

# Use of correlated potential harmonic basis functions for the description of the ${}^4\text{He}$ trimer and small clusters

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A correlated many-body basis function is used to describe the  ${}^4\text{He}$  trimer and small helium clusters ( ${}^4\text{He}_N$ ) with  $N = 4-9$ . A realistic helium dimer potential is adopted. The ground state results of the  ${}^4\text{He}$  dimer and trimer are in close agreement with earlier findings. But no evidence is found for the existence of Efimov state in the trimer for the actual  ${}^4\text{He}$ - ${}^4\text{He}$  interaction. However, decreasing the potential strength we calculate several excited states of the trimer which exhibit Efimov character. We also solve for excited state energies of these clusters which are in good agreement with Monte Carlo hyperspherical description. © 2011 American Institute of Physics. [doi:10.1063/1.3583365]

## I. INTRODUCTION

Three-body atomic systems are of great interest due to the possibility of finding Efimov states. Out of them, the helium trimer has drawn particular interest for more than one decade. Although,  ${}^4\text{He}_3$  looks a very simple system, the question of whether it supports or not a bound state is a long term question. In 1970, Efimov proposed that if two spin zero neutral bosons interact resonantly then the addition of a third identical particle leads to the appearance of an infinite number of bound levels.<sup>1,2</sup> This is related to the divergence of the  $s$ -wave scattering length ( $a_s$ ). As the two-body scattering length  $|a_s|$  greatly exceeds the range of the two-body interactions, the scattering length characterizes the dynamics of the whole system showing universal behaviour. Efimov states are highly exotic as they result when there is a zero or near-zero energy two-body bound state. Although halo states (which are very weakly bound three-body states, which have no bound two-body subsystem) are quite familiar in nuclear systems, there is no clear example of Efimov states in any naturally occurring system. Efimov states will also not exist in atomic systems due to the long-range Coulomb interaction; but they may exist in systems of spinless neutral atoms.

Although the Efimov physics was formulated in 1970,<sup>1-3</sup> only very recently, experimental evidence of Efimov states in ultracold caesium and potassium trimers have been reported.<sup>4</sup> In such ultracold atoms in a magnetic field, the two-body interaction is tunable using Feshbach resonances and the conditions necessary for the existence of Efimov states can be tailor made to be valid. However, no evidence of Efimov states in naturally occurring trimer systems have so far been reported. As observed by several authors,  ${}^4\text{He}_3$  is the most promising system in this category, as the  ${}^4\text{He}$  dimer has only one very weakly bound state ( $E_0 \sim 1$  mK), whose binding energy is extremely small on the molecular scale. Because of

such weak binding it was difficult to detect it earlier. The  ${}^4\text{He}$  dimer has been observed experimentally by Luo *et al.*<sup>5,6</sup> In subsequent experiments Schöllkopf and Toennies<sup>7,8</sup> were able to determine helium trimer and tetramer. But no experiment verifies Efimov states in helium trimer. Theoretically, the main difficulties arise from the fact that the number of Efimov states is highly sensitive to the binding energy of the dimer and even a 1% decrease of the strength of two-body interaction makes the system unbound. He-dimer potential is also not uniquely known. However, several sophisticated helium dimer interaction potentials have been developed. The review of Janzen and Aziz<sup>9</sup> presented several potential curves of He-He potential. Some *ab initio* and widely used He-He potentials are LM2M2,<sup>10</sup> Tang, Tonnies, and Yiu (TTY),<sup>11</sup> and HFD-HE2 (Ref. 12) potentials, which are widely used in He-cluster calculations. All these interactions support only a single bound state of  ${}^4\text{He}$  dimer. The  ${}^4\text{He}$ - ${}^4\text{He}$  scattering length is of the order of few tens of Bohr radius which is very large compared to the range of two-body interaction potentials. The limit of large scattering length corresponds to near zero two-body binding energy. The corresponding three-body system will have an infinite series of bound states called Efimov states. Both the ground and the excited states (which has been claimed by some authors as an Efimov state) have been well studied in Refs. 13-29. But experimentally  ${}^4\text{He}$  trimer has been observed in its ground state only and no experiment has been able to see the excited state.<sup>7,30</sup>

Our present work mainly concerns the spectrum of the helium trimer and small  ${}^4\text{He}$  clusters. It is along the same line of earlier investigations but using a different basis function. As the Efimov state is highly elusive, very small uncertainties in the helium dimer interaction may lead to different conclusions. Since,  ${}^4\text{He}$  systems are strongly correlated due to high  ${}^4\text{He}$ - ${}^4\text{He}$  repulsion at short separation, the effect of interatomic correlation must be taken properly into account. Although different approaches have been taken in earlier works to calculate ground state properties, the calculations of excited states are limited. The main difficulty comes from the very time consuming computations with increase of the

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number of particles, especially because of the very slow rate of convergence for such a weakly bound system.

