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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 special; on 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 analyze 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/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.

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Introduction. At the beginning of the 1980s strong efforts were made to calculate the ground-state properties of ^{4}He and ^{3}He droplets containing a specific number N of atoms [1–4]. After computing the energy per particle, E_N/N, and the rms radii of the droplets it was possible to study the evolution of these quantities as $N \to \infty$. For example, a liquid-drop formula was proposed to fit E_N/N in terms of $x = N^{-1/3}$:

$$E_N/N = E_v + E_s x + E_c x^2 \tag{1}$$

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 $\langle r^2\rangle^{1/2}$, as $r_0(N) = \sqrt{5/3}\,\langle r^2\rangle^{1/2} N^{-1/3}$. Extrapolated results for the infinite liquid were obtained from calculations on droplets using different values of N. The motivations for that study were twofold. On one hand, the theoretical results obtained with realistic interatomic potentials could be compared to experimental results. In 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.* [5], 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 the 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 $t = E_s/4\pi r_0^2(\infty)$ 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. Note 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 1990s due to the fact that the dimer composed by two ^{4}He atoms is very loosely bound. Its energy is $E_2 \approx 1$ mK, and the two-body scattering length, $a \approx 100$ Å, has a very large value if compared to the typical length of the system, the van der Waals length $\ell_{\rm vdW}$, which for two helium atoms is $\ell_{\rm vdW} \approx 2.5$ Å. When $a \gg \ell_{\rm vdW}$ 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, $E_2 \approx \hbar^2/(ma^2)$, with m the boson mass, vanishes at the unitary limit, corresponding to $a \to \infty$. As demonstrated by Efimov in a series of papers [6,7], 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 [8].

At present, there is intense experimental activity [9–12] dedicated to the study of the behavior of few-body systems close to the unitary limit. In 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 intense experimental activity using ultracold jets of helium going through a diffraction grating [13]. Although 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 states 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 [15,16]. In particular, in Ref. [17] a diffusion Monte Carlo (DMC) method has been used to study clusters up to ten atoms interacting through the Tang, Toennies, and Yiu potential [18]. From a more general perspective, trimers and tetramers have been studied with different interactions in which the potential strength has been varied in order to drive the system to the unitary limit [19–22]. When a two-boson system interacting via a short-range potential is close to the unitary limit, the three-boson system

shows universal behavior. Its spectrum is governed by the two-body scattering length a and the three-body parameter κ_* defines the energy of the n_* level at the unitary limit, $\hbar^2\kappa_*^2/m$. The system manifests a discrete scale invariance; the ratio of binding energies for two consecutive states is $E_3^n/E_3^{n+1} = e^{2\pi/s_0}$, with the universal number $s_0 \approx 1.006\,24$ [23]. The studies using potential models have shown that this description is very well fulfilled if range corrections are taken into account [24].

A three-boson system close to the unitary limit can be described using an effective field theory (EFT) [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 determines the values of a and κ_*. This kind of study has 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 differences) obtained from comparisons to experimental data or results obtained with more realistic interactions can be analyzed. This strategy has been explored in Refs. [27–29] in which the results for the ground-state energy of small clusters of helium calculated using a soft potential model are extremely close (within a few percent) to that obtained using a realistic helium-helium interaction.

