting particles to come too close to each other. We thus choose a Gaussian potential of strength V_0 and range r_0

$$V(r_{ij}) = V_0 e^{-r_{ij}^2/r_0^2}. \tag{36}$$

Choosing appropriate values of V_0 and r_0, the potential can be made either soft or stiff. A particular experimental situation at the low temperature limit is characterized by the s-wave scattering length (a_{sc}). For given values of V_0 and r_0, one can calculate a_{sc} by solving the two-body radial Schrödinger equation for positive energies, in the zero energy limit. Alternately, for a suitably chosen value of r_0 and an experimentally known value of a_{sc} one can find V_0 numerically from the solution of the two-body Schrödinger equation in the $E \rightarrow 0+$ limit. In Fig. 1, we present a plot of calculated a_{sc} as a function of V_0 for r_0=0.0855 o.u. As is well known, a_{sc} is positive and monotonically continuous for $V_0 > 0$. The scattering length becomes negative as V_0 becomes negative and continues to $-\infty$ at a particular negative value of V_0. At this point, a_{sc} has an infinite discontinuity and as V_0 decreases further, a_{sc} starts from $+\infty$ and decreases continuously to $-\infty$ at a second particular value of V_0. The first, second, ..., branch of the curve (as V_0 decreases from positive values) correspond respectively to zero, one, ..., two-body bound states. For a stable BEC, we choose the first branch of the curve. From Fig. 1, one notices that for r_0 =0.0855 o.u., the first discontinuity occurs at about V_0 =−184 o.u. For r_0=0.005 o.u., this value is much more nega-

tive (-8.18963×10^5 o.u.). In the same figure, we also plot the Born approximation for a_{sc} (corresponding to r_0 =0.0855 o.u.), given by [12]

$$a_{sc}^{(B)} = \frac{m}{2\pi\hbar^2} \int d^3r \ V(\vec{r}). \tag{37}$$

For a Gaussian interaction this integral can be done analytically and gives

$$a_{sc}^{(B)} = \frac{2m}{\hbar^2} V_0 r_0^3 \frac{\sqrt{\pi}}{4}. \tag{38}$$

From Fig. 1, it is seen that the Born approximation is good only for small values of $|V_0|$. In this work, we use the exact result and not the Born approximation. For repulsive potentials, we choose a conveniently small value of r_0 and calculate V_0 by the exact procedure.

Choosing a smaller value of r_0, V_0 increases in magnitude and the potential becomes stiffer. For very small values of r_0, $V(r_{ij})$ simulates a δ-function. For attractive interactions, we perform a model calculation with chosen values of r_0 and V_0.

C. Results

With this choice of potential we have solved the CDE Eq. (28) for various number of particles. We use oscillator units (o.u.) in which energy and length are expressed in units of oscillator energy and oscillator length ($\hbar\omega$ and $\sqrt{\hbar/m\omega}$, respectively, where ω is the circular frequency of the harmonic confining potential). The matrix element, Eq. (31), has been calculated by a multipoint Gauss-Jacobi quadrature, the number of points being decided by the condition of convergence of a typical matrix element. We first verify that our results are independent of the choice of r_0, if V_0 is appropriately calculated using two-body Schrödinger equation, so that a_{sc} has the same value (100 bohr for ^{87}Rb, which has a repulsive interaction). In a few representative calculations, the ground state energy and low lying excitation spectrum of the condensate containing A particles have been found to be stable within numerical errors, for several values of r_0 ranging from 0.1 o.u. to 0.005 o.u. As for example, the ground state energy per particle for a condensate containing $A=10$ bosons approaches a convergence as r_0 decreases from 0.1 to 0.005. Relative change in the energy per particle from r_0 =0.01 o.u. to 0.005 o.u. is only about 0.012%. As r_0 decreases, the calculation of the matrix elements as also the solution of Eq. (34) become extremely CPU time consuming. This is because for very small r_0, one has to introduce very fine r-mesh intervals (typically 10^{-5} o.u.), which increases CPU time enormously. To keep the numerical calculations manageable, we choose r_0=0.005 o.u. and V_0=3.1985 $\times 10^6$ o.u. (which corresponds to JILA ^{87}Rb experiments with a_{sc}=100 bohr and trap frequency ν=200 Hz). We next test the convergence of our results as K_{max} increases by calculating the ground state energy per particle of the condensate for V_0=3.1985$\times 10^6$ o.u. and r_0=0.005 o.u. Our results are presented in Table I. It is seen that the energy per particle converges quite rapidly as K_{max} increases. For example, for A=20, the change in energy is less than 0.001% as K_{max}

