Bosonic drops with two- and three-body interactions close to the unitary limit

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Abstract. When the binding energy of a two-body system goes to zero the two-body system shows a continuous scaling invariance governed by the large value of the scattering length. In the case of three identical bosons, the three-body system in the same limit shows the Efimov effect and the scale invariance is broken to a discrete scale invariance. As the number of bosons increases correlations appear between the binding energy of the few- and many-body systems. We discuss some of them as the relation between the saturation properties of the infinite system and the low-energy properties of the few-boson system.

Keywords: Few-Boson Systems, Efimov Physics, Helium drops

1 Introduction

The ground state properties of $^4\text{He}$ and $^3\text{He}$ droplets with $N$ atoms have been studied in a series of papers \cite{1,2,3,4}. The energy per particle, $E_N/N$ can be described, as $N \to \infty$, using a liquid-drop formula in terms of $x = (N-1)/3$

$$E_N/N = E_v + E_s x + E_c x^2$$

where $E_v$, $E_s$ and $E_c$, are the volume, surface and curvature terms respectively. Results for the infinite liquid can be obtained from calculations at fixed values of $N$. Since the value at saturation can be obtained independently, these studies probe the validity of the extrapolation formulas used to predict the properties of the infinite system typically computed in droplets having a few hundred atoms.

More recently helium drops have been studied using modern helium-helium interactions \cite{5,6}. In Ref. \cite{7} a diffusion Monte Carlo (DMC) method has been used to study clusters up to 10 atoms interacting through the Tang, Toennies, and Yiu (TTY) potential \cite{8}. Helium trimers and tetramers have been studied around the unitary limit varying the potential strength \cite{9,10,11,12}. It has been shown that with a very small reduction of the strength (about 3%) the binding
energy of the helium dimer disappears. In fact the helium dimer is very close to the unitary limit having a two-body binding energy of about 1.3 mK and a large two-body scattering length of about 189 a_0 (a_0 is the Bohr radius).

We can observe two, very different, descriptions of light helium clusters. On one hand, several models of the helium-helium interaction are available. On the other hand, the large value of the helium-helium scattering length locates the small clusters of helium close to the unitary limit in which universal behavior can be observed. Accordingly, the particular form of the potential is not important, many properties are determined from a few parameters as the two-body scattering length a and the trimer ground state energy E_3^0 (or the first excited state E_3^1). Specific (soft) potential models can be constructed in order to reproduce those data and used to calculate binding energies of droplets and the saturation properties of the infinite system [13]. In this way, a direct link between the low energy scale (or long-range correlations) and the high energy energy scale (or short-range correlations) can be established.

2 Helium dimer and trimer with soft potential models

In the following we study the ground state energy of the N = 2, 3 boson systems using a soft gaussian potential constructed to reproduce the low-energy behavior of the system. We define the two-body interaction as

\[ V(r_{ij}) = V_0 e^{-r_{ij}^2/d_0^2} \]

with the two gaussian parameters, V_0 and d_0, determined from the dimer energy, E_2, and the two-body scattering length a. Realistic helium-helium potentials can be used to calculate E_2 and a, subsequently used to fix V_0 and d_0. In this way, the gaussian interaction results in a low-energy representation of the original potential. Using the LM2M2 interaction [14], widely used in the description of helium clusters, as the reference interaction, the values V_0 = −1.2343566 K and d_0 = 10.0 a_0 can be used. To study correlations between observables we can start analyzing the Efimov radial law

\[ E_n^3/(\hbar^2/ma^2) = \tan^2 \xi \]

\[ \kappa_a = e^{(n-n^*)\pi/s_0} e^{-\Delta(\xi)/2s_0} \cos \xi , \]

that gives, in the zero-range limit, the three-boson spectrum E_3^n in terms of the universal function \( \Delta(\xi) \) and the three-body parameter \( \kappa_a \), defined by the energy at the unitary limit of the reference level \( n^* \), \( E_3^{n^*} = \hbar^2 \kappa_a^2/m \). Eq.(4) indicates that the product \( \kappa_a a \) is a function of the angle \( \xi \). Assuming that for real systems the product \( \kappa_a a \) is still a function of \( \xi \) we can propose:

\[ \kappa_a a = [\kappa_a a]_G \]

where \([\kappa_a a]_G\) is the value of the product calculated with the gaussian potential at the angle \( \xi \). To verify this hypothesis we consider the ground state binding
energies of the dimer $E_2 = 1.303$ mK and trimer $E_3 = 126.4$ mK as given by the LM2M2 potential defining the angle $\xi$ as $E_3/E_2 = \tan^2 \xi = 97.0$. Modifying the strength of the gaussian potential to $V_0 = -1.24294$ K and calculating the dimer and trimer energies, the same angle is obtained. Moreover, a gaussian potential has the property that its three-body parameter verifies $\kappa = 0.488/d_0$ [15,16].