In the present communication we use the set of correlated basis functions, called potential harmonics (PH) basis,<sup>31</sup> which is a subset of the complete hyperspherical harmonics (HH) basis. This subset incorporates long-range two-body correlations and its choice would have been adequate for taking care of full two-body correlations, provided sufficient number of PH basis functions (leading to convergence of the wave function in the entire interval) were taken. However, due to very strong two-body repulsion at very short separations (arising from the nucleus-nucleus repulsive core of the  ${}^4\text{He}$ - ${}^4\text{He}$  potential), the  $(ij)$ -interacting pair Faddeev component becomes vanishingly small for  $r_{ij} \rightarrow 0$  (where  $r_{ij}$  is the  $(ij)$ -pair separation). Since the leading members of the PH basis are non-vanishing for  $r_{ij} \rightarrow 0$ ,<sup>31</sup> the rate of convergence of the PH expansion is very slow. This has been observed in our numerical calculations. To improve the rate of convergence we multiply the PH basis with a suitable short-range correlation function, which ensures that the probability of interaction of two atoms at distances  $r < r_c$  is very small, where  $r_c$  is the radius of the short-range repulsive core. This short-range correlation function reproduces the correct short-range behaviour of the dimer wave function and is obtained by solving the two-body Schrödinger equation with the chosen two-body potential, in the appropriate energy limit. However, inclusion of this short-range correlation function makes the PH basis non-orthogonal, treatment of which is discussed in Sec. II.

The binding energies of light  ${}^4\text{He}_N$  clusters (with  $N$  small) are quite small, compared with the molecular energy scale. Hence, such systems are very weakly bound and extended spatially, the average  ${}^4\text{He}$ - ${}^4\text{He}$  separation being large. Therefore, one expects that three- and higher-body correlations, as also three-body forces are negligible. This justifies *a priori* our choice of the PH basis. However as  $N$  increases, the net pairwise attraction increases as  $N(N-1)/2$ . Consequently, for large  $N$ , the average inter-particle separation decreases and higher-body correlations are no more negligible. For still larger  $N$ , three-body (and even higher-body) forces come into play, making a solution of the many-body problem a nearly impossible task.

Our purpose is then twofold. Firstly to apply the correlated basis functions to describe correlated  ${}^4\text{He}$  systems. We thus investigate how accurately the two-body correlated basis sets will reproduce the observed spectrum of the  ${}^4\text{He}$  trimer which naturally addresses the question of the applicability of the correlated PH basis for diffuse He cluster. Secondly to reconsider the question of the existence of Efimov states in the  ${}^4\text{He}$  trimer, in view of the recent experimental finding which gives negative result for the existence of Efimov trimers.<sup>30</sup>

In addition, we also investigate how far we can use the simple PH basis, as  $N$  increases. We find that this is possible up to  $N = 9$ . We also investigate the excited states as a function of cluster size with up to  $N = 9$   ${}^4\text{He}$  atoms.

Section II deals with the methodology which uses correlated PH basis. Section III presents the results and discussions. Section IV contains our main conclusions.

## II. CORRELATED PH BASIS

The Hamiltonian for a system of  $(N+1)$  atoms (each of mass  $m$ ) and interacting via two-body potential has the form,

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N+1} \nabla_i^2 + \sum_{i>j=1}^{N+1} V(\vec{x}_i - \vec{x}_j), \quad (1)$$

where  $V(\vec{x}_i - \vec{x}_j) = V(\vec{r}_{ij})$  is the He-He two-body potential described later. We use the standard Jacobi coordinates defined as  $\vec{\zeta}_i = (\frac{2i}{i+1})^{\frac{1}{2}} [\vec{x}_{i+1} - \frac{1}{i} \sum_{j=1}^i \vec{x}_j]$ , ( $i = 1, 2, \dots, N$ ) and the center of mass through  $\vec{R} = \frac{1}{N+1} \sum_{i=1}^{N+1} \vec{x}_i$ . Then the relative motion of the atoms is described in terms of  $N$  Jacobi vectors  $(\vec{\zeta}_1, \dots, \vec{\zeta}_N)$  as<sup>31</sup>

$$\left[ -\frac{\hbar^2}{m} \sum_{i=1}^N \nabla_{\zeta_i}^2 + V(\vec{\zeta}_1, \dots, \vec{\zeta}_N) - E \right] \Psi(\vec{\zeta}_1, \dots, \vec{\zeta}_N) = 0. \quad (2)$$

As the  ${}^4\text{He}$  atoms are spinless bosons, we decompose  $\Psi$  in Faddeev components,

$$\Psi(\vec{x}) = \sum_{ij>i}^{N+1} \psi_{ij}(\vec{x}). \quad (3)$$

As explained earlier, due to large spatial extent of the  ${}^4\text{He}$  clusters, only two-body correlations are important. Hence  $\psi_{ij}$  is a function of two-body separation vector only, besides the global length (hyperradius, see below). Here,  $\psi_{ij}$  (symmetric under  $P_{ij}$ ) satisfy the Schrödinger equation,

$$(T - E)\psi_{ij}(\vec{x}) = -V(\vec{r}_{ij}) \sum_{k,l>k} \psi_{kl}(\vec{x}), \quad (4)$$