From the above discussion we observe two, very distinctive, descriptions of light helium clusters. On one hand, strong efforts have been made to determine the best possible helium-helium interaction. Different models exist 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 behavior. The particular form of the potential is not important and many features can be determined from a few experimental data, such as a and the trimer ground-state energy E_3^0 (or first excited state E_3^1). Accordingly, a soft potential model can be constructed in order to reproduce those observables. Here we want to determine the saturation properties of the infinite system from calculations on helium drops described using a soft potential model making a direct link between the low-energy scale (or long-range correlations) and the high-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 expand the many-body wave function in the hyperspherical harmonic (HH) basis and calculate the ground-state energy for increasing values of the grand orbital quantum number K. The method using two- and three-body potentials is described in Refs. [30,31]. Depending on the range of the three-body force the pattern of convergence in terms of K could not be sufficiently fast to guarantee a converged value for the energy (the maximum value of $K = 16$ has been used). In this case an extrapolation formula is needed to estimate the ground-state energy. In order to decrease the uncertainty introduced by the extrapolation procedure we implemented a DMC algorithm which is known to provide very good estimates of the ground-state energies. For low values of N ($N \leqslant 10$) the HH and DMC results are in complete agreement. For greater values of N and, in particular, for the shorter three-body force ranges considered, the DMC method provides a converged value for the energy, whereas the HH and DMC results coincide only after the extrapolation procedure mentioned above. Due to the big numerical effort needed for the DMC at high N values, we use this method for selected cases. From the combination of the two methods we obtain converged values for the ground-state energy.

The potential model. To study the ground-state energy of the N boson system, as a reference we use calculations on helium drops interacting through the HFDHE2 potential. Results using the Green's function Monte Carlo (GFMC) method are available as well as results using a variational Monte Carlo (VMC) approach. The soft potential model is constructed using a Gaussian representation of the HFDHE2 potential as

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

in which the two parameters, V_0 and d_0, are determined from the dimer energy, $E_2 = 0.830\,12$ mK, and the two-body scattering length $a = 235.547a_0$, with a_0 the Bohr radius. These quantities are described with good accuracy using $V_0 = 1.208\,018$ K and $d_0 = 10.0485a_0$ (with $\hbar^2/m = 43.281\,307\,\mathrm{K}\,a_0^2$). It should be noticed that with the simultaneous description of a and E_2 the correct value of the effective range $r_{\mathrm{eff}} = 13.977a_0$ is obtained as the three quantities are related by the effective range formula, which in the case of shallow states is $k_d = 1/a + r_{\mathrm{eff}}k_d^2/2$, with the binding momentum defined from the relation $E_2 = \hbar^2k_d^2/m$. The particular selection of the Gaussian parameters results in a good description of the low-energy physics in the two-body sector. Moving to the three-body sector, using the Gaussian 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

$$W(\rho_{ijk}) = W_0 e^{-2\rho_{ijk}^2/\rho_0^2}, \tag{3}$$

where $\rho_{ijk}^2 = (2/3)(r_{ij}^2 + r_{jk}^2 + r_{ki}^2)$ and the strength W_0 and range ρ_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 of 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 ρ_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 ρ_0, with low values giving a better description. To show the sensitivity to the range of the three-body force and to analyze the behavior of the energy per particle E_N/N, in

