Three dimensional bosonic cluster states of Efimov character near the unitary

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We study three-dimensional bosonic cluster interacting through van der Waals potential at large scattering length. We use Faddeev-type decomposition of the many-body wave function which includes all possible two-body correlations. At large scattering length, a series of Efimov-like states appear which are spatially extended and exhibit the exponential dependence on the state number. We also find the existence of generalized Tjon lines for $N$-body clusters. Signature of universal behaviour of weakly bound clusters can be observed in experiments of ultracold Bose gases.

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I. INTRODUCTION

One of the most interesting topic of quantum physics in recent days is the characterization of universal properties of bosonic many-body system in the unitary regime [1–8]. By using the Feshbach resonance the two-body scattering length $a_s$ is tuned to very large values. The unitary regime is characterized by simple universal laws. For weakly interacting dilute Bose gas, the gas like state becomes unstable as $a_s$ increases [9]. However the Efimov effect in quantum three-body systems leads to different concept of universality. Efimov effect appears in the three-body level ($N=3$) where the attractive two-body interaction is such that the scattering length is much larger than the range of the interaction. Under such condition, a series of weakly bound and spatially extended states of Efimov character appears in the system. Although the Efimov character and ultracold behaviour of Fermi gas is well understood, the exhaustive study of bosonic system with large scattering length are few. Helium trimer $^4\text{He}_3$ is a well studied quantum three-body system in this direction [10, 11]. its first excited state is theoretically claimed as of Efimov state, however no experimental observation is still reported. Whereas the recent experimental observations of Efimov phenomena in ultracold gases has drawn interest in the study of universality in few-body quantum systems [12–13]. But the extension of Efimov physics for larger system ($N > 3$) is not straightforward. There are several studies in this direction which predicted the universality of the system [2, 12–19]. Though predictions and conclusions made in these works are qualitatively similar quantitative differences exist. This necessitates further study of universal properties of bosonic cluster state having Efimov character.

In this work we consider few-bosonic clusters of $^{85}\text{Rb}$ atoms interacting with van der Waals interaction. Our motivation also comes from recent experiments of weakly bound molecules created from ultracold Bose gas. Utilizing the Feshbach resonance the effective interatomic interaction can be essentially tuned to any desired value. For weakly interacting dilute systems, the Efimov state appears at unitary ($|a_s| = \infty$). Our motivation is to study the near threshold behaviour of weakly bound three-dimensional clusters. To characterize this delicate system we prescribe two-body correlated basis function for the many-body cluster interacting through shape-dependent two-body van der Waals potential. We expect that our present study will explore the generic behaviour of three-dimensional bosonic cluster near the unitary. The usage of realistic potential with a short range repulsive core and long-range attractive tail $(-C/r^6)$ may give qualitative conclusion as before but different quantitative behaviours are expected.

The paper is organized as follows. In Sec. II we discuss the many-body Hamiltonian and numerical calculation. Sec. III considers the results and exhibit the signature of universal cluster states with Efimov character. Sec. IV concludes with a summary.
II. FORMALISM

A. Many-body Hamiltonian and numerical calculations

We approximately solve the many-body Schrödinger equation by Potential harmonic expansion method (PHEM). We have successfully applied PHEM to study different properties of Bose Einstein condensate and atomic clusters. The method has been described in detail in our earlier works. We briefly describe the method below for interested readers.

We consider a system of \( N = (A + 1) \) \(^{85}\)Rb atoms, each of mass \( m \) and interacting via two-body potential. The Hamiltonian of the system is given by

\[
H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i,j>i}^{N} V(\vec{r}_i - \vec{r}_j).
\]

Here \( V(\vec{r}_i - \vec{r}_j) \) is the two-body potential and \( \vec{r}_i \) is the position vector of the \( i \)th particle. It is usual practice to decompose the motion of a many-body system into the motion of the center of mass where the center of mass coordinate is \( \vec{R} = \frac{1}{N} \sum_{i=1}^{N} \vec{r}_i \) and the relative motion of the particles in center of mass frame. For atomic clusters, the center of mass behaves like a free particle in laboratory frame and we set its energy zero. Hence, we can eliminate the center of mass motion by using standard Jacobi coordinates, defined as

\[
\vec{\zeta}_i = \sqrt{\frac{2i}{i+1}} (\vec{r}_{i+1} - \frac{1}{i} \sum_{j=1}^{i} \vec{r}_j) \quad (i = 1, \ldots, A),
\]

and obtain the Hamiltonian for the relative motion of the atoms

\[
H = -\frac{\hbar^2}{m} \sum_{i=1}^{A} \nabla_i^2 + V_{\text{int}}(\vec{\zeta}_1, \ldots, \vec{\zeta}_A) .
\]