where  $T$  being the total kinetic energy; operating  $\sum_{i,j>i}$  on both sides of Eq. (4) we get back the original Schrödinger equation. The hyperradius is defined as  $r = \sqrt{\sum_{i=1}^N \zeta_i^2}$ . The hyperradius and  $(3N-1)$  hyperangles (denoted by  $\Omega_N$ ) together constitute  $3N$  hyperspherical variables. The choice of Jacobi coordinates is not fixed as the labeling of the particle indices is arbitrary. We choose a particular set for the  $(ij)$  interacting pair, called the  $(ij)$ -partition, by taking  $\vec{r}_{ij}$  as  $\vec{\zeta}_N$ , and  $(\vartheta, \phi)$  are two spherical polar angles of the separation vector  $\vec{r}_{ij}$ . The angle  $\phi$  is defined through  $r_{ij} = r \cos \phi$ . For the remaining  $(N-1)$  Jacobi coordinates we define the hyperradius for the partition  $(ij)$  as  $\rho_{ij} = [\sum_{k=1}^{N-1} \zeta_k^2]^{\frac{1}{2}}$  such that  $\rho_{ij}^2 + r_{ij}^2 = r^2$  and  $\rho_{ij} = r \sin \phi$ . With this choice, the hyperspherical coordinates are

$$(r, \Omega_N) = (r, \phi, \vartheta, \phi, \Omega_{N-1}), \quad (5)$$

where  $\Omega_{N-1}$  involves  $(3N-4)$  variables:  $2(N-1)$  polar angles associated with  $(N-1)$  Jacobi vectors  $\vec{\zeta}_1, \dots, \vec{\zeta}_{N-1}$  and  $(N-2)$  angles defining the relative lengths of these Jacobi vectors.<sup>31</sup> Then the Laplacian in  $3N$ -dimensional space has the form,

$$\nabla^2 \equiv \sum_{i=1}^N \nabla_{\zeta_i}^2 = \frac{\partial^2}{\partial r^2} + \frac{3N-1}{r} \frac{\partial}{\partial r} + \frac{L^2(\Omega_N)}{r^2}, \quad (6)$$

where  $L^2(\Omega_N)$  is the grand orbital operator in  $D = 3N$  dimensional space. Potential Harmonics for the  $(ij)$ -partition

are defined as the eigenfunctions of  $L^2(\Omega_N)$  corresponding to zero eigenvalue of  $L^2(\Omega_{N-1})$ . The corresponding eigenvalue equation satisfied by  $L^2(\Omega_N)$  is<sup>31</sup>

$$[L^2(\Omega_N) + \mathcal{L}(\mathcal{L} + D - 2)]\mathcal{P}_{2K+l}^{l,m}(\Omega_{ij}) = 0, \quad \mathcal{L} = 2K + l. \quad (7)$$

This new basis is a subset of the HH and it does not contain any function of the coordinate  $\vec{\zeta}_i$  with  $i < N$  and is given by<sup>31</sup>

$$\mathcal{P}_{2K+l}^{l,m}(\Omega_{(ij)}) = Y_{lm}(\omega_{ij}) {}^{(N)}P_{2K+l}^{l,0}(\phi)\mathcal{Y}_0(D-3), \quad (8)$$

where  $Y_{lm}(\omega_{ij})$  is the spherical harmonics and  $\omega_{ij} = (\vartheta, \varphi)$ . The function  ${}^{(N)}P_{2K+l}^{l,0}(\phi)$  is expressed in terms of Jacobi polynomials and  $\mathcal{Y}_0(3N-3)$  is the HH of order zero in the  $(3N-3)$  dimensional space, spanned by  $\{\vec{\zeta}_1, \dots, \vec{\zeta}_{N-1}\}$  Jacobi vectors.<sup>31</sup> Thus the contribution to the grand orbital quantum number comes only from the interacting pair and the  $3N$  dimensional Schrödinger equation reduces effectively to a four-dimensional equation. The relevant set of quantum numbers are three – orbital  $l$ , azimuthal  $m$ , and grand orbital  $2K+l$  for any  $N$ . The full set of quantum numbers are

$$l_1 = l_2 = \dots = l_{N-1} = 0, \quad l_N = l, \quad (9)$$

$$m_1 = m_2 = \dots = m_{N-1} = 0, \quad m_N = m, \quad (10)$$

$$n_2 = n_3 = \dots = n_{N-1} = 0, \quad n_N = K. \quad (11)$$

We expand  $(ij)$ -Faddeev component,  $\psi_{ij}$ , in the complete set of potential harmonics appropriate for the  $(ij)$  partition:

$$\psi_{ij} = r^{-(\frac{3N-1}{2})} \sum_K \mathcal{P}_{2K+l}^{lm}(\Omega_N^{(ij)}) u_K^l(r), \quad (12)$$

which includes only two-body correlations. Taking projection of the Schrödinger equation on a particular PH, a set of coupled differential equations (CDE) is obtained<sup>32</sup>

$$\left[ -\frac{\hbar^2}{m} \frac{d^2}{dr^2} + \frac{\hbar^2}{mr^2} \{\bar{\mathcal{L}}(\bar{\mathcal{L}} + 1) + 4K(K + \alpha + \beta + 1)\} - E \right] U_{Kl}(r) + \sum_{K'} f_{Kl} V_{KK'}(r) f_{K'l} U_{K'l}(r) = 0, \quad (13)$$

