

Quality of potential harmonics expansion method for dilute Bose–Einstein condensate

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Abstract. We present and examine an approximate but *ab initio* many-body approach, viz., potential harmonics expansion method (PHEM), which includes two-body correlations for dilute Bose–Einstein condensates. Comparing the total ground state energy for three trapped interacting bosons calculated in PHEM with the exact energy, the new method is shown to be very good in the low density limit which is necessary for achieving Bose–Einstein condensation experimentally.

Keywords. Bose–Einstein condensation; hyperspherical harmonics method; potential harmonics.

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1. Introduction

Bose–Einstein condensation (BEC) was first experimentally achieved in the year 1995 in supercooled dilute alkali atomic vapours [1–3]. This was considered as a milestone in physics and since then tackling it theoretically [4–6] is a challenging problem. Gröss–Pitaevskii (GP) equation of mean field theory is generally considered as a good starting point, where individual atoms lose their identity and the whole condensate is described by a single wave function [4]. The success of the mean field theory in very dilute regime where the effect of correlation is negligible is quite satisfactory. But in recent experiments using Feshbach resonance one can change the effective interaction to any desired value simply by tuning the external field. It implies the possibility of BEC even in strongly interacting systems. The use of GP equation is questionable in such dense systems as it cannot take into account the effect of atomic correlations. Naturally, a many-body approach becomes essential. Some useful attempts have already been taken in this direction. In our recent publications [7,8] we proposed a nice treatment called potential harmonics expansion method (PHEM) for dilute trapped bosons. The PHEM has already been proved

as a nice and economical way which can successfully reproduce the static and thermodynamic properties of ^{87}Rb and ^{23}Na condensate [7,8]. In the present work, we are interested in studying the success of PHEM over a broad region – from dilute to dense condensates. Comparing with the hyperspherical harmonics expansion method (HHEM), which is basically exact and includes all types of correlations, we investigate the condition for the applicability of our new approach. Since exact HHEM, without approximations, is practicable only for three particles, we compare PHEM with HHEM for a condensate containing three atoms. The agreement is quite good over a wide range of scattering length corresponding to dilute to dense condensates. In §2, we briefly describe the potential harmonics expansion method. Section 3 presents the comparison between PHEM and HHEM for three particles whereas §4 explains the numerical results. Section 5 draws the conclusion.

2. Potential harmonics expansion method for trapped interacting bosons

The relative motion of A interacting bosons trapped in a spherically symmetric confining potential is described by N ($=A - 1$) Jacobi coordinates $\vec{\zeta}_i$ in many-body hyperspherical approach. For hyperspherical variables, one replaces the $3N$ coordinates by hyperradius r and a set of $(3N - 1)$ hyperangles Ω_N [9]. The Schrödinger equation for relative motion then takes the form

$$\left[-\frac{\hbar^2}{m} \left\{ \frac{1}{r^\nu} \frac{\partial}{\partial r} \left(r^\nu \frac{\partial}{\partial r} \right) - \frac{\hat{K}^2(\Omega_N)}{r^2} \right\} + \sum_{i>j=1}^A V_{ij} + \frac{1}{4} m \omega^2 r^2 - E_{\text{rel}} \right] \psi(r, \Omega_N) = 0, \quad (1)$$

where $\nu = 3N - 1$ and $\hat{K}^2(\Omega_N)$ is the hyperangular momentum operator in the $(3N - 1)$ -dimensional hyperangular space. The complete expression can be found in ref. [9]. Next, by expanding the total wave function $\psi(r, \Omega_N)$ in the complete set of hyperspherical harmonics (HH) $\mathcal{Y}_{K\alpha}(\Omega_N)$ (which are the eigenfunctions of $\hat{K}^2(\Omega_N)$) one gets a set of coupled differential equations (CDE) [9]

$$\left[-\frac{\hbar^2}{m} \frac{d^2}{dr^2} + \frac{\hbar^2}{m} \frac{K(K + 3N - 2)}{r^2} + \frac{1}{4} m \omega^2 r^2 - E_{\text{rel}} \right] u_{[K]}(r) + \frac{A(A - 1)}{2} \sum_{[K']} \langle \mathcal{Y}_{[K]}^{(s)}(\Omega_N) | V_{12} | \mathcal{Y}_{[K']}^{(s)}(\Omega_N) \rangle u_{[K']}(r) = 0, \quad (2)$$

where V_{12} stands for (1–2) pair interaction and $\mathcal{Y}_{[K]}^{(s)}(\Omega_N)$ is the totally symmetric HH basis element, which is symmetric under any pair exchange. Till now there is no approximation and thus this is considered as an exact *ab initio* many-body tool. But in reality its application is severely restricted to $A = 3$ due to extreme complexity in the symmetrization of the HH basis and the calculation of the matrix element. Under permutation of the particle indices, N Jacobi vectors get mixed up

into another set of N Jacobi vectors. The simplest permutation P_{12} changes only $\vec{\zeta}_1$ to $-\vec{\zeta}_1$ and thus introduces a factor $(-1)^{l_1}$. But the effect of general P_{ij} is very complicated and in practice it is almost impossible to do the calculations.