Here \( V_{\text{int}}(\vec{\zeta}_1, \ldots, \vec{\zeta}_A) \) is the sum of all pair-wise interactions expressed in terms of Jacobi coordinates. The Hyperspherical harmonic expansion method (HHEM) is an ab-initio complete many-body approach and includes all possible correlations. The hyperspherical variables are constituted by the hyperradius \( r = \sqrt{\sum_{i=1}^{A} \zeta_i^2} \) and \((3A - 1)\) hyperangular variables which are comprised of 2A spherical polar angles \((\vartheta_j, \varphi_j; j = 1, \ldots, A)\) associated with \( A \) Jacobi vectors and \((A - 1)\) hyperangles \((\phi_2, \phi_3, \ldots, \phi_A)\) given by their lengths. However the calculation of potential matrix elements of all pairwise potentials becomes a formidable task and the convergence rate of the hyperspherical harmonic expansion becomes extremely slow for \( N > 3 \), due to rapidly increasing degeneracy of the basis. Thus HHEM is not suitable for the description of large diffuse atomic clusters. But for a diffuse cluster like Rb-cluster, only two-body correlation and pairwise interaction are important. Therefore we can decompose the total wave function \( \Psi \) into two-body Faddeev component for the interacting \((ij)\) pair as

\[
\Psi = \sum_{i,j>i}^{N} \phi_{ij}(\vec{r}_{ij},r) .
\]

It is important to note that \( \phi_{ij} \) is a function of two-body separation \((\vec{r}_{ij})\) and the global \( r \) only. Therefore for each of the \( N(N-1)/2 \) interacting pair of a \( N \) particle system, the active degrees of freedom is effectively reduced to only four, viz., \( \vec{r}_{ij} \) and \( r \) and the remaining irrelevant degrees of freedom are frozen. Since \( \Psi \) is decomposed into all possible interacting pair Faddeev components, all two-body correlations are included. Thus the physical picture for a given Faddeev component is that when two particles interact, the rest of the particles behave as inert spectators. Thus the effect of two-body correlation comes through the two-body interaction in the expansion basis. It is to be noted that \( \phi_{ij} \) is symmetric under the exchange operator \( P_{ij} \) for bosonic atoms and satisfy the Faddeev equation

\[
[T - E] \phi_{ij} = -V(\vec{r}_{ij}) \sum_{k,l>k}^{N} \phi_{kl} \]

where \( T = -\frac{\hbar^2}{m} \sum_{i=1}^{A} \nabla_i^2 \) is the total kinetic energy operator. Applying the operator \( \sum_{i,j>i}^{N} \) on both sides of Eq. 5, we get back the original Schrödinger equation. Since we assume that when \((ij)\) pair interacts the rest of the bosons are inert spectators, the total hyperangular momentum and the orbital angular momentum of the whole system is contributed by the interacting pair only. Next the \((ij)\)th Faddeev component is expanded in the set of potential harmonics (PH) (which is a subset of hyperspherical harmonic (HH) basis and sufficient for the expansion of \( V(\vec{r}_{ij}) \)) appropriate for the \((ij)\) partition as

\[
\phi_{ij}(\vec{r}_{ij},r) = r^{-\frac{3A-1}{2}} \sum_{K} P_{2K+1}^{l_m}((\Omega_A^{ij})u_K^l(r) .
\]

\( \Omega_A^{ij} \) denotes the full set of hyperangles in the \( 3A \)-dimensional space corresponding to the \((ij)\) interacting pair and \( P_{2K+1}^{l_m}((\Omega_A^{ij}) \) is called the PH. It has an analytic expression:

\[
P_{2K+1}^{l_m}((\Omega_A^{ij}) = Y_{lm}(\omega_{ij}) \binom{A}{l} P_{2K+1}^{l_m}(\phi) Y_0(D-3); \quad D = 3A
\]

