Saturation properties of helium drops from a Leading Order description

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Saturation properties are directly linked to the short-range scale of the two-body interaction of the particles. The case of helium is particular, from one hand the two-body potential has a strong repulsion at short distances. On the other hand, the extremely weak binding of the helium dimer locates this system very close to the unitary limit allowing for a description based on an effective theory. At leading order of this theory a two- and a three-body term appear, each one characterized by a low energy constant. In a potential model this description corresponds to a soft potential model with a two-body term purely attractive plus a three-body term purely repulsive constructed to describe the dimer and trimer binding energies. Here we analyse the capability of this model to describe the saturation properties making a direct link between the low energy scale and the short-range correlations. We will show that the energy per particle, $E/N$, can be obtained with reasonable accuracy at leading order extending the validity of this approximation, characterizing universal behavior in few-boson systems close to the unitary limit, to the many-body system.

Introduction. At the beginning of the eighties strong efforts were done to calculate ground state properties of $^4$He and $^3$He droplets containing specific number $N$ of atoms [1–4]. After computing the energy per particle, $E/N$, and the rms radii of the droplets it was possible to study the evolution of these quantities as $N → ∞$. For example, a liquid-drop formula was proposed to fit $E/N$ in terms of $x = N^{-1/3}$

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

with $E_v$, $E_s$ and $E_c$, the volume, surface and curvature terms respectively. A similar behavior, in powers of $x$, has been proposed for the unit radius, defined in terms of the rms radius $(r^2)^{1/2}$, as $r_0(N) = \sqrt{\frac{2}{3N}} (r^2)^{1/2} N^{-1/3}$. Extrapolated results for the infinite liquid were obtained from calculations on droplets using different values of $N$. The motivations for that study were twofold, from one side the theoretical results obtained with realistic interatomic potentials could be compared to experimental results. To this respect the calculation on the infinite system, liquid $^4$He at equilibrium density, predicts a value $E_v = -7.11$ K using the high quality potential HFDHE2 from Aziz et al. [3], in very good agreement with the experimental value of $-7.14$ K at a density of 0.0219 Å$^{-3}$. This can be seen as a successful application of the potential theory to describe ground state properties of liquid helium. A second motivation was to analyze the capability of the extrapolation formulas to predict the properties of the infinite system using results computed in droplets having at most a few hundred atoms. It was shown that stable values of $E_v$ and the surface tension $t = E_s/4\pi r_0^2(∞)$ could be obtained in agreement with those calculated in the infinite system. This analysis gave support to the liquid-drop formulas used in nuclear physics to predict nuclear matter properties. To be noticed that whereas different properties can be measured in infinite liquid helium this is not the case for infinite nuclear matter.

Droplets of bosonic helium attracted attention in the nineties due to the fact that the dimer composed by two $^4$He atoms is very loosely bound. Its energy is $E_2 ≈ 1$ mK, and the two-body scattering length, $a ≈ 100$ Å, has a very large value if compared to the typical length of the system, the van der Waals length $\ell_{vdw}$, which for two helium atoms is $\ell_{vdw} ≈ 2.5$ Å. When $a \gg \ell_{vdw}$ the system can be studied in first approximation in the zero-range limit. It provides a good approximation for shallow states in which the particles stay most of the time outside the interaction region and, accordingly, the low energy dynamics does not depend on the details of the interaction. Moreover $E_2 ≈ \hbar^2/(ma^2)$, with $m$ the boson mass, vanishes at the unitary limit, corresponding to $a → ∞$. As demonstrated by Efimov in a series of papers [1–4], the three-body system has a geometrical series of excited states that accumulate at zero energy. This is called the Efimov effect and was experimentally confirmed more than three decades after its prediction [5].