Here PHEM offers an approximate but greatly simplified approach which is very appropriate to the experimentally achieved dilute BEC. In the dilute regime, as only two-body interaction is physically relevant and the effect of three- and higher-body correlation is absent, instead of taking full HH basis, which includes all $(3N - 1)$ angular variables, we can choose a subset of HH, whose members depend only on the interacting pair separation and a global length. Naturally the number of hyperspherical variables will be drastically reduced to just four – one is hyperradius r and the other three are related with the Jacobi vector chosen as the separation vector of the interacting pair. This new basis set is called potential harmonics (PH) basis, since it is the necessary and sufficient basis set for the expansion of the potential of the interacting pair. The PH basis has the form [10]

$$\mathcal{P}_{K=2n+l}^{l,m}(\Omega_{ij}) \equiv \mathcal{Y}_{[K]}(\Omega_N) = Y_{lm}(\omega_{ij}) \binom{N}{2n+l} P_{2n+l}^{l,0}(\phi) \mathcal{Y}_0(3N - 3), \quad (3)$$

where $\mathcal{Y}_0(3N - 3)$ is the HH of order zero in $3(N - 1)$ -dimensional space [7], $Y_{lm}(\omega_{ij})$ is the spherical harmonics and $\binom{N}{2n+l} P_{2n+l}^{l,0}$ is a function involving Jacobi polynomial. Thus for our new basis, the active variables are $\{r, \vec{r}_{ij}\}$ and PH basis is independent of all hyperspherical variables associated with $(N - 1)$ Jacobi vectors. Let us decompose the full A -body wave function in Faddeev components

$$\psi(r, \Omega_{3N}) = \sum_{i,j>i}^A \Phi_{ij}(r, \vec{r}_{ij}). \quad (4)$$

Naturally ψ will be totally symmetric under any pair exchange if Φ_{ij} is required to be symmetric under $i \leftrightarrow j$. Thus the relative motion for trapped interacting bosons can be written in Faddeev component as [7]

$$\left(T + \frac{1}{4} m \omega^2 r^2 - E_{\text{rel}} \right) \Phi_{ij}(r, \vec{r}_{ij}) = -V(\vec{r}_{ij}) \sum_{k,l}^A \Phi_{kl}(r, \vec{r}_{kl}). \quad (5)$$

As now Φ_{ij} is simply the function of r and \vec{r}_{ij} we expand Φ_{ij} in the complete set of PH basis, eq. (3), which results in the set of CDE [7]

$$\left[-\frac{\hbar^2}{m} \frac{d^2}{dr^2} + \frac{\hbar^2}{m} \frac{\mathcal{L}_n(\mathcal{L}_n + 1)}{r^2} + \frac{1}{4} m \omega^2 r^2 - E_{\text{rel}} \right] u_{nl}(r) + \sum_{n'} f_{n'l}^2 V_{nn'}(r) u_{n'l}(r) = 0, \quad (6)$$

where the interaction matrix has the form

$$V_{nn'}(r) = (h_n^{\alpha\beta} h_{n'}^{\alpha\beta})^{-1/2} \int \mathcal{P}_{2n+l}^{l,m}(\Omega_{ij}) V(r_{ij}) \mathcal{P}_{2n'+l}^{l,m}(\Omega_{ij}) d\Omega_{ij}. \quad (7)$$

3. Comparison of PHEM with HHEM for three trapped interacting bosons

The density of alkali atomic vapours in actual experimental condition is extremely low, the interatomic distance is much larger than the atomic scattering length a_{sc} , which characterizes the strength of two-body interaction. For experimental condensate of ^{87}Rb , $a_{sc} \simeq 100$ Bohr, na_{sc}^3 for this system $\simeq 2.5 \times 10^{-4} \ll 1$, n being the particle density. This extreme diluteness of the condensate is ideally suitable for the choice of potential harmonics basis. The success of PHEM has already been established particularly for ^{87}Rb condensate [7]. But recent interest is to achieve BEC even in high density Tango–Bose gas. So the application of PHEM in a wide range of density is essential and a comparison with HHEM result will show the effect of higher-body correlations. As HHEM becomes unmanageable for more than the three-body system, for the present comparative calculations we fixed $A = 3$.