\( Y_0(D-3) \) is the HH of order zero in the \((3A-3)\) dimensional space spanned by \( \{\zeta_1, \ldots, \zeta_{A-1}\} \) Jacobi vectors; \( \phi \) is the hyperangle between the \( A \)-th Jacobi vector \( \vec{\zeta}_A = \vec{r}_{ij} \) and the hyperradius \( r \) and is given by \( \zeta_A = r \cos \phi \). For the remaining \((A-1)\) noninteracting bosons we define
hyperradius as
\[
\rho_{ij} = \sqrt{\sum_{K=1}^{A-1} \zeta_K^2} = r \sin \phi. \tag{8}
\]
such that \(r^2 = r_{ij}^2 + \rho_{ij}^2\). The set of \((3A-1)\) quantum numbers of HH is now reduced to only 3 as for the \((A-1)\) non-interacting pair
\[
l_1 = l_2 = \ldots = l_{A-1} = 0, \tag{9}
\]
\[
m_1 = m_2 = \ldots = m_{A-1} = 0, \tag{10}
\]
\[
n_2 = n_3 = \ldots = n_{A-1} = 0, \tag{11}
\]
and for the interacting pair \(l_A = l, m_A = m\) and \(n_A = K\).

Thus the 3\(A\) dimensional Schrödinger equation reduces effectively to a four dimensional equation with the relevant set of quantum numbers: Energy \(E\), orbital angular momentum quantum number \(l\), azimuthal quantum number \(m\) and grand orbital quantum number \(2K + l\) for any \(N\).

Substituting Eq. (11) in Eq. (8) and projecting on a particular PH, a set of coupled differential equation for the partial wave \(u_K^l(r)\) is obtained
\[
\left[ \frac{-\hbar^2}{m} \frac{d^2}{dr^2} + \frac{\hbar^2}{mr^2} \left( \mathcal{L}(\mathcal{L} + 1) + 4K(K + \alpha + \beta + 1) \right) - E \right] U_{Kl}(r) + \sum_{K'} f_{Kl} V_{KK'}(r) f_{K'l} U_{K'l}(r) = 0 \tag{12}
\]
where \(\mathcal{L} = l + \frac{3N-6}{2}, U_{Kl} = f_{Kl} u_K^l(r), \alpha = \frac{3N-8}{2}\) and \(\beta = l + 1/2\).

\(f_{Kl}\) is a constant and represents the overlap of the PH for interacting partition with the sum of PHs corresponding to all partitions [28]. The potential matrix element \(V_{KK'}(r)\) is given by
\[
V_{KK'}(r) = \int P_{2K+1}^{\pi l} (\Omega_A^{ij}) V(r_{ij}) P_{2K'+1}^{\pi l} (\Omega_A^{ij}) d\Omega_A^{ij}. \tag{13}
\]
We do not require the additional short-range correlation function \(\eta(r_{ij})\) as mentioned in Ref. [25].

III. RESULTS

A. Universal Cluster states

It is already pointed out that the universal properties of ultracold dilute atomic gas in the unitary regime is characterized when the two-body scattering length \(a_s\) is tuned to very large values by using the Feshbach resonance. Although the unitary Fermi gas has been largely investigated both experimentally and theoretically [18], the bosonic unitary regime is a formidable challenge in the many-body theories. Even though the range of the interaction is small compared with the particle separation, interatomic correlations are very important and the standard mean-field theories are inadequate.