At present days there is an intense experimental activity [6–12] dedicated to study the behavior of few-body systems close to the unitary limit. To this respect the helium trimer was indicated as a candidate for a direct observation of an Efimov type excited state. The possibility of observing Efimov states in small clusters of helium has triggered an intense experimental activity using ultracold jets of helium going through a diffraction grating [13]. Though it was not possible to extract specific energy values, the diffraction patterns were used to identify the number of atoms in the droplets. This research culminated recently with a measurement of the ground and excited state of the helium trimer giving a direct confirmation of the existence of Efimov states [14].

Helium drops have been studied using modern helium-
helium interactions \cite{15,16}. In particular in Ref. \cite{17} 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{18}. From a
greater perspective, trimers and tetramers have been
studied with different interactions in which the poten-
tial strength has been varied in order to drive the
system to the unitary limit \cite{19–22}. When a two-boson
system interacting via a short-range potential is close
to the unitary limit, the three-boson system shows uni-
versal behavior. Its spectrum is governed by the two-
body scattering length $a$ and the three-body parameter
$\kappa_s$ defines the energy of the $n_s$ level at the unitary limit,
$\hbar^2\kappa_s^2/m$. The system manifests a discrete scale invariance
(DSI), the ratio of binding energies for two consecutive
states is $E_n^*/E_{n+1}^* = e^{2\pi/s_0}$, with the universal number
$s_0 \approx 1.00624$ \cite{23}. The studies using potential models
have shown that this description is very well fulfilled if
range corrections are taken into account \cite{24}.

A three-boson system close to the unitary limit can be
described using an effective field theory (EFT) \cite{25,26}.
At leading order (LO) the effective Hamiltonian includes
a two-body and a three-body contact term. The strength
of the two terms determine the values of $a$ and $\kappa_s$. This
kind of studies have triggered the idea of describing the
dimer and trimer using a soft potential model consisting
in a two- plus a three-body term in which the strengths
can be fixed to describe some particular observables, for
example the dimer and trimer binding energies. This
Hamiltonian can be used to solve the Schrödinger equation
for systems with $N > 3$ and the agreement (or differ-
ces) obtained from comparisons to experimental data
or results obtained with more realistic interactions can be
analysed. This strategy has been explored in Refs. \cite{27–
29} in which the ground state energy of small clusters of
helium calculated using a soft potential model results ex-
tremely close (within a few percent) to that one obtained
using a realistic helium-helium interaction.

From the above discussion we observe two, very dis-
tinctive, descriptions of light helium clusters. On one
hand, strong efforts have been done to determine the best
possible helium-helium interaction. Different models ex-
ist in the literature and they have been tested in drops
as well as in infinite liquid. On the other hand the large
scattering length of the helium-helium system indicates
that the helium trimer and tetramer show universal behav-
ior. The particular form of the potential is not im-
portant and many features can be determined from a few
experimental data, such as $a$ and the trimer ground state
energy $E_3^*$ (or first excited state $E_3^*$). Accordingly a soft
potential model can be constructed in order to reproduce
those observables. Here we want to determine saturation
properties of the infinite system from calculations on he-
lium drops described using a soft potential model making
a direct link between the low energy scale (or long-range
correlations) and the high energy energy scale (or short-
range correlations). Moreover this analysis will clarify
whether a four-body force is needed at a LO description.