where  $U_{Kl}(r) = f_{Kl} u_K^l(r)$ ,  $\bar{\mathcal{L}} = l + \frac{3N-3}{2}$ ,  $\alpha = \frac{3N-5}{2}$ ,  $\beta = l + \frac{1}{2}$ ,  $l$  being the orbital angular momentum contributed by the interacting pair and  $K$  is the hyperangular momentum quantum number.  $f_{Kl}$  is a constant representing the overlap of the PH for interacting partition with the full set, which is given in Ref. 32. The potential matrix element  $V_{KK'}(r)$  is given by<sup>32</sup>

$$V_{KK'}(r) = \int \mathcal{P}_{2K+l}^{l,m*}(\Omega_N^{ij}) V(r_{ij}) \mathcal{P}_{2K'+l}^{l,m}(\Omega_N^{ij}) d\Omega_N^{ij}. \quad (14)$$

The quantities  $\mathcal{L}_K$  and  $f_{Kl}^2$  are given by

$$\mathcal{L}_K = 2K + l + \frac{3N-3}{2}, \quad (15)$$

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

the latter being the overlap of the PH for the  $(ij)$ -partition (corresponding to only the  $(ij)$ -pair interacting) with the sum of PH for all partitions.

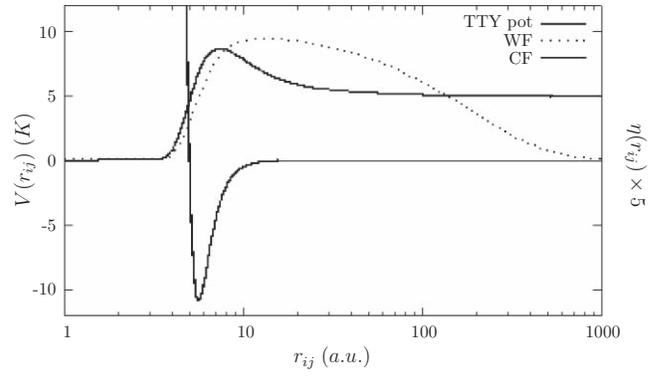


FIG. 1. Plot of TTY potential ( $V(r_{ij})$ ; TTY pot), He-dimer wave function and correlation function ( $\eta(r_{ij})$ ; CF) as a function of  $r_{ij}$ . Note the logarithmic scale for  $r_{ij}$ .

So far we have disregarded the effect of the strong short-range correlation in the PH basis. The He-He potential becomes suddenly very strongly repulsive below a certain value of interatomic separation. This causes a very strong short-range two-body correlation in the many-body wave function. Then we introduce this correlation function in the expansion basis and call it as correlated potential harmonics (CPH) basis,

$$[\mathcal{P}_{2K+l}^{l,m}(\Omega_{(ij)})]_{corr} = Y_{lm}(\omega_{ij}) {}^{(N)}P_{2K+l}^{l,0}(\phi) \times \mathcal{Y}_0(3N-3)\eta(r_{ij}), \quad (16)$$

where  $\eta(r_{ij})$  is the short-range correlation function. It is practically zero for very small  $r_{ij}$  ( $r_{ij} < r_c$ , where  $r_c$  is the size of the repulsive core). Its role is to enhance the speed of convergence of the expansion basis. The correlation function is plotted in Fig. 1. It perfectly reproduces the same short-range behaviour of the dimer wave function. We obtain  $\eta(r_{ij})$  as the zero energy solution of  $(ij)$ -pair relative motion in the potential  $V(r_{ij})$ ,

$$-\frac{\hbar^2}{m} \frac{1}{r_{ij}^2} \frac{d}{dr_{ij}} \left( r_{ij}^2 \frac{d\eta(r_{ij})}{dr_{ij}} \right) + V(r_{ij})\eta(r_{ij}) = 0. \quad (17)$$

The correlation function quickly attains its asymptotic form  $C(1 - \frac{a_{ij}}{r_{ij}})$  for large  $r_{ij}$ . The asymptotic normalization is chosen to make the wave function positive at large  $r_{ij}$ .<sup>33</sup> The correlated potential matrix element  $V_{KK'}(r)$  is now given by

$$V_{KK'}(r) = (h_K^{\alpha\beta} h_{K'}^{\alpha\beta})^{-\frac{1}{2}} \int_{-1}^{+1} \left\{ P_K^{\alpha\beta}(z) V \left( r \sqrt{\frac{1+z}{2}} \right) P_{K'}^{\alpha\beta}(z) \eta \left( r \sqrt{\frac{1+z}{2}} \right) w_l(z) \right\} dz. \quad (18)$$