The interaction strength of sufficiently dilute atomic cloud is parameterized by a single parameter—the \(s\)-wave scattering length. However for our present study to explore the generic behavior near the unitary, we consider the van der Waals potential characterized by two parameters: the cutoff radius of the repulsive hard core \(r_c\) and the strength of the long-range tail \(C_6\). Thus keeping \(C_6\) fixed, it is possible to tune the value of \(r_c\). Solving the two-body Schrödinger equation it is possible to calculate the scattering length for each choice of \(r_c\). We solve the zero-energy two-body Schrödinger equation for the two-body wave function \(\eta(r_{ij})\) as
\[
-\frac{\hbar^2}{m} \frac{1}{r_{ij}^2} \frac{d}{dr_{ij}} \left( r_{ij}^2 \frac{d\eta(r_{ij})}{dr_{ij}} \right) + V(r_{ij}) \eta(r_{ij}) = 0. \tag{14}
\]

Where \(V(r_{ij}) = \infty\) for \(r_{ij} \leq r_c\) and \(-\frac{C_6}{r_{ij}^6}\) for \(r_{ij} > r_c\). The asymptotic form of \(\eta(r_{ij})\) is \(C(1 - \frac{1}{r_{ij}^6})\), \(C\) is the normalization constant. The solution of two-body equation shows that the value of \(a_s\) changes from negative to positive passing through an infinite discontinuity. In Fig. 1 we plot the zero-energy scattering length \(a_s\) as a function of \(r_c\). At each discontinuity, one extra node in the two-body wave function appears which corresponds to one extra two-body bound state. However for our present study we fix \(r_c\) such that it corresponds to zero node in the two-body wave function. We impose the constraint just to avoid the formation of the molecules, otherwise when \(a_s\) sufficiently increases, the rate of three-body collisions will increase which deplete the density by forming molecules.

With the above set of parameters we solve the set of

![FIG. 1: Plot of zero energy scattering length \(a_s\) (in Bohr) as a function of \(r_c\) (in Bohr). Here only one branch corresponding to zero node in two-body wave function is shown. Blue horizontal line shows the \(a_s\) = 0.](image)
matrix including the diagonal hypercentrifugal repulsion for a fixed value of \( r \). The CDE is then decoupled approximately into a single uncoupled differential equation
\[
\left[ -\frac{\hbar^2}{m} \frac{d^2}{dr^2} + \omega_0(r) - E_R \right] \zeta_0(r) = 0 ,
\]
which is known as extreme adiabatic approximation (EAA) and the lowest eigenvalue \( \omega_0(r) \) is the effective potential in which the hyperradial motion takes place. The above equation is solved to obtain the energy and wave function with appropriate boundary conditions on \( \zeta_0(r) \).

In Fig. 2 we plot the calculated bosonic cluster ground state energies in the negative scattering length near the unitary for different cluster sizes with \( N = 3, 4, 5, 6, 7 \) as a function of the scattering length \( a_s \) (in Bohr). It is to be noted that the effective interaction of the bosonic cluster is determined by \( \int V(r_{ij}) d^3r_{ij} \). With increase in particle number, the number of interacting pair \( \left( \frac{N(N-1)}{2} \right) \) also increases and the energy becomes more negative as expected.

**B. Signature of Efimov states**

For two particles the infinite scattering length corresponds to a bound state at zero energy. For three particles the Efimov effect appears at \( a_s \sim 0 \), and for \( \frac{1}{a_s} = 0 \), infinitely many three-body bound states with smaller binding energy and larger radii will appear. Moving in the opposite by decreasing the attraction, these states cease to be bound one by one. We have calculated the spectrum of bosonic clusters and in Fig. 3 we plot \( E_{n0} \) as a function of the state number \( n \) of the negative energy states. The radii of Efimov states \( r_{av} \) as a function of state number \( n \) is shown in Fig. 4. Points on the curve correspond to the bound states.

**C. Structural properties and correlation**

Finally we analyse the structural properties of the cluster states by calculating the pair-correlation function

\[
\rho_{ij}(r) = \frac{1}{N!} \frac{1}{(2\pi \hbar)^3} \int \frac{d^3p}{(2\pi \hbar)^3} \frac{d^3q}{(2\pi \hbar)^3} \frac{\psi^*(p)\psi^*(q)\psi(r-p-q)\psi(r-q)}{(E_n - E_0\pm \hbar \omega_0(r))^2},
\]

where \( \psi \) is the wave function and \( E_n \) is the energy of \( n \)-body system.
$R_2(r_{ij})$ which determines the probability of finding the $(ij)$ pair of particles at a relative separation $r_{ij}$. Fig. 5 presents the pair correlation function for $N = 3 - 7$ at unitarity. $R_3(r_{ij})$ is considered as a more effective quantity in the description of structural properties as the interatomic interaction plays a crucial role. When atoms try to form clusters, due to the attractive part of van der Waals interaction, the short range hard core repulsion has the effect of repulsion, Thus $R_2(r_{ij})$ is zero for $r_{ij}$ smaller than the hard core radius $r_c$. We calculate $R_2(r_{ij})$ by

