Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Structural and quantum properties of van der Waals cluster near the unitary regime

M.L. Lekala [a], B. Chakrabarti [b,*], S.K. Haldar [c,d], R. Roy [b], G.J. Rampho [a]

[a] Department of Physics, University of South Africa, P.O. Box 392, Pretoria 0003, South Africa
[b] Department of Physics, Presidency University, 86/1 College Street, Kolkata 700 073, India
[c] Theoretical Physics Division, Physical Research Laboratory, Navrangpura, Ahmedabad 380009, India
[d] Department of Physics, University of Haifa, Kyriat Tivon 36006, Haifa, Israel

ARTICLE INFO

Article history:
Received 20 January 2017
Received in revised form 4 May 2017
Accepted 5 May 2017
Available online xxxx
Communicated by V.A. Markel

Keywords:
VdW cluster
Unitary limit
Structural property
Correlated basis function

ABSTRACT

We study the structural and several quantum properties of 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, we observe spatially extended states which exhibit the exponential dependence on the state number. The cluster ground state energy shows universal nature at large negative scattering length. 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. We also study the spectral statistics of the system. We calculate both the short-range fluctuation and long-range correlation and observe semi-Poisson distribution which interpolates the Gaussian Orthogonal Ensemble (GOE) and Poisson statistics of random matrix theory. It indicates that the van der Waal cluster near the unitary becomes highly complex and correlated. However additional study of $P(r)$ distribution (without unfolding of energy spectrum) reveals the possibility of chaos for larger cluster.

1. Introduction

Computation of energy levels and the study of various structural and quantum properties of several rare gas clusters is a long standing problem in many-body physics and several remarkable works have been published in this direction [1–7]. The properties of these clusters are mainly calculated using variational Monte Carlo methods. It has been observed that in contrast to helium, the rare gases have more classical behaviour. The interaction potential is generally taken as the Lennard-Jones potential. The energetics and structural properties of super Borromean N-body clusters have also been reported recently [8].

Our present study mainly involves the characterization of universal properties of bosonic clusters in the unitary regime and interacting with van der Waals potential. The effective interatomic interaction at ultracold temperature can be essentially tuned to any desired value by utilizing Feshbach resonances. By changing the external magnetic field the evidence for the formation of Efimov trimer states has been reported [9,10]. The study of universalities in few-body quantum system ($N > 3$) is not straightforward. There are several studies in this direction which predict the universality of these systems [11–20], though predictions and conclusions made in these works are qualitatively similar, quantitative difference exists [21–26]. This is to be noted that energy level statistics and spectral analysis of van der Waals clusters are reported earlier by our group [27,28]. However the earlier calculations consider diffuse cluster and weakly interacting trapped bosons. Whereas the present study considers the atomic cluster at very large scattering length when the system becomes highly correlated and complex. The comparison with the diffuse cluster is made in a separate section later.

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 [18]. However in quantum few-body systems it leads to different concept of universality. Universalities appear when 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 appear in the system.

* Corresponding author.
E-mail address: barnali.physics@presiuniv.ac.in (B. Chakrabarti).

http://dx.doi.org/10.1016/j.physleta.2017.05.009
0375-9601/

Although the behaviour of ultracold Fermi gas is well understood, the exhaustive study of bosonic system with large scattering length is not properly presented in literature. Helium trimer $^4He_3$ is a well studied quantum three-body system in this direction [19,20].

In this work we consider few-bosonic clusters of ^{85}Rb atoms interacting with van der Waals interaction. In some recent experiments it has been revealed that the range of the interaction between atoms is typically the van der Waals length characterized by $r_{vdw} = \frac{1}{2}\left(\frac{mC_6}{\hbar^2}\right)^{\frac{1}{4}}$, which is associated with the $-\frac{C_6}{r^6}$ tail [29,30]. To characterize this delicate system we prescribe two-body correlated basis function for the many-body cluster. At large scattering length the ground state energy exhibits the universality for few atoms (N up to 7) in the cluster. A series of spatially extended states are observed which exhibit exponential dependence on the state number. We also find the existence of generalized Tjon lines for N-body clusters.

The study of energy level statistics of such complex clusters is another important area of our present study. We are able to calculate the full energy spectrum for $N = 7$ cluster and calculate nearest-neighbour level spacing distribution $P(s)$ and $\triangle_3$ statistics. Our numerical result strongly resembles the semi-Poisson distribution for the lower levels which interpolates the GOE (Gaussian Orthogonal Ensemble) and Poisson statistics. We also present the $P(r)$ distribution of the ratio of the consecutive level spacing (r) and the average $< \tilde{r} >$ which are presently considered as the most useful statistical measures to distinguish order and chaos in the energy levels.