Here,  $h_K^{\alpha\beta}$  and  $w_l(z)$  are, respectively, the norm and weight function of the Jacobi polynomial  $P_K^{\alpha\beta}(z)$ .<sup>31</sup> Note that the inclusion of the short-range correlation function,  $\eta(r_{ij})$  makes the PH basis non-orthogonal. This introduces an overlap matrix on the eigenvalue side of the matrix eigenvalue equation. One can use the standard procedure for handling a non-orthogonal basis, by introducing a transformation using the eigenvalues of the overlap matrix to convert the eigenvalue

equation into the standard diagonalization of a symmetric matrix. However, we see from Fig. 1 that  $\eta(r_{ij})$  differs from a constant value only by a small amount in a relatively small interval. Hence to simplify the calculation, we project Eq. (4) on to a particular PH, *viz.*,  $\mathcal{P}_{2K+l}^{lm}(\Omega_N^{(ij)})$ . The dependence of the overlap  $\langle \mathcal{P}_{2K+l}^{lm}(\Omega_N^{(ij)}) | \mathcal{P}_{2K+l}^{lm}(\Omega_N^{(kl)}) \eta(r_{kl}) \rangle$  on the hyperradius  $r$  is quite small. Disregarding derivatives of this overlap with respect to the hyperradius, we approximately get back Eq. (13), with  $V_{KK'}(r)$  given by Eq. (18). The effect of the overlap being different from unity is represented by the asymptotic constant  $C$  of  $\eta(r_{ij})$ . The physical picture is that the effective interaction between pairs of  $^4\text{He}$  atoms at very low energy becomes  $V(r_{ij})\eta(r_{ij})$ . Note that at very low kinetic energy, the atoms have a very large de Broglie wavelength and do not approach each other close enough to “see” the *actual*  $^4\text{He}$ - $^4\text{He}$  interaction. In the limit of zero energy, the scattering cross section becomes  $4\pi|a_s|^2$  and the effective interaction is governed by the  $s$ -wave scattering length  $a_s$ , through the asymptotic form of  $\eta(r_{ij})$ . This also justifies the use of  $s$ -wave scattering length, which essentially disregards all angular correlations of the pair separation vectors. Clearly at such small relative kinetic energies, only  $l = 0$  angular momentum comes into play.

### III. RESULTS

As mentioned in the Introduction, several accurate He-He potentials are available in the literature. We choose the TTY potential for the dimer potential, which is one of the most commonly used accurate potentials. This potential has the form,<sup>11,18</sup>

$$V(x) = A[V_{ex}(x) + V_{disp}(x)], \quad (19)$$

where  $x$  represents the interparticle distance. The part  $V_{ex}$  has the form  $V_{ex}(x) = Dx^p e^{-2\gamma x}$  with  $p = \frac{7}{2\gamma} - 1$ . The other part  $V_{disp}$  is given as  $V_{disp}(x) = -\sum_{n=3}^{12} C_{2n} f_{2n}(x) x^{-2n}$ . The coefficients  $C_{2n}$  are calculated using the recurrence relation  $C_{2n} = (\frac{C_{2n-2}}{C_{2n-4}})^3 C_{2n-6}$ ;  $C_6 = 1.461$ ,  $C_8 = 14.11$ ,  $C_{10} = 183.5$ ,  $A = 315766.2067 K$ ,  $D = 7.449$ , and  $\gamma = 1.3443 (a.u.)^{-1}$ . The function  $f_{2n}$  is given by  $f_{2n}(x) = 1 - e^{-bx} \sum_{k=0}^{2n} \frac{(bx)^k}{k!}$  with  $b(x) = 2\gamma - \frac{p}{x}$ .

For our numerical solution, the set of CDEs [Eq. (13)] is solved by hyperspherical adiabatic approximation (HAA).<sup>34</sup> In HAA, one assumes that the hyperradial motion is slow compared to the hyperangular motion. The effective potential for the hyperradial motion (obtained by diagonalizing the potential matrix together with the diagonal hypercentrifugal repulsion for each value of  $r$ ) is obtained as a parametric function of  $r$ . We choose the lowest eigenpotential ( $\omega_0(r)$ ) as the effective potential. Thus in HAA, energy and wave function are obtained approximately by solving a single uncoupled differential equation,

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

subject to appropriate boundary conditions on  $\zeta_0(r)$ . The third term is a correction to the lowest order HAA approximation.<sup>34</sup>

TABLE I. The  $^4\text{He}$ -dimer energy using TTY potential.

Expt.	$\epsilon_d$ (mK)	
1.1 <sup>+0.3</sup> <sub>-0.2</sub>	Present method	-1.254
(Ref. 37)	DMC (Ref. 35)	-1.243
	Other (Ref. 18)	-1.309
	Other (Ref. 17)	-1.313

Here,  $\chi_{K0}(r)$  is the  $K$ th component ( $K$  being the hyperangular momentum quantum number) of the eigenvector of the potential plus hypercentrifugal matrix, corresponding to the lowest eigenvalue  $\omega_0(r)$ , as a parametric function of  $r$ . This is called uncoupled adiabatic approximation, whereas disregarding the third term corresponds to the extreme adiabatic approximation. The principal advantage of the present method is twofold. First, the correlated PH (CPH) basis set correctly takes care of the effect of strong short-range correlation of He-He interaction. Second, the use of HAA basically reduces the multidimensional problem to an effective one-dimensional problem introducing the effective potential. The effective potential ( $\omega_0$ ) gives clear qualitative as well as quantitative pictures. For our numerical calculation, we study  $l = 0$  states and truncate the CPH basis to a maximum value  $K = K_{max}$ , requiring proper convergence.