In order to treat the helium clusters with increasing
number of particles we use two different methods. We ex-
and the trimer ground state
energy $E_3^*$ (or first excited state $E_3^*$). Accordingly a soft
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\begin{align*}
V(r_{ij}) &= V_0 e^{-r_{ij}/r_0^2} \\
\kappa &= \frac{\hbar^2\kappa_s^2}{m} \\
E_n &= \frac{\hbar^2}{2m} \kappa_s^2 n_s \pi/\pi \\
E_0 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{n_s^2} \pi/\pi \\
E_1 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-1)^2} \pi/\pi \\
E_2 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-2)^2} \pi/\pi \\
E_3 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-3)^2} \pi/\pi \\
E_4 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-4)^2} \pi/\pi \\
E_5 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-5)^2} \pi/\pi \\
E_6 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-6)^2} \pi/\pi \\
E_7 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-7)^2} \pi/\pi \\
E_8 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-8)^2} \pi/\pi \\
E_9 &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-9)^2} \pi/\pi \\
E_{10} &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-10)^2} \pi/\pi \\
E_{11} &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-11)^2} \pi/\pi \\
E_{12} &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-12)^2} \pi/\pi \\
E_{13} &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-13)^2} \pi/\pi \\
E_{14} &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-14)^2} \pi/\pi \\
E_{15} &= \frac{\hbar^2}{2m} \kappa_s^2 \frac{1}{(n_s^2-15)^2} \pi/\pi
\end{align*}
body scattering length $a = 235.547 \, a_0$, with $a_0$ the Bohr radius. These quantities are described with good accuracy using $V_0 = 1.208018 \, \text{K}$ and $r_0 = 10.0485 \, a_0$ (with $\hbar^2/m = 43.281307 \, \text{K} \, a_0^2$). Using this potential the binding energy of the trimer ground state is 139.8 mK, this value is greater than the value obtained with the HFDHE2 potential of 117.3 mK. Accordingly the two-body soft potential has to be supplemented with a slightly repulsive three-body force. This well known characteristic corresponds, in terms of EFT, to a LO description. Following Refs. 27–31 we introduce a three-body force depending on the relative distances of three particles

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

where $\rho_{ijk}^2 = (2/3)(r_{ij}^2 + r_{jk}^2 + r_{ki}^2)$ and the strength $W_0$ and range $\rho_0$ are parameters to be fixed in order to have a reasonable description of the light clusters ground state binding energies $E_N$. In the following we employ the soft-gaussian potential (SGP) model consisting on a two-body plus a three-body term. The SGP ground state binding energies up to $N = 10$ are shown in Fig. 1 (red dots) as a function of the three-body range parameter $\rho_0$. In each case the strength $W_0$ is fixed to reproduce the trimer ground state of the HFDHE2 potential (117.3 mK). The SGP results are compared to those of the HFDHE2 potential [3] given in the figure as the (black) solid lines. As can be seen from the figure there is a slight dependence on the range $\rho_0$, with low values giving a better description. To show the sensitivity to the range of the three-body force and to analyse the behavior of the energy per particle $E_N/N$, in Fig. 2 we show this quantity as a function of $N$. We can observe that, for the values of $N$ given in the figure, $E_N/N$ calculated with the HFDHE2 interaction has an almost linear behavior. The results of the SGP follow this tendency though a spread depending on $\rho_0$ appears as $N$ increases.

In the present study the strength and range of the two-body gaussian potential are determined from $E_2$ and $a$. In a more general perspective a gaussian potential can be thought of as regularized contact interaction and the observables in the different $N$-body sectors can be studied in terms of the range of the gaussian defined as the inverse of the cutoff $r_0 = \Lambda^{-1}$ (for a recent discussion see Ref. 32). In this context the range of the two- and three-body forces are related. Here we follow a different strategy in which the two-body potential is fixed by two data in the $N = 2$ sector. The strength of the three-body potential is determined by $E_3$ for different values of its range $\rho_0$. In this way the evolution of $E_N/N$ can be studied as a function of the parameter $\rho_0$. To be noticed that the two- and three-body potential terms evolve differently with $N$ since one is proportional to the number of pairs and the other to the number of triplets. The intention of using $\rho_0$ as an independent parameter is to keep the evolution of these two terms as close as possible to the results of the original potential. Eventually a particular value of $\rho_0$ can be detected as the optimum value to use in the description of the saturation properties of the infinite system.