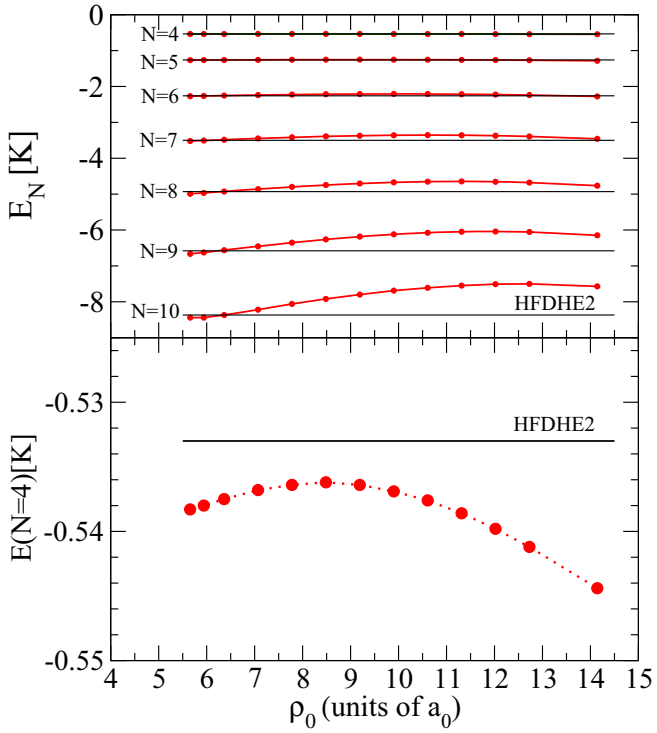

FIG. 1. Binding energies using the SGP for different values of the three-body force range ρ_0 (red dots) at the indicated N values (upper panel). The specific case of $N = 4$ is shown in the lower panel. As a reference, the values of the HFDHE2 potential are also shown (black solid lines).

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, although a spread depending on ρ_0 appears as N increases.

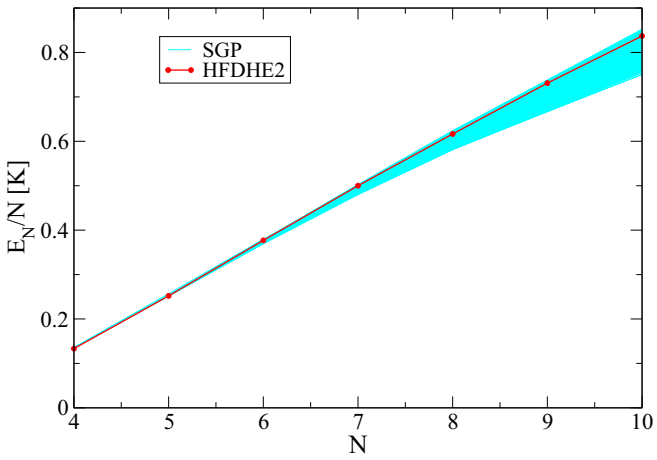

FIG. 2. Binding energy per particle as a function of the number of particles N. The results of the SGP for different values of the three-body force range ρ_0 are shown as the cyan band. As a reference, the values of the HFDHE2 potential from Ref. [3] are shown as solid (red) circles.

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 a 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 $d_0 = \Lambda^{-1}$ (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 ρ_0. In this way the evolution of E_N/N can be studied as a function of the parameter ρ_0. Note 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 ρ_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 ρ_0 can be detected as the optimum value to use in the description of the saturation properties of the infinite system. A similar strategy has been recently used in nuclear physics [33] and in boson systems at unitary [34].

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 $N \leqslant 10$, 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 analyze 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 ρ_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 ρ_0 can be identified. From inspection of the results this particular value is $\rho_0 \approx 8.5a_0$ 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 ρ_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 $20 \leqslant N \leqslant 112$ we obtain (in K)

$$E_N/N = 6.98–18.6x + 10.3x^2 \qquad (4)$$

to be compared to the values (in K) $E_v = 7.02$, $E_s = -18.8$, and $E_c = 11.2$ and $E_v = 6.91$, $E_s = -18.9$, and $E_c = 12.0$ obtained with the GFMC and VMC methods, respectively, using the HFDHE2 interaction.

The infinite unit radius $r_0(\infty)$ can be obtained from a second-order expansion in terms of $x = N^{-1/3}$. The SGP results for the optimum ρ_0 value predict $r_0(\infty) = 2.24$ Å, close to the GFMC result for the HFDHE2 interaction of 2.22 Å and a surface tension $t = E_s/4\pi r_0^2(\infty)$ of 0.29 K Å^{-2}, close to the experimental value of 0.27 K Å^{-2} and the HFDHE2 GFMC result of 0.28 K Å^{-2}. We consider the capability of the SGP of following the energy per particle and the unit radius (giving a reasonable prediction of the surface tension) a consequence