For the two-body interaction, we choose a simple Gaussian of depth V_0 and range r_0

$$V(r_{ij}) = V_0 e^{-r_{ij}^2/r_0^2}. \quad (8)$$

The choice of this potential already gives very accurate results in our previous calculations [7,8]. With adjustable parameters V_0 and r_0 (provided $r_0 \ll a_{sc}$) we solve the two-body Schrödinger equation for positive energy in the zero energy limit such that it reproduces the desired scattering length. We choose $\sqrt{\hbar/m\omega}$ as the unit of length in oscillator unit (o.u.) and $\hbar\omega$ as the unit of energy in o.u. We choose the trap frequency $\omega = 150$ Hz. Keeping the frequency fixed, we increase the strength of the two-body interaction simply by increasing a_{sc} and compare the PHEM results with exact HHEM result.

For the three-body system, the two Jacobi vectors $\vec{\zeta}_1$ and $\vec{\zeta}_2$ are given in terms of hyperradius r and hyperspherical angle ϕ as

$$\begin{aligned} \zeta_2 &= r \cos \phi, \\ \zeta_1 &= r \sin \phi. \end{aligned} \quad (9)$$

Restricting to the system with orbital angular momentum $L = 0$ ($l_2 = l_1$) and $M = 0$, the hyperspherical harmonics for a three-body system in the coupled basis is given by [9]

$$\begin{aligned} \mathcal{Y}_{[K]}(\Omega_2) &= {}^{(2)}P_K^{l_1 l_1}(\phi) [Y_{l_1 m_1}(\hat{\zeta}_1) Y_{l_1 - m_1}(\hat{\zeta}_2)]_{00} \\ &= {}^{(2)}P_K^{l_1 l_1}(\phi) \sum_{m_1} \langle l_1 m_1 l_1 - m_1 | 00 \rangle Y_{l_1 m_1}(\hat{\zeta}_1) Y_{l_1 - m_1}(\hat{\zeta}_2), \end{aligned} \quad (10)$$

where $[K]$ represents the set of five quantum numbers (which are $K, l_1, l_1, 0, 0$) in coupled angular momentum representation. Now $\mathcal{Y}_{[K]}(\Omega)$ must be totally symmetric under any pair exchange. This is done by introducing a three-dimensional vector

$$\vec{Z}(\eta) = \vec{\zeta}_1 \sin \eta + \vec{\zeta}_2 \cos \eta, \quad (11)$$

Table 1. Comparison of the calculated total ground state energy (in o.u.) of three trapped bosons interacting via two-body interactions represented by the s-wave scattering length (a_{sc}) given in o.u.

a_{sc} (o.u.)	Total energy of the system	
	by PHEM	by exact HHEM
0.001	4.500808	4.501048
0.003	4.502884	4.503772
0.005	4.505898	4.507802
0.007	4.510536	4.514174
0.009	4.518120	4.525052
0.010	4.523730	4.533476
0.012	4.540864	4.561268
0.014	4.569738	4.615784
0.016	4.614026	4.721060
0.018	4.673294	4.909786
0.020	4.742576	5.198074

where η is a parameter. As $\vec{\zeta}_1 = \vec{x}_2 - \vec{x}_1$ and $\vec{\zeta}_2 = \sqrt{3}(\vec{x}_3 - \vec{X})$ [9], where \vec{x}_i is the position vector of the i th particle ($i = 1, 2, 3$) and \vec{X} is the center of mass coordinate, it can be easily shown that for $\eta = \frac{\pi}{2}, \frac{\pi}{2} - \frac{2\pi}{3}$ and $\frac{\pi}{2} + \frac{2\pi}{3}$, $\vec{Z}(\eta)$ becomes $(\vec{x}_2 - \vec{x}_1)$, $(\vec{x}_3 - \vec{x}_2)$ and $(\vec{x}_1 - \vec{x}_3)$ respectively [9]. Thus three specific values of η correspond to three cyclic permutations of the particle indices. Thus $\mathcal{Y}_{[K]}^{(s)}(\Omega) = \sum_c \mathcal{Y}_{[K]}(\Omega, \eta)$, where \sum_c represents a cyclic sum, is a totally symmetric basis function. Such HH basis states for two different partitions of the particle indices are connected by a unitary transformation

$$\mathcal{Y}_{Kl_1l_2LM}(\Omega_2, \eta) = \sum_{l'_1l'_2} \langle l'_1l'_2|l_1l_2 \rangle_{KL}^{(\eta)} \mathcal{Y}_{Kl'_1l'_2LM}(\Omega), \quad (12)$$

where $\langle l'_1l'_2|l_1l_2 \rangle_{KL}^{(\eta)}$ is the Raynal–Revai coefficient [11] associated with a particular partition (η) . The symmetrized HH basis set is given by

$$\mathcal{Y}_{Kl_1l_2LM}^{(s)}(\Omega) = \mathcal{N}_{Kl_1l_2} \sum_{l'_1l'_2} \left(\sum_c \langle l'_1l'_2|l_1l_2 \rangle_{KL}^{\eta} \right) \mathcal{Y}_{Kl'_1l'_2LM}(\Omega), \quad (13)$$

where $\mathcal{N}_{Kl_1l_2}$ is a normalization constant. Next we calculate the potential matrix element with this symmetrized basis. After truncating the K value to a maximum K_{\max} we solve the set of coupled differential equations, eq. (2), by renormalized Numerov algorithm [12]. The results are compared with those of eq. (6) obtained by PHEM.