TABLE I. Calculated ground state energy per particle (in o.u.) of the condensate containing A particles for various K_{max} values, showing convergence trend as K_{max} increases ($V_0 = 3.1985 \times 10^6$ o.u. and $r_0 = 0.005$ o.u.).

K_{max}	2	4	6	8	10	12
A						
3	1.50041	1.50031	1.50026	1.50023	1.50021	1.50019
5	1.50123	1.50117	1.50112	1.50108	1.50104	1.50101
10	1.50350	1.50348	1.50346	1.50344	1.50342	1.50340
15	1.50453	1.50451	1.50450	1.50449	1.50449	
20	1.50539	1.50538	1.50537	1.50536	1.50536	
25	1.50618	1.50617	1.50617	1.50616	1.50616	
30	1.50693	1.50692	1.50692	1.50691		
35	1.50764	1.50763	1.50763	1.50766		

FIG. 3. Plot of $\omega_0(r)$ as a function of r (dotted and continuous curves together) for $A = 10$ (subcritical number) for a model attractive two-body interaction ($V_0 = -100$ o.u., $r_0 = 0.0855$ o.u.), which corresponds to $a_{sc} = -0.1176$ o.u.

increases from 2 to 10. Another interesting observation is that the ground state energy *decreases* as K_{max} increases, which is consistent with the Rayleigh-Ritz principle. Thus it is reassuring that our method is working satisfactorily and is fast converging.

However a numerical difficulty appears as the particle number (A) and K_{max} increase. The quantity α increases rapidly with A (e.g., $\alpha = 0.5$ for $A = 3$ and $\alpha = 71$ for $A = 50$), while β remains constant at $\frac{1}{2}$ (for $l = 0$). Thus the Jacobi polynomial $[P_n^{\alpha,\beta}(z)]$ as also its weight function $[w_l(z)]$ are highly asymmetric functions in the interval $[-1, 1]$ (see Ref. 24). They have tremendous variation in their values (e.g., 2^α to zero) as the argument varies from -1 to $+1$ for large A. Furthermore $w_l(z)$ increases from 0 to 2^α within a *very small interval* close to $z = -1$, for large α. In addition, $P_n^{\alpha,\beta}(z)$ has n nodes in the interval $[-1, 1]$. Hence unavoidable numerical error creeps into the numerical integration of the potential matrix, using Eq. (31). Consequently the calculated energy per particle and other physical quantities show irregularity for $A \geq 40$, as also for smaller A with large K_{max}. Therefore we have restricted A to 35. Even for $15 \leq A \leq 35$, some results for large K_{max} are not reliable. Hence these have been
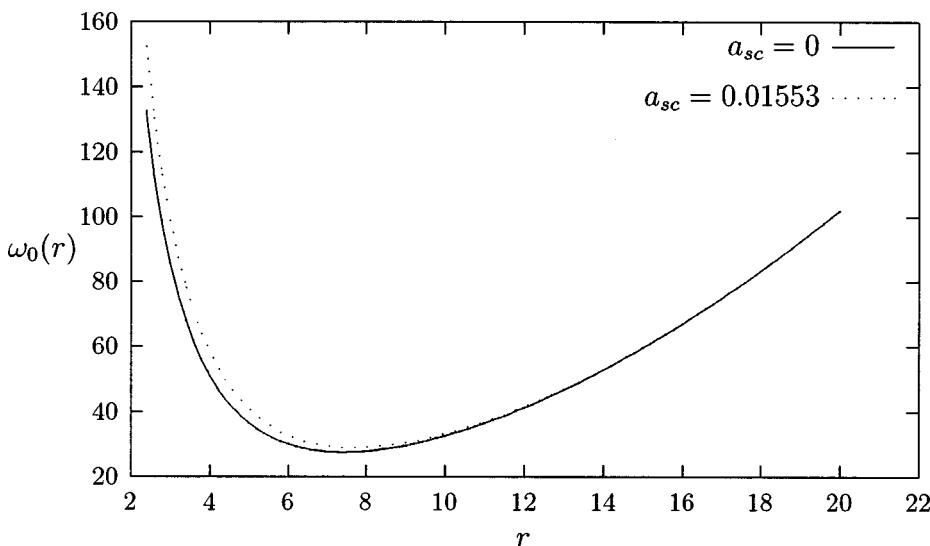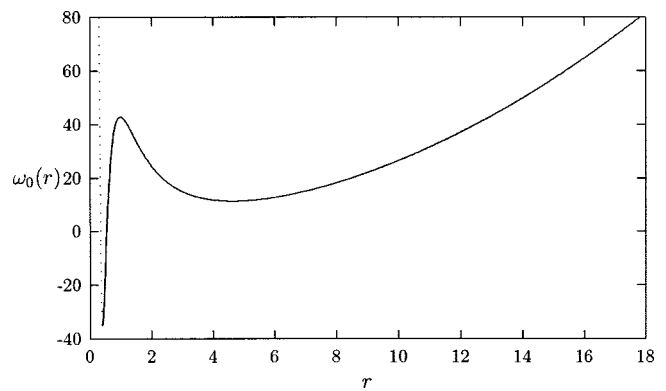
left out in Table I. In all subsequent calculations, we keep $K_{max} = 4$. We are at present trying to overcome these difficulties for large A by improved numerical techniques.