$$R_2(r_{ij}) = \int_{\tau''} |\psi|^2 d^3 \tau''$$ \hspace{1cm} (16)

where $\psi$ is the many-body wave function and the integral over the hypervolume excludes the integration over $r_{ij}$. The position of the maximum is shifted to larger $r_{ij}$ with increase in $N$ and peak height reduces. However we do not observe any structure in the correlation function. It says that the extremely diffuse cluster behaves just like diffuse liquid blob as observed in earlier work [2]. It is already mentioned that while the universal

![FIG. 5: Plot of pair-correlation function of van der Waals cluster of different sizes $N$ near the unitarity.](image)

behaviours of the trimer are quite well understood, much less is known about the larger systems. In this context the investigation of correlations between energies of three and four-particle systems is indeed required. The earlier studies in this direction are mainly focused on the Tjon line which refers to the approximately linear correlation between the energies of three-nucleon and four-nucleon systems [18, 19]. It is expected that the bosonic cluster energy close to the unitarity, for different cluster states should follow the generalized Tjon line. It says that the energies are linearly correlated to each other and a two-parameter relation is maintained.

$$\frac{E_{N+1}}{E_{N-1}} = \rho_N + \zeta_N \frac{E_N}{E_{N-1}}$$ \hspace{1cm} (17)

In Fig. 6 we present the energy ratio $\frac{E_{N+1}}{E_{N-1}}$ as a function of $\frac{E_N}{E_{N-1}}$ for different cluster sizes $N = 4, 5, 6$. Solid lines show linear fits of the form $\frac{E_{N+1}}{E_{N-1}} = \rho_N + \zeta_N \frac{E_N}{E_{N-1}}$. The fitting parameters are summarized in Table I. We refer the approximate linear fitting of the energy ratios of clusters as the generalized Tjon line. We observe that the values of the fitting parameters gradually decreases with increasing $N$ and this is consistent with earlier finding [2].

| $N$ | $\rho_N$ | $\zeta_N$ |
|-----|--------|--------|
| 4   | -1.76107 | 2.5346 |
| 5   | -0.898113 | 2.02464 |
| 6   | -0.8666535 | 1.98111 |

This definitely opens the possibilities of future investigations of how the behaviour of the generalized Tjon lines are related in the description of the universal properties of diffuse bosonic clusters.

IV. CONCLUSION

The physics of weakly bound few-body systems and their universal behaviour near the unitary is a challenging research area in recent days. The recent experimental observation of Efimov phenomena in ultracold Bose gases has renewed the interest in universal few-body physics. The theoretical study of three-dimensional bosonic cluster with more than three particles is also challenging and the numerical treatment becomes complicated with $N > 3$. The cluster is weakly bound as the kinetic and potential energy nearly cancel. It needs to include interatomic correlation. In the present study we utilize two-body correlated basis function for the study of $N$-boson systems. Use of realistic van der Waals potential presents the actual feature of such delicate systems. We calculate the energy spectrum of $N$-body cluster with $N$ upto 7 atoms. At large scattering length, which is much larger than the range of interaction, the ground state energy of $N$-body cluster shows universal behaviour. Next, to exhibit the Efimov like character of the energy states we calculate the Efimov like character of the energy states we present the exponential dependence on the state number. We also calculate the r.m.s radii of the spatially extended systems and also shows their exponential dependence on the state number. Calculation of two-body pair correlation exhibit the expected feature and does not show any structure. It says that the weakly interacting cluster behaves just like a single quantum stuff. We also calculate the energy correlation between two clusters differing by one atom and shows that they maintain a two parameter linear relation. We refer the Tjon line as the characteristic of universal behaviour of bosonic cluster.

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FIG. 6: Plot of $E_{N+1}$ as function of $E_N$ for different cluster sizes $N$. The + signs shows the numerical data and the blue dotted line represent our two-parameter linear fitting (see text) - the Tjon line.