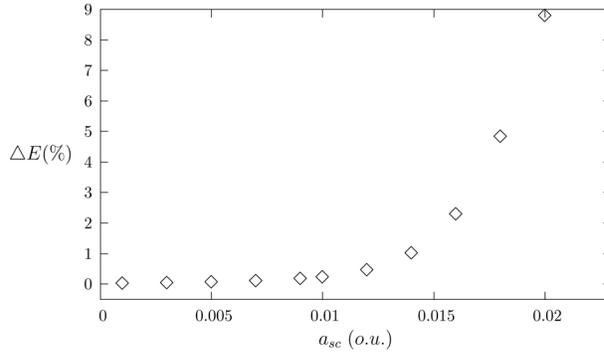


Figure 1. The percentage error (ΔE) of the calculated energies by PHEM, as a function of the scattering length.

4. Numerical results

The PHEM equation (eq. (6)) is solved by extreme adiabatic approximation [13], which gives slight overbinding. Our results of PHEM and HHEM are presented in table 1 for various values of a_{sc} . Energies by PHEM are lower than the exact ones, as expected. For smaller values of a_{sc} (0.001 o.u.–0.007 o.u.) the agreement between PHEM and HHEM results is very good. The difference starts to increase with increased value of a_{sc} . The value of a_{sc} for ^{87}Rb condensate is 0.00433 o.u. which belongs to the above limit. The percentage error of the calculated energies (ΔE) is shown in figure 1 as a function of interaction strength a_{sc} . Next we calculate the correlation energy. Although the correlation energy is rigorously defined as the energy difference between the configuration interaction energy and the Hartree–Fock energy in quantum chemistry, in many-body BEC it is simply the difference of the exact many-body energy (which includes correlations) and the GP energy which considers no correlation. We define a correlation fraction (C) as the difference of PHEM (or HHEM) energy and GP energy divided by the former. We present C for different values of $a_{sc} < 0.01$ in table 2, and the agreement is extremely good. Note that HHEM includes both two- and three-body correlations, whereas PHEM includes only two-body correlation. As the correlation fraction calculated from PHEM is very close to that calculated in HHEM, we can conclude that in the dilute system only the effect of two-body correlation is relevant and one can safely ignore the effect of three-body correlation. So our new approach would be considered as a nice complement of HHEM.

5. Conclusions

In this paper, we have reviewed the general hyperspherical harmonics expansion procedure for a A -body system and found that its practical application for $A > 3$ is very difficult and the difficulty increases immensely as A increases. On the other hand, for a dilute and confined A -body system, the method can be greatly simplified by disregarding the higher than two-body correlations, resulting in the

Table 2. Correlation fraction by PHEM and HHEM for different a_{sc} .

a_{sc} (o.u.)	$C(\text{PHEM})$	$C(\text{HHEM})$
0.001	0.0000377	0.0000155
0.003	0.001745	0.001547
0.005	0.002646	0.002222
0.007	0.003119	0.002311
0.009	0.005953	0.004412

potential harmonic expansion method. The PHEM in principle can be used for any finite A . It appears to be an ideal tool for the Bose–Einstein condensation of a small number of trapped bosons in dilute regime. However, one has to ascertain the contributions of the disregarded higher than two-body correlations. Since the HHEM is practically manageable for $A = 3$ only, we considered a system of three trapped, interacting bosons and compared the two results for various values of s-wave scattering length of the two-body interaction. We find that the PHEM compares very well with the exact results for the range of a_{sc} usually encountered in the BEC experiments. Thus our calculation suggests that the neglect of three-body correlation is justified in the dilute limit, as in the case of a typical BEC.

The potential harmonics has a particularly simple expression. The Faddeev decomposition of the total wave function together with restricting l values of $\mathcal{P}_{K=2n+l}^{lm}(\Omega_{ij})$ to even integers, guarantee that the wave function is totally symmetric under any pair exchange. Thus the symmetrization, which was a major stumbling block in HHEM, is tremendously simplified in the PHEM. Finally calculation of the matrix element also simplifies to a single one-dimensional integral for a central potential. The restrictive assumption for the PHEM is that the system should be very dilute – this is manifestly true for the experimentally achieved BEC. Thus the PHEM is an ideal and very handy tool for the investigation of BEC.

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