In Fig. 2, we present a plot of the lowest eigenpotential in EAA for $A = 20$, for a model repulsive interaction with $V_0 = 20$ o.u. and $r_0 = 0.1$ o.u. (dotted curve) corresponding to $a_{sc} = 0.01553$ o.u. (224.3 bohr). In the same figure, we also include the noninteracting ($V_0 = 0$, $a_{sc} = 0$) case (continuous curve), which naturally lies below the repulsive interaction ($a_{sc} > 0$) curve. In Fig. 3, we plot $\omega_0(r)$ for an attractive interaction, viz., $V_0 = -100$ o.u., $r_0 = 0.0855$ o.u. (note from Fig. 1 that this corresponds to zero two-body bound state and $a_{sc} = -0.1176$ o.u.) for $A = 10$. Since we cannot go to large values of A due to numerical problems mentioned above, we keep A small and increase V_0 to study the critical behavior (see below) at a lower value of A. Both these curves have the general features same as those found in earlier calculations using K-harmonics approximation [13]. Figure 3 shows a metastable region with a local minimum of $\omega_0(r)$, which is preceded by a collapse region for smaller r. As A increases above a critical value (A_{cr}), the metastable region disappears. This is seen in Fig. 4 for $A = 16$ for the same V_0 and r_0. These

FIG. 2. Lowest eigenpotential for $A = 20$ as a function of r. Continuous curve is for $a_{sc} = 0$ (no two-body interaction) and the dotted curve is for a repulsive interaction ($a_{sc} = 0.01553$ o.u.).
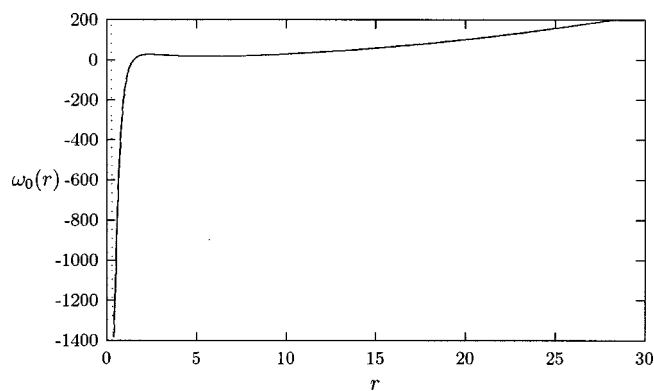
FIG. 4. Plot of $\omega_0(r)$ as a function of r (dotted and continuous curves together) for $A=16$ (critical number) for the same attractive two-body potential as in Fig. 3.