$E_N/N$ using a soft potential model. Here we extend the study of $E_N/N$ for increasing values of $N$. The calculations of Ref. 3 using the HFDHE2 potential show that this quantity has an almost linear behavior for $N \leq 10$, as discussed before. As $N$ is increased further $E_N/N$ saturates following the trend given by Eq. (1). This behavior is confirmed by the rms radius which increases almost linearly with $N^{1/3}$ for $N > 20$, resembling a liquid drop. Now we want to analyse the evolution of the binding energy using the SGP. To this aim, we calculate $E_N/N$ and radii up to $N = 112$, this value seems to be sufficient to determine $E_v$ from Eq. (1). The results are given in Fig. 3. There is a large spread in both quantities depending on the three-body range $\rho_0$ given as the cyan band for $E_N/N$ and as error bars for the rms radii. The HFDHE2 results are inside the energy per particle band therefore an optimum value of $\rho_0$ can be identified. From inspection of the results this particular value is $\rho_0 \approx 8.5 \, a_0$ and corresponds to the range needed to get the closest value to the exact tetramer binding energy, as can be seen in the lower panel of Fig. 1. Using this 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 $20 \leq N \leq 112$ we obtain (in K)

$$E_N/N = 6.98 - 18.6 \, x + 10.3 \, x^2$$

(4)
to be compared to the values (in K) $E_v = 7.02$, $E_s =$
can propose the following formula

\[ E_N = E^{(0)}_v \left(1 - \frac{3}{N} \right)^{1/4} \left(1 + \frac{3E_3}{4E_4} \right), \tag{5} \]

where the exponent of 1/4 in the numerator and the energy coefficient in the denominator are optimal choices to describe the GFMC results. Using Eq. (5) to fit the GFMC results in the region 4 \( \leq N \leq 112 \) the value \( E^{(0)}_v \approx 6.8 \) is obtained with a comparable overall accuracy to Eq. (1) as shown in Fig. 3 by the dashed line. If the range of the fit is limited to the region 4 \( \leq N \leq 10 \), where the energy per particle increases almost linearly, the value \( E^{(0)}_v \approx 6.5 \) is obtained. A characteristic of Eq. (5) is that \( E^{(0)}_v \) can be determined using a single value of \( E_N/N \). Making explicit the \( N=4 \) case we obtain

\[ \frac{E^{(0)}_v}{E_4} = 3.602 \left(1 + \frac{9E_3}{16E_4} \right). \tag{6} \]

This relation gives the saturation energy in units of \( E_4 \). Using the GFMC ratio \( E_4/E_3 = 4.55 \) we obtain \( E^{(0)}_v/E_4 = 12.8 \). From this analysis it could be thought that, besides range corrections (to evaluate in a forthcoming analysis), the saturation energy of the droplets could be proportional to \( E_4 \) as \( E^{(0)}_v = \xi_4 E_4 \) with \( \xi_4 \) approaching a universal number at unitary in a similar way in which is defined the Bertsch parameter in the case of a Fermi gas [32].

Conclusions. There are two distinct approaches to describe bosonic helium drops. It is possible to use a realistic atomic interaction obtained from a detailed description of the electronic properties. These potentials are able to describe many observables in the low and high energy domains, as well as transport properties. A different view which puts in evidence the fact that the helium system is close to the unitary limit, is to construct a very simple potential model able to reproduce a few data as the dimer and trimer energies and the large value of the two-body scattering length. This model is constructed as a sum of a two-body (attractive) and a three-body (repulsive) soft terms. It can describe with good approximation properties that emerge as quasi universal, as for example the ratio \( E_0^3/E_3 \) between the ground and excited states of the helium trimer or the ratios \( E_4^3/E_3^3 \) and \( E_4^1/E_3^1 \) between the ground state trimer and the two levels of the tetramer [34]. Our main conclusion is that the universal properties observed in light drops propagate with the number of particles allowing an estimate of the saturation energy from the energy of very light drops. The limiting case is given by Eq. (5) in which the saturation energy can be determined by the ratio \( E_4/E_3 \) and one of the two values. Following some ideas discussed in the literature [32, 33], we have speculated about the universal characteristic of the ratio \( E^{(0)}_v/E_4 \) at unitarity.

A second observation of the present work is that a four-body interaction is not needed to describe the saturation properties at LO. We can conclude that the soft-gaussian potential captures the physics of the system close to uni-
tarity building a bridge between few- and many-body physics.

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