The ground state properties of  $^4\text{He}$  dimer is obtained by numerical solution of the two-body Schrödinger equation by Runge-Kutta algorithm. The dimer energy  $\epsilon_d$  using TTY potential as well as the results from other references are presented in Table I. Note that there is appreciable difference in the dimer energy calculated by different authors, even though all solve the same Schrödinger equation with the same potential. This appears to be due to the fact that the dimer energy is extremely small in molecular energy scale. Hence, inevitable numerical errors (which depend on the depth of the two-body potential) appear appreciable for the dimer binding energy. The dimer bound state wave function along with the TTY potential and correlation function are shown in Fig. 1, as a function of interparticle distance  $r_{ij}$ . This shows that the spatial extension of the wave function is much larger than the range of the interatomic potentials. The rms value of  $r_{ij}$  is calculated as 98.596  $a.u.$ , in agreement with the fact that the helium dimer is one of the largest diatomic molecules. The very low value of binding energy of the dimer and the large spatial extension of the ground state wave function is a consequence that the ground state of the helium dimer is very loosely bound.

The trimer ground state energy, as well as the results obtained in earlier investigations by other authors are presented in Table II for different potentials. In Fig. 2 we plot the lowest eigenpotential curve together with the ground state wave function for the trimer. The rms value of hyperradius is 21.389  $a.u.$ . Thus our correlated PH basis successfully reproduces the energy values which are in very close agreement with other sophisticated calculations.<sup>17,18,35-39</sup>

Although we have performed detailed calculations of the  $^4\text{He}$  trimer ground state energy, the other goal of the present work is to study trimer excited states which are claimed to be Efimov states. There is still some considerable contro-

TABLE II. The absolute value of  $^4\text{He}$ -trimer ground state energy (in units of mK) obtained via different methods.

Potential	PHEM	Variational	Faddeev	Adiabatic	DMC
TTY	125.51	126.40 (Ref. 38)	126.4 (Ref. 27)	...	125.46 (Ref. 39)
LM2M2	126.37	126.40 (Ref. 39)	126.4 (Ref. 27)	125.2 (Ref. 14)	
HFDHE2	120.28		117.1 (Ref. 27)	98.1 (Ref. 13)	

versy and one can find wide range of discussions regarding whether one or both states should be considered as Efimov state.<sup>13–29</sup> As it is expected to be strongly influenced even by a small variation of the pairwise interaction, we study the behavior of  $^4\text{He}$  trimer excited state as a function of pairwise interaction,

$$V_{He-He} = \lambda V_{TTY}, \quad (21)$$

where  $\lambda$  is a dimensionless constant, which fixes the strength of two-body interaction. Here,  $\lambda = 1$  is the physical value. Efimov proposed that the resonant type of interaction corresponds to the divergence of scattering length and near the singular point the number of three-body bound levels is given by

$$N \simeq \frac{1}{\pi} \ln \left( \frac{|a_s|}{r_e} \right), \quad (22)$$

where  $a_s$  is the two-body scattering length and  $r_e$  is the effective range of two-body potential. Hence, the two-body potential which produces a two-body bound state with vanishing binding energy will support an infinite number of three-body bound states. This situation corresponds to the divergence of  $|a_s|$ . Thus the usual way to characterize Efimov states is to analyse the spectrum by varying the two-body interaction strength.  $\lambda = 0$  corresponds to free particle limit, when neither two-body nor three-body bound states appear. We found that by increasing  $\lambda$  from a small value, the trimer starts to support an excited state at  $\lambda = 0.978$ . Then the binding energy of this state gradually increases with increase in

$\lambda$  and attains its maximum value at  $\lambda = 0.984$ , then it decreases gradually and finally it dissociates into trimer fragments as a dimer and a monomer. We found that the first excited state disappears for both increasing and decreasing  $\lambda$  and it is clearly the signature of Efimov states. Table III summarizes energies of the first four excited states ( $\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4$ ) of the  $^4\text{He}$  trimer, calculated by the CPH procedure, for different strength ( $\lambda$ ) of the two-body interaction. However, our calculation does not find the Efimov-like state with actual physical interaction which corresponds to  $\lambda = 1.0$ . Our calculations show that at  $\lambda = 1$ , the system supports only one state with energy 125.51 mK and the corresponding scattering length is  $a_s = 192.95$  a.u., which is again in perfect agreement with the other previous theoretical results.<sup>17,18</sup> However, this two-body potential does not reproduce any excited state in the corresponding three-body system. As we decrease the strength to  $\lambda = 0.994$ , the first excited state appears. As  $\lambda$  decreases towards  $\lambda = \lambda_{Efimov} = 0.984$ , it starts to be strongly bound. It is characterized as a virtual state. The number of three-body bound states increases rapidly as  $\lambda$  approaches  $\lambda_{Efimov}$ . Table III shows that maximum accumulation of bound states occurs at  $\lambda = 0.984$  and then decreases rapidly as  $\lambda$  decreases beyond  $\lambda_{Efimov}$ . For  $\lambda$  less than 0.978, the first excited state disappears again. The region between  $\lambda = 0.978$  and  $\lambda = 0.984$  is in close agreement with the earlier observation.<sup>16</sup> Beyond  $\lambda_{Efimov}$ , the states start to disappear. But the striking result of our calculation is that this region excludes  $\lambda$