FIG. 5. Three low-lying excitation frequencies for various values of particle number (A), corresponding to the JILA experiment with ^{87}Rb atoms ($a_{sc}=100$ bohr; oscillator frequency $=200$ Hz). Energies are in oscillator units.

features are the same as reported earlier [13]. However, in our case, since $V(r)$ is finite for $r \rightarrow 0$, and the repulsive centrifugal term goes as $1/r^2$, there is no real collapse. For very small r, $\omega_0(r)$ becomes strongly repulsive even for an attractive two body interaction. This is represented by the dotted lines in Figs. 3 and 4. Note that the dotted and continuous parts together constitute the entire calculated $\omega_0(r)$ curve. The small r (repulsive) part is plotted with a different (dotted) curve to emphasize that the remaining part (continuous portion) of $\omega_0(r)$ has the same behavior as obtained with attractive contact interaction in Ref. 13. Only the dotted part differs remarkably from the corresponding part in Ref. 13. In reality for $A>A_{cr}$, there is a very narrow and deep well at a small value of r; hence all the particles will be trapped within this well. As the particles come within a small region, corresponding to a small value of r, the density of the condensate increases, and due to increased three and higher body collisions, molecule formation takes place with the disappearance of the BEC. The deep and narrow well in $\omega_0(r)$ near the origin, for an attractive two-body interaction with $A>A_{cr}$, can support a lowlying, highly localized bound state, which describes the formation of molecules. Although this is the lowest lying state in the corresponding $\omega_0(r)$, it does not represent the ground state of the condensate, which has already "collapsed." This gives a realistic scenario of what happens as A increases above A_{cr} for attractive interactions. For an attractive δ-function interaction, the lack of a rigorous solution fails to give a realistic picture and one talks of a "collapse of the condensate" in a qualitative fashion.

We next calculate first three excited states for different number of particles (A) in the condensate. These are shown in Fig. 5. Values of E_n^{ex} for $n=1,2,3$ have been represented by diamonds, pluses, and squares, respectively. The excitation energy increases slowly with A. They agree fairly well with the K-harmonic approximation [13]. In Table II, we present numerical values and notice that the excitation energies increase gradually with A.

In Fig. 6, we plot the ground state wave function, $\zeta_0(r)$, as a function of the global length r for various values of A. It is seen that as the particle number increases, the peak of $\zeta_0(r)$ shifts towards larger values of r. This is understandable, since for large A, the total repulsion of all the pairs increases
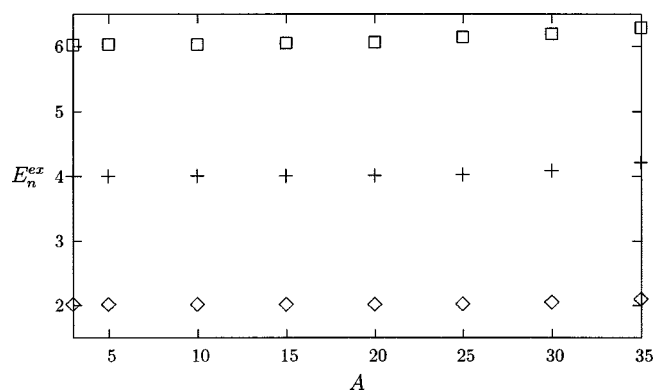
as A^2 and particles are pushed outwards, by the A-dependent hypercentrifugal repulsion in Eq. (28).

Finally we calculate and plot the ground state energy per particle $\left(E_0/A - \frac{3}{2}\hbar\omega\right)$ as a function of Aa_{sc} for selected values of A (10, 20, and 30) for a repulsive interaction in Fig. 7. Corresponding curves are from the bottom upwards respectively. We compare these with the corresponding values calculated from the GP equation. This curve is the topmost in Fig. 7. One notices that our results approach the GP result as A increases for a fixed Aa_{sc}, as expected. We also note that our energies are below those of the GP equation, indicating once again a better result from the variational point of view. Figure 7 agrees qualitatively with a similar figure of Ref. [19], where exact diagonalization of the Hamiltonian was performed for one and two dimensional condensates, respectively.