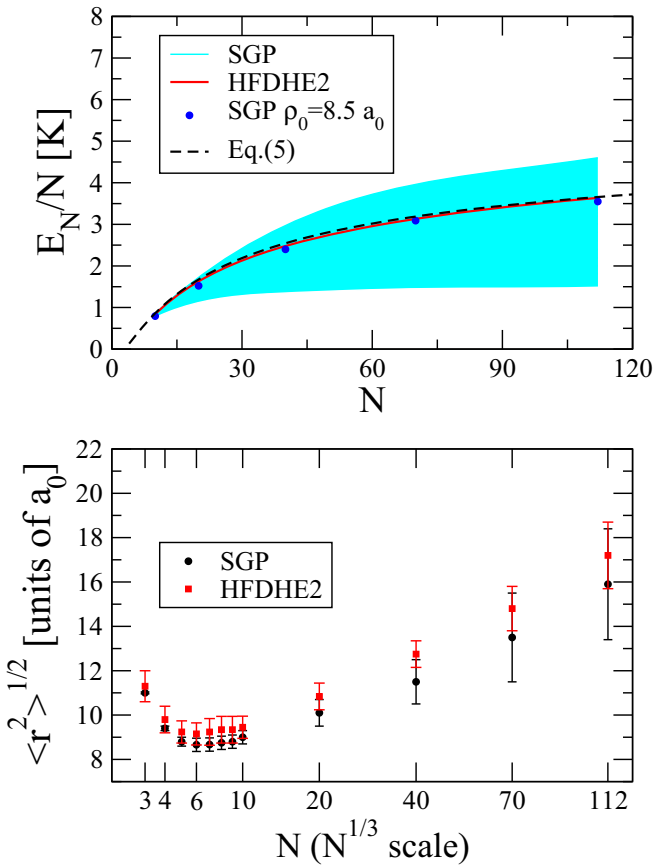

FIG. 3. Binding energy per particle (upper panel) and rms radii (lower panel) as a function of the number of particles N. The different values of the range ρ_0 of the SGP are shown as the cyan band (for E/N) or as error bars (rms radii). The dashed line is the prediction of Eq. (5) (see text). The values of the HFDHE2 potential are also presented.

of the propagation of the universal behavior observed in the three-body sector to the infinite system. This is an unexpected result. Accordingly, we can think in a different expansion of E_N/N in terms of N incorporating explicitly the energy values of the light droplets. Considering that $E_3/3$ is almost negligible compared to E_N/N as $N \to \infty$, we can propose the following formula:

$$\frac{E_N}{N} = E_v^{(0)} \frac{1-(3/N)^{1/4}}{1+\frac{3E_4}{4E_3}(3/N)}, \tag{5}$$

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 $4 \leqslant N \leqslant 112$ the value $E_v^{(0)} \approx 6.8$ 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 $4 \leqslant N \leqslant 10$, where the energy per particle increases almost linearly, the value $E_v^{(0)} \approx 6.5$ is obtained. A characteristic of Eq. (5) is that $E_v^{(0)}$ can be determined using a single value of E_N/N. Making explicit the $N = 4$ case, we obtain

$$\frac{E_v^{(0)}}{E_4} = 3.602\left(1+\frac{9E_4}{16E_3}\right). \tag{6}$$

This relation gives the saturation energy in units of E_4. Using the GFMC ratio $E_4/E_3 = 4.55$ we obtain $E_v^{(0)}/E_4 = 12.8$. 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 $E_v^{(0)} = \xi_4 E_4$ with ξ_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 [35].

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 cloud. These potentials are able to describe many observables in the low- and high-energy domains, as well as transport properties. A different view which evidences 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 such 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 term. It can describe with good approximation properties that emerge as quasiuniversal, as, for example, the ratio E_3^0/E_3^1 between the ground and excited states of the helium trimer or the ratios E_4^0/E_3^0 and E_4^1/E_3^0 between the ground-state trimer and the two levels of the tetramer [36]. 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 [32,37], we have speculated about the universal characteristic of the ratio $E_v^{(0)}/E_4$ 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 unitarity building a bridge between few- and many-body physics.

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