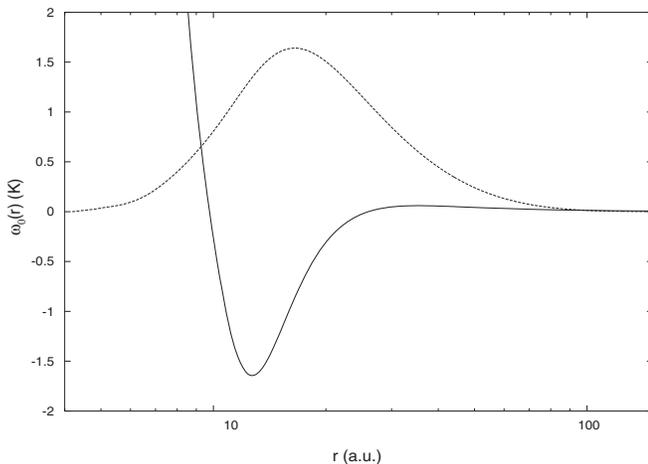


FIG. 2. Lowest eigenpotential (solid line) and ground state wave function (dashed line, arbitrary unit) for the  $^4\text{He}$  trimer with TTY potential as a function of hyperradius  $r$ . Note the logarithmic scale for  $r$ .

TABLE III. Calculated energies of the first four excited states ( $\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4$ ) of the  $^4\text{He}$  trimer for different two-body interaction strength ( $\lambda$ ) together with the number of bound states for each  $\lambda$ . Energy values are in Kelvin (K).

$\lambda$	$\epsilon_1$	$\epsilon_2$	$\epsilon_3$	$\epsilon_4$	$N$
0.978	-0.0050				2
0.980	-0.0522				2
0.982	-5.481	-0.3107	-0.0757		4
0.983	-31.67	-6.245	-0.9619		6
0.984	-482.0	-369.6	-273.1	-191.0	19
0.985	-100.6	-71.09	-54.27	-39.56	10
0.986	-46.86	-25.62	-15.43	-7.43	6
0.987	-13.23	-10.24	-5.58	-4.8	5
0.988	-7.61	-1.87			3
0.989	-4.56	-0.06			3
0.990	-2.703				2
0.991	-1.56				2
0.992	-0.83				2
0.993	-0.37				2
0.994	-0.09				2
0.995					1

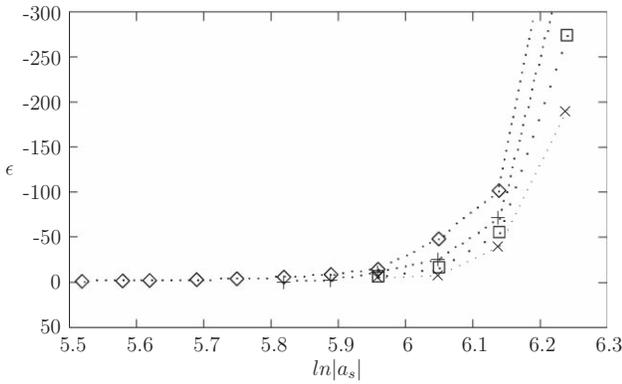


FIG. 3. Plot of three-body energy ( $\epsilon$ ) against  $\ln|a_s|$ , where  $a_s$  is the two-body scattering length for helium trimer. Energies of first, second, third, and fourth excited state are given by the symbols  $\diamond$ ,  $+$ ,  $\square$ ,  $\times$ , respectively.

$= 1$  which is the actual two-body physical interaction. Thus the states which disappear into the continuum are the Efimov states. The ground state energy for the three-body system increases as  $\lambda$  increases and are characterized as normal states. As  $\lambda$  approaches  $\lambda_{Efimov}$ , accumulation of states near the  $\epsilon = 0$  energy, clearly signifies the presence of Efimov effect. In Fig. 3, we present the Efimov diagram. Note that there is an infinite number of Efimov states close to zero energy as  $|a_s|$  increases. Efimov showed that if two-body scattering length is large then the corresponding three-body system exhibits universal properties. The sequence of three-body bound states near zero energy is in agreement with Efimov observation. However, as discussed above this region does not include the physical interaction. In our correlated many-body approach, we do not get any signature of the existence of Efimov state in the  $^4\text{He}$ -trimer, using the actual  $^4\text{He}$ - $^4\text{He}$  interaction potential. However, the Efimov state appears when the interaction strength is decreased. This perfectly confirms the experimental findings,<sup>7,30</sup> which have been unable to find any trimer excited state which can be claimed as an Efimov state. This also supports the claim of Geltman,<sup>36</sup> where a complete theoretical framework is presented explaining why Efimov state will not appear. However, we do not absolutely claim that trimer excited state does not exist at all as there is a large body of work based on many methods.<sup>13-29</sup> It may be the limitation of our basis set which is unable to produce such an elusive state. It may be improved using more sophisticated potential recently used in Ref. 23 which includes retardation and non-additive three-body term in the dimer potential.