IV. CONCLUSIONS

In this paper, we have investigated the $T=0$ properties of a Bose-Einstein condensate (BEC), consisting of A atoms (bosons) trapped by an external field and interacting *via* realistic two-body interactions. An *ab initio* treatment of the Schrödinger equation involves $3(A-1)$ degrees of freedom

TABLE II. Calculated excitation energies (in o.u.) of the first three excited states for different numbers (A) of ^{87}Rb atoms (parameters as in Table I).

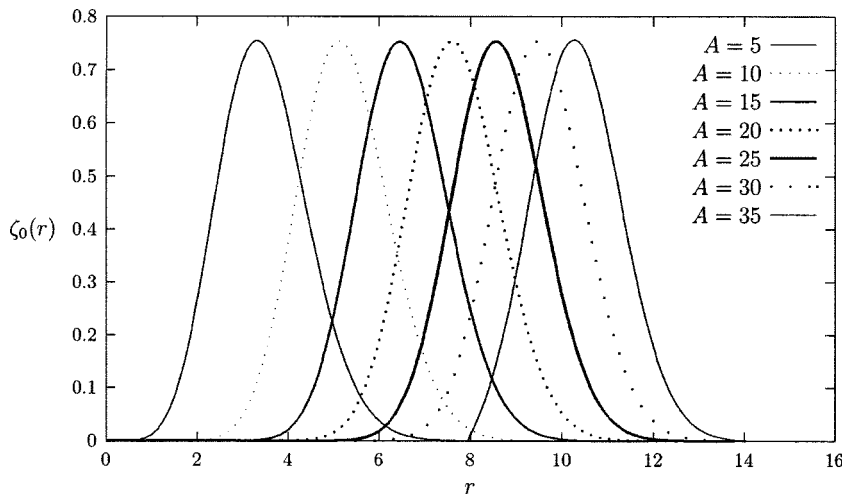| A	1st	2nd	3rd
3	2.00116	4.00283	6.00494
5	2.00130	4.00428	6.00962
10	2.00231	4.00705	6.01268
15	2.00355	4.0130	6.03147
20	2.00471	4.01647	6.04604
25	2.00671	4.03225	6.12762
30	2.03276	4.08846	6.17127
35	2.08319	4.10225	6.27118

FIG. 6. Plot of ground state wave function as a function of hyperradius (r) for various indicated values of A, in the chosen trap.

for the relative motion. Use of traditional hyperspherical harmonics expansion (HHE) method is impossible for $A > 3$, due to tremendous and mounting complexity of the method as particle number increases beyond three. We circumvent this difficulty by exploiting the subset of potential harmonics (PM) basis, instead of the full set of hyperspherical harmonics (HH) basis. The PH basis is obtained as the subset of HH needed for expanding the two-body potential for the interacting pair. The choice of PH basis corresponds to inclusion of two-body correlations and disregard of all higher-body correlations in the condensate. On the other hand, two-body correlations are very important in BEC and cannot be disregarded as in mean field theories or the GP equation. This assumption is exactly appropriate for the BEC, since for practical realization of BEC, the density of atoms must be kept so low that there are practically no three and higher body collisions. Existence of the latter type of collisions would facilitate formation of molecules and consequent depletion of the condensate. As a consequence of this assumption, *only four* active degrees of freedom of the condensate (instead of a total of $3A - 3$ degrees of freedom for the relative motion of the A particle system) are physically important—these are constituted by the global length (hyperradius, r) and the three active angle variables of the PH. In effect one *freezes* the remaining $(3A - 7)$ angle variables of PH. This leads to a tremendous simplification of the actual

numerical calculation. Since we make Faddeev like decomposition of the full wave function, an appropriate symmetrization of the wave function under exchange of the interacting pair guarantees full symmetrization. Moreover, the potential matrix elements involve integrals over *only three* angle variables, leading to an immense reduction in the complexity of the numerical procedure for A particles. Since there are no theoretical restrictions on A, this opens the possibility of an approximate, but very reliable, *ab initio* solution of the large but finite body condensate. However, a numerical difficulty arises due to the fact that the parameter α [$=(3A-8)/2$] of the Jacobi polynomials, $P_n^{\alpha,\beta}(x)$, and its associated weight function, become very large as A increases. These cause numerical problems, for $A \geqslant 40$. We are at present attempting to remove this difficulty by appropriate numerical procedure. In the present report, we restrict ourselves to $A \leqslant 35$, for which reliable calculations are possible.