The paper is organized as follows. In Sec. 2 we discuss the many-body Hamiltonian and numerical calculation. Sec. 3 considers the results and exhibits the signature of universal cluster states. Comparison is made with diffuse cluster. It also presents calculation of energy level statistics. Sec. 4 concludes with a summary.

2. 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 [31–33] and atomic clusters [34,27,28]. The method has been described in detail in our earlier works [31–33]. 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

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

Here $V(\mathbf{r}_i - \mathbf{r}_j)$ is the two-body potential and $\mathbf{r}_i$ is the position vector of the ith 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 $\mathbf{R} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{r}_i$ 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 to zero. Hence, we can eliminate the center of mass motion by using standard Jacobi coordinates, defined as [35–37]

$$\zeta_i = \sqrt{\frac{2i}{i+1}}(\mathbf{r}_{i+1} - \frac{1}{i}\sum_{j=1}^{i}\mathbf{r}_j) \qquad (i = 1, \cdots, A), \tag{2}$$

and obtain the Hamiltonian for the relative motion of the atoms

$$H = -\frac{\hbar^2}{m}\sum_{i=1}^{A}\nabla_{\zeta_i}^2 + V_{int}(\zeta_1, ..., \zeta_A)\ . \tag{3}$$

Here $V_{int}(\zeta_1, ..., \zeta_A)$ 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 $(\vartheta_j, \varphi_j;\ j = 1, \cdots, A)$ associated with A Jacobi vectors and $(A-1)$ hyperangles $(\phi_2, \phi_3, \cdots, \phi_A)$ 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 and complex atomic clusters. However we may assume that only two-body correlation and pairwise interaction are present and the total wave function Ψ can be decomposed into two-body Faddeev component for the interacting (ij) pair as

$$\Psi = \sum_{i,j>i}^{N}\phi_{ij}(\mathbf{r}_{ij}, r)\ . \tag{4}$$

ϕ_{ij} is a function of two-body separation $(\mathbf{r}_{ij})$ 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 are effectively reduced to only four, *viz.*, $\mathbf{r}_{ij}$ and r and the remaining irrelevant degrees of freedom are frozen. Since Ψ 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. The two-body correlation enters through the two-body expansion basis and as ϕ_{ij} is symmetric under the exchange operator P_{ij}, the Faddeev equation can be written as

$$[T - E]\,\phi_{ij} = -V(\mathbf{r}_{ij})\sum_{kl>k}^{N}\phi_{kl} \tag{5}$$

where $T = -\frac{\hbar^2}{m}\sum_{i=1}^{A}\nabla_{\zeta_i}^2$ is the total kinetic energy operator. Applying the operator $\sum_{i,j>i}$ 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 are contributed by the interacting pair only. The (ij)th Faddeev component is then expanded in the subset of hyperspherical harmonics, which we call as potential harmonic (PH) basis as

$$\phi_{ij}(\mathbf{r}_{ij}, r) = r^{-(\frac{3A-1}{2})}\sum_{K}\mathcal{P}^{lm}_{2K+l}(\Omega_A^{ij})u^l_K(r)\ . \tag{6}$$

$\mathcal{P}^{lm}_{2K+l}(\Omega_A^{ij})$ is called the PH. It has an analytic expression:

$$\mathcal{P}^{l,m}_{2K+l}(\Omega_A^{(ij)}) = Y_{lm}(\omega_{ij})\ {}^{(A)}P^{l,0}_{2K+l}(\phi)\mathcal{Y}_0(D-3); \qquad D = 3A, \tag{7}$$

$\mathcal{Y}_0(D-3)$ is the HH of order zero in the $(3A-3)$ dimensional space. The global hyperradius r is further defined as $r^2 = r_{ij}^2 + \rho_{ij}^2$, where r_{ij} is the separation between (ij) interacting pair and ρ_{ij} is basically the global size of the remaining noninteracting bosons. As the angular momentum contribution from the noninteracting $(A-1)$ bosons is zero, the $3A$ quantum number of HH is now reduced to only four as energy E, orbital angular momentum quantum number l, azimuthal quantum number m, grand orbital quantum number $2K + l$ for any N. We substitute Eq. (4) in Eq. (5) and take a projection on a particular PH basis and obtain a set of coupled differential equations in the partial wave $U_{Kl}(r)$.

Please cite this article in press as: M.L. Lekala et al., Structural and quantum properties of van der Waals cluster near the unitary regime, Phys. Lett. A (2017), http://dx.doi.org/10.1016/j.physleta.2017.05.009