The results discussed above depend largely on small changes of  $\lambda$ . Since  $\lambda_{Efimov}$  does not differ much from the physical value  $\lambda = 1$ , it is important to have an error estimate on the value of  $\lambda_{Efimov}$ . We do this in the following manner. Errors can arise from inaccuracies in energy calculation due to the CPH approximation, disregard of three-body force and purely numerical error. Since no exact calculation including three-body force is possible in the present context, error estimates for the first two are not possible. In the absence of these, we look for an error estimate purely due to numerical errors. We first look for convergence in trimer ground state energy ( $E_{00}$ ) as  $K_{max}$  is increased. Once the convergence is reached,

TABLE IV. Energies  $E_{0n}^{PHEM}$  (where  $n$  is the number of excitations) for  $^4\text{He}_N$  cluster,  $N = 4 - 9$ , calculated by correlated PH basis. Comparison with MC hyperspherical ( $E_{0n}^{MC}$ ) and other available results is also presented. Energy values are in  $\text{cm}^{-1}$ .

$N$	$n$	$E_{0n}^{PHEM}$	$E_{0n}^{MC}$ (Refs. 35 and 39)	$E_{0n}^{others}$
4	0	-0.388	-0.389	-0.387 (Ref. 35)
	1	-0.124	-0.0922	-0.088 (Ref. 40)
5	0	-0.905	-0.910	
	1	-0.418	-0.415	
	2	-0.208		
	3	-0.048		
6	0	-1.605	-1.619	
	1	-0.894	-0.936	
	2	-0.453		
	3	-0.266		
	4	-0.132		
	5	-0.029		
7	0	-2.330	-2.478	
	1	-1.483	-1.624	
	2	-0.875		
	3	-0.466		
	4	-0.214		
	5	-0.077		
	6	-0.014		
8	0	-2.896	-3.506	
	1	-1.982	-2.539	
	2	-1.287		
	3	-0.780		
	4	-0.431		
	5	-0.207		
	6	-0.078		
9	0	-3.097	-4.645	
	1	-2.189	-3.565	
	2	-1.480		
	3	-0.946		
	4	-0.562		
	5	-0.301		
	6	-0.136		
7	-0.044			

we estimate the fluctuation ( $\Delta E_{00}$ ) in  $E_{00}$  by increasing  $K_{max}$  beyond the convergence requirement. It is found to be random and about 0.75% of  $E_{00}$ . This represents the purely numerical error introduced through the complicated multistep numerical procedure. Next we find the change  $\Delta\lambda$  in  $\lambda$ , around the physical value ( $\lambda = 1$ ) which produce  $\Delta E_{00}$ . It is found to be  $\Delta\lambda = 8.9 \times 10^{-5}$ . Taking this into consideration, three places of decimal are significant in  $\lambda$ . This is the error estimate within the present approximation. The values of  $\lambda$  presented here and in Table III conform to this.

Inspired by the fact that our correlated basis function can very accurately reproduce the ground state energy, we repeat our calculation for ground and excited states of tetramer and small clusters. In Table IV, we present energies ( $E_{0n}^{PHEM}$ ) up to nine atoms and comparison with Monte Carlo (MC) hyperspherical description<sup>35,39</sup> and other available results<sup>40</sup> is presented. Notice that  $^4\text{He}$  clusters with  $N > 3$  are still weakly bound compared to other rare gas clusters. However, the MC hyperspherical description calculates the ground state and the

first excited state energy. The main difficulty is again the rapid increase in the computer time. We are not aware of any other existing calculations which report higher excited states. However, the good agreement for the ground and the first excited state energies with the essentially exact MC calculation points out the efficiency of our correlated basis function for floppy systems. But deviation grows with increase in  $N$  gradually which clearly shows that PHEM is not valid for bulk system or larger cluster which definitely requires three-body correlations, as also many-body forces.

#### IV. CONCLUSION

We have applied correlated potential harmonics basis to calculate the spectrum of helium trimer and small clusters which are commonly known as van der Waals clusters. We use one of the widely used helium interaction potentials introducing a correlation function in the expansion basis to reproduce correctly the short-range behaviour of the interatomic potential. The dimer system is found to be barely bound which leads to large positive scattering length. This is in perfect agreement with earlier observations. The trimer ground state is also reproduced correctly in our calculation and is in perfect agreement with DMC results. At present there is still controversy regarding the existence of Efimov states in the helium trimer: a number of theoretical works either confirming or disproving the existence of Efimov states have been published, although there is no experimental verification at present. This motivates us to apply a correlated basis function to revisit the problem as these are highly sensitive to two-body interaction. We find several excited states which exhibit Efimov-type behaviour as they disappear with increase in two-body interaction strength. However, this two-body interaction does not contain the actual  ${}^4\text{He}$ - ${}^4\text{He}$  physical interaction. Decreasing the two-body interaction strength we observe accumulation of a large number of states near the zero-energy continuum. Next, we have applied the CPHEM for a system containing few helium atoms. Our results agree well with the DMC results. However, deviation starts with increasing number of atoms which definitely require inclusion of three-body correlations. We conclude that the correlated potential harmonic expansion method is a very useful and simple method for  ${}^4\text{He}$  trimer and also small He clusters.

We also remark that this correlated basis function should be applicable for other diffuse clusters such as  ${}^{87}\text{Rb}$ . The accuracy of the PHEM will depend on the floppiness of the system and for very extended systems, PHEM is expected to be very accurate even for large  $N$ . But for compact clusters one needs to incorporate higher-body correlations.

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