We have compared our results with earlier calculations for $A = 3$ [12], K-harmonic approximation [13], exact diagonalization of the Hamiltonian in one and two dimensions [19] as also with the predictions of the GP equation [8]. As a preliminary calculation we have taken two-body Gaussian interactions of varying range. Our results agree qualitatively with the previous ones, most of which use a contact interaction. This demonstrates the reliability and feasibility of our method. Thus a reliable *ab initio* calculation for a large but
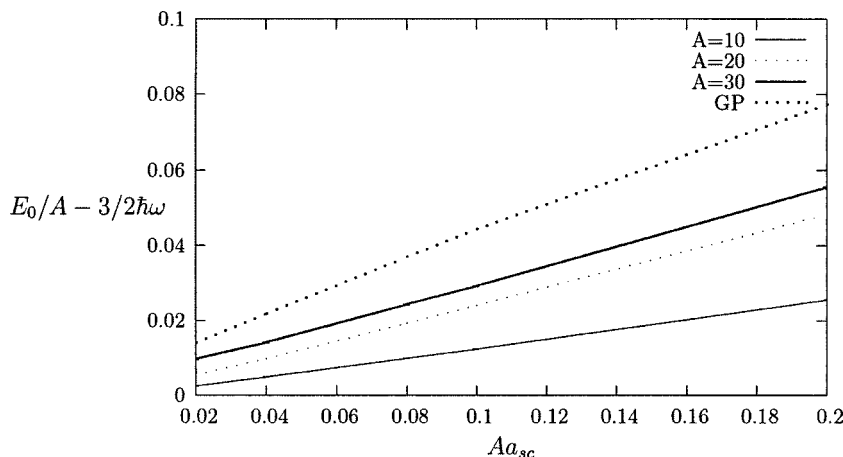

FIG. 7. Plot of ground state energy per particle ($E_0/A - 3/2\hbar\omega$) as a function of Aa_{sc} for a repulsive interaction for indicated values of A and the GP results.

finite number of atoms in a condensate, where individual particles interact via realistic two-body interactions, appears feasible. Extension of our method to a larger number of particles as also use of more realistic two-body interaction is underway.

APPENDIX: HYPERSPHERICAL VARIABLES AND HYPERSPHERICAL HARMONICS

1. Hyperspherical variables

The relative motion of the $A=(N+1)$ particle system is described in terms of N Jacobi coordinates defined by Eq. (8) and having $3N$ degrees of freedom. An equivalent set of hyperspherical variables is constituted by the hyperradius (r) defined by Eq. (11), $2N$ spherical polar angles of $\vec{\zeta}_1, \vec{\zeta}_2 \ldots \ldots, \vec{\zeta}_N$ and ($N-1$) hyperangles $\{\phi_2, \phi_3, \ldots, \phi_N\}$ giving the length of the Jacobi vectors $\vec{\zeta}_1, \vec{\zeta}_2 \ldots \ldots, \vec{\zeta}_N$, through

$$\zeta_N = r \cos \phi_N,$$

$$\zeta_{N-1} = r \sin \phi_N \cos \phi_{N-1},$$

$$\zeta_{N-2} = r \sin \phi_N \sin \phi_{N-1} \cos \phi_{N-2},$$

$$\vdots$$

$$\zeta_2 = r \sin \phi_N \sin \phi_{N-1} \ldots . \sin \phi_3 \cos \phi_2,$$

$$\zeta_1 = r \sin \phi_N \sin \phi_{N-1} \ldots . \sin \phi_3 \sin \phi_2,$$

$$(\phi_1 = 0). \tag{A1}$$

Equation (A1) automatically satisfies Eq. (11).