The two-body scattering length using the modified strength is $a = 170.50$ a$_0$. Accordingly, we can estimate the three-body parameter $\kappa_*$ of the LM2M2 interaction, knowing that the scattering length is $189.41$ a$_0$, as

$$[\kappa_*]_{LM2M2} = \frac{170.5}{189.41} \cdot 0.488/d_0 \cdot$$

(6)

The obtained value is $\kappa_* = 0.044$ a$_0^{-1}$ in complete agreement with the LM2M2 value given in the literature. We have shown that the three-body parameter can be determined by three quantities, the dimer and trimer energies and the two-body scattering length.

3 Saturation properties of the N-boson system

In the following we analyze correlations between the saturation properties of the infinite system and the low-energy behavior of the few-boson systems. To this end we use as the reference interaction the Aziz HFDHE2 potential used in Ref. [3] to compute binding energies of helium droplets. A low energy representation of the HFDHE2 potential is obtained by defining the parameters of the gaussian potential $V_0 = -1.208018$ K and $d_0 = 10.0485$ a$_0$, giving a trimer ground state binding energy of $E^0_3 = 139.8$ mK. This value is substantially greater than the value obtained using the HFDHE2 potential: $E^0_3 = 117.3$ mK. It is well known that to tune the trimer binding energy to the expected value a slightly repulsive three-body force has to be introduced. As proposed in Refs. [17,18,19,20,21] we define the following three-body force

$$W(\rho_{ijk}) = W_0 e^{-2\rho_{ijk}/\rho_0^2},$$

(7)

where $\rho_{ijk}$ is the hyperradius of particles $i$, $j$, $k$ defined as $\rho_{ijk}^2 = (2/3)(r_{ij}^2 + r_{jk}^2 + r_{ki}^2)$. For selected values of the range $\rho_0$, the strength $W_0$ is fixed to reproduce the HFDHE2 trimer ground state binding energy $E^0_3$. The binding energy of the droplets $E_N$ can be computed using this soft gaussian potential (SGP) and can be studied as a function of the range $\rho_0$. In Fig.1 the binding energies of helium drops up to $N = 10$ are shown as a function of $\rho_0$ and compared to the HFDHE2 values from Ref.[3] using the Green Function Monte Carlo (GFMC) method. Though a small dependence on $\rho_0$ can be seen, an overall good description is obtained.

The $\rho_0$ dependence is analyzed in Fig.2 in the case of the tetramer binding energy. It can be seen that there is a value of $\rho_0$, around 8.5 a$_0$, that gives the best description of this quantity. The next step is to compute the droplets binding energies up to $N \approx 100$ and extract the saturation energy from Eq.(1). This is
shown in Fig.3 where the results for different values of \( \rho_0 \) form the dark band. The results using the optimum value of \( \rho_0 = 8.5 \ a_0 \) are shown as (blue) points. They follow, with acceptable accuracy, the GFMC results using the HFDHE2 potential shown as the (red) solid line. Using the optimum value of \( \rho_0 \) it is possible to determine \( E_v, E_s \) and \( E_c \) defined in Eq. (1). From the results of the SGP in the range \( 20 \leq N \leq 112 \) the following values are obtained (in K)

\[
E_N/N = 6.98 - 18.6 x + 10.3 x^2.
\]

They can be compared to the values (in K) obtained with the GFMC method \( E_v = 7.02, E_s = -18.8 \) and \( E_c = 11.2 \) using the HFDHE2 interaction.

We conclude that after tuning the range of the three-body force to reproduce as better as possible the tetramer binding energy, the soft gaussian potential, consisting of a two- and a three-body term, with the four parameters determined by the dimer, trimer and tetramer binding energies and the two-body scattering length is able to estimate with good accuracy the energy per particle of the infinite system.

4 Conclusions

In the present work we have analyzed correlations between different observables imposed by the proximity of the system to the unitary limit. Due to the large value of the two-body scattering length, helium drops are well suited to study
these phenomena. Correlations of this type can also be studied in nuclear systems, since the $n-n$ and $n-p$ scattering lengths are large [22,23]. Here we have shown results for helium drops using a gaussian soft interaction to determine the three-body parameter $\kappa^*$. Noticeably, the result was in extremely good agreement with the values given in the literature calculated directly using the LM2M2 potential. Secondly, using the HFDHE2 as the reference potential, we have calculated binding energies for helium drops up to $N = 112$ and, using a liquid-drop formula, we have extracted the saturation energy. We have observed that using the optimum value for the range of the three-body interaction a good estimate of the experimental saturation energy is obtained. In this way we have clarified the existing correlations between different observables imposed by the unitary limit in many-body systems close to the unitary limit.

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Fig. 3. The binding energy of the droplets as a function of the number of particles $N$.