2. Grand orbital operator

The general grand orbital operator, $L^2(\Omega_N)$ of Eq. (15) is defined through [14]

$$L_i^2(\Omega_i) = \frac{\partial^2}{\partial \phi_i^2} + [3(i-2)\cot \phi_i + 2(\cot \phi_i - \tan \phi_i)]\frac{\partial}{\partial \phi_i}$$

$$+ \frac{l^2(\omega_i)}{\cos^2 \phi_i} + \frac{L_{i-1}^2(\Omega_{i-1})}{\sin^2 \phi_i}$$

$$= 4(1 - z_i^2)\frac{\partial^2}{\partial z_i^2} + 6[2 - i(1 + z_i)]\frac{\partial}{\partial z_i} + 2\frac{l^2(\omega_i)}{1 + z_i}$$

$$+ 2\frac{L_{i-1}^2(\Omega_{i-1})}{1 - z_i} \quad (i = 2, \ldots, N), \tag{A2}$$

where $z_i = \cos 2\phi_i$, ω_i represents the set of two polar angles of $\vec{\zeta}_i$ and ϕ_i's are given by Eq. (A1). Note that $L_1^2(\Omega_1) = l^2(\omega_1)$ and $L_N^2(\Omega_N) \equiv L^2(\Omega_N)$ appear in Eq. (15).

3. Hyperspherical harmonics

An eigenfunction of $L^2(\Omega_N)$ is called hyperspherical harmonics (HH) and is given (without angular momentum coupling) by [34]

$$Y_{[\mathcal{L}]}(\Omega_N) = Y_{l_1 m_1}(\omega_1)\prod_{j=2}^{N} Y_{l_j m_j}(\omega_j)^{(j)}P_{\mathcal{L}_j}^{l_j, \mathcal{L}_{j-1}}(\phi_j), \tag{A3}$$

where

$$^{(j)}P_{\mathcal{L}_j}^{l_j, \mathcal{L}_{j-1}}(\phi_j) = \left\{ \frac{2\nu_j\Gamma(\nu_j - n_j)\Gamma(n_j + 1)}{\Gamma\left(\nu_j - n_j - l_j - \frac{1}{2}\right)\Gamma\left(n_j + l_j + \frac{3}{2}\right)} \right\}^{1/2}$$

$$\times (\cos \phi_j)^{l_j}(\sin \phi_j)^{\mathcal{L}_{j-1}}P_{n_j}^{\nu_{j-1}, l_j + 1/2}(\cos 2\phi_j)$$

$$(j = 2, 3, \ldots, N), \tag{A4}$$

with

$$\nu_j = \nu_{j-1} + 2n_j + l_j + \frac{3}{2}$$

$$= \mathcal{L}_j + \frac{3j}{2} - 1$$

$$= \mathcal{L}_{j-1} + 2n_j + l_j + \frac{3j}{2} - 1 \quad (j = 2, 3, \ldots, N). \tag{A5}$$

In Eq. (A4) $P_n^{\alpha, \beta}(x)$ is a Jacobi polynomial. In Eq. (A3), $[\mathcal{L}]$ represents the set of quantum numbers $\{(l_1, m_1), (l_2, m_2), \ldots, (l_N, m_N), n_2, n_3, \ldots, n_N\}$ for a fixed value of grand orbital quantum number $\mathcal{L} = \mathcal{L}_N$. The quantum number $\mathcal{L}_i$ is defined through

$$\mathcal{L}_i = \mathcal{L}_{i-1} + 2n_i + l_i, \tag{A6}$$

with $\mathcal{L}_1 = l_1$. Hence

$$\mathcal{L} \equiv \mathcal{L}_N = l_1 + \sum_{j=2}^{N} (2n_j + l_j). \tag{A7}$$

The HH of Eq. (A3) forms the uncoupled basis. For systems with a good orbital angular momentum $\vec{L} = \vec{l}_1 + \vec{l}_2 + \cdots + \vec{l}_N$, one has to couple the individual orbital angular momenta—then the projection quantum numbers $m_1, m_2, \ldots, m_N$ are replaced by the ($N-1$) intermediately coupled angular momenta and the projection M of $\vec{L}$.

The potential harmonics (PH) given by Eq. (17) corresponds to $l_N = l$, $l_1 = l_2 = l_3 = \cdots = l_{N-1} = 0$, such that $L = l_N = l$, $M = m_N = m$ and grand orbital $\mathcal{L} \equiv \mathcal{L}_N = 2K + l$ with $n_2 = n_3 = \cdots = n_{N-1} = 0$ and $K = n_N$. Substitution of these in Eqs. (A3)–(A5) gives the PH of Eq. (17).

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