Universal nature and finite-range corrections in elastic atom-dimer scattering below the dimer breakup threshold

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Abstract

We investigate universal behavior in elastic atom-dimer scattering below the dimer breakup threshold calculating the atom-dimer effective-range function $ak \cot \delta$. Using the He-He system as a reference, we solve the Schrödinger equation for a family of potentials having different values of the two-body scattering length $a$ and we compare our results to the universal zero-range form deduced by Efimov, $ak \cot \delta = c_1(ka) + c_2(ka) \cot[s_0 \ln(\kappa_s a) + \phi(ka)]$, for selected values of the three-body parameter $\kappa_s$. Using the parametrization of the universal functions $c_1, c_2, \phi$ given in the literature, a good agreement with the universal formula is obtained after introducing a particular type of finite-range corrections. Furthermore, we show that the same parametrization describes a very different system: nucleon-deuteron scattering below the deuteron breakup threshold. Our analysis confirms the universal character of the process, and relates the pole energy in the effective-range function of nucleon-deuteron scattering to the three-body parameter $\kappa_s$.

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I. INTRODUCTION.

Scattering of two particles at very low energy shows universal behavior encoded in the scattering length $a$ and in the effective range $r_s$. In fact, systems with different interactions sharing the same scattering length and the same effective range have the same effective range function, $k \cot \delta = -1/a + r_s k^2/2$, and, accordingly, the same low energy behavior. In the limit $a \gg r_0$, where the scattering length is much greater than the typical range of the potential $r_0$, not only the scattering process is universal, but also some bound-state properties. When $a \to +\infty$ (known as unitary limit), the two-particle system has a shallow-bound state with the bound-state energy $E_2 \approx \hbar^2/ma^2$ fixed by the scattering length. In this limit, the physics is scale invariant.

In the 1970s, V. Efimov [? ? ] showed that the scale invariance is broken in the $s$-wave three-body sector of a bosonic system. The residual symmetry is the discrete scale invariance (DSI); namely, the physics is invariant under the rescaling $r \to \Lambda^n r$, where the constant is usually written $\Lambda = e^{\pi/s_0}$, with $s_0 \approx 1.00624$ an universal number that characterizes a system of three-identical bosons. One consequence is that at the unitary limit the three-body spectrum consists of an infinite number of states that accumulate to zero with the ratio between two consecutive states being $E_{n+1}^3/E_n^3 = e^{-2\pi/s_0}$. For finite scattering length, the binding energies satisfy the Efimov’s equation

$$E_n^3 + \frac{\hbar^2}{ma^2} = e^{-2(n-n_*)\pi/s_0} \exp \left[ \Delta(\xi)/s_0 \right] \frac{\hbar^2 \kappa_*^2}{m},$$

with $\tan \xi = -(mE_n^3/\hbar^2)^{1/2}a$. The function $\Delta(\xi)$ is universal and a parametrization in the interval $[-\pi, -\pi/4]$ is given in Ref. [? ]. The three-body parameter $\kappa_*$ is the wave number of the $n = n_*$ state at the unitary limit.

The DSI constrains the form of the observables to be log-periodic functions of the control parameters. One example is the atom-dimer scattering length which has the general form

$$a_{AD}/a = d_1 + d_2 \tan \left[ s_0 \ln(\kappa_* a) + d_3 \right],$$

where $d_1, d_2, d_3$ are universal constants whose value has been determined in the zero-range limit [? ]. For collisions below the dimer breakup threshold, DSI imposes the following universal form for the effective range function

$$ka \cot \delta = c_1(ka) + c_2(ka) \cot \left[ s_0 \ln(\kappa_* a) + \phi(ka) \right]$$

(3)
with $\delta$ the atom-dimer phase-shift and $c_1, c_2, \phi$ universal functions of the dimensionless variable $ka$, where $k^2 = (4/3)E/(\hbar^2/m)$, being $E$ the center of mass energy of the process. As $k \to 0$, $ka \cot \delta \to -a/a_{AD}$ and at $k = 0$ the constants $d_1, d_2, d_3$ and $c_1(0), c_2(0), \phi(0)$ are related by simple trigonometric relations. A parametrization of the universal constants and functions can be found in Ref. [? ].

In this paper we study in detail the universal behavior of $a_{AD}$ and of the effective range function $ka \cot \delta$. To this aim, we use the family of atomic $^4$He–$^4$He potentials derived in Ref. [?] for several values of $a$, running from $a \approx 440\, a_0$ to $a \approx 50\, a_0$. The corresponding dimer energies range from $E_2 \approx 0.22\, \text{mK}$ to $E_2 \approx 21\, \text{mK}$ covering two order of magnitude. For selected values of $a$ in the mentioned interval we calculate $a_{AD}$ and the $s$-wave phase-shift in order to construct the effective range function below the dimer breakup threshold. As predicted by Eq. (3), when the value of $a$ increases we observe that $a_{AD}$ changes sign tending to $-\infty$. This behavior produces a pole in the effective range function. More specifically, our numerical results are used to analyze the universal form of Eqs. (2) and (3), and, as the calculations are done using finite-range interactions, to extract finite-range corrections by comparing our results to the zero-range theory. Interestingly, for the explored zone of positive scattering length, the range corrections can be taken into account by a shift in the variable $\kappa a$.

This study is of interest for several fields of research, ranging from cold-atoms to nuclear physics and, in particular, in halo nuclei where a cluster description is justified. In atomic physics, where the Efimov effect has been observed for the first time [? ], discrepancies arise between the theoretical prediction and the experimental determination of the ratio between $a_+\text{ and } a_-\text{ [? ? ] }$, that means between the scattering lengths at which an Efimov state disappears in the atom-dimer and in the three-atom continuum, respectively. The solution to this puzzle is probably hidden in finite-range corrections to the universal formulas (see Ref [?] and references therein for a recent account of the problem). In halo nuclei there has been a lot of interest in the observation of universal aspects in the scattering of a neutron on a neutron-halo nucleus having a large scattering length, as for example the $n - ^{19}\text{C}$ system (see Refs. [? ? ] and Ref. [?] for a recent review). In this context we make use of the universal character of the effective range function to evaluate a very different system: low energy nucleon-deuteron scattering. It is well known that the nucleon-deuteron effective range function presents a pole structure that has been related to the presence of a virtual
state. First observations of this particular behavior have been done in Refs. [397] whereas in Ref.[397] an explicit calculation of the effective range function has been done using a semi-realistic nucleon-nucleon potential. In this last reference the calculations allowed to extract the energy of the pole after fitting the effective range formula with the form suggested by Delves [397]. In the present work, we show that the pole structure of the effective range function can be quantitatively related to the universal form given by Eq.(3) and, using the parametrization determined in the atomic three-helium system, we apply that equation to describe nucleon-deuteron scattering as well. In particular, using the universal function \( \phi \), the energy of the pole can be used to extract the three-body parameter \( \kappa_* \). In this way, the universal behavior imposed by the DSI is analyzed in systems with natural lengths that differ of several order of magnitude.

II. THE THREE-BOSON MODEL.

We construct the model using the LM2M2 [397], one of the most used \(^4\text{He}-^4\text{He}\) potentials, as the reference interaction, with the mass parameter \( \hbar^2/m = 43.281307 \, (a_0)^2 \, \text{K} \). In order to change the value of the scattering length, we have modified the LM2M2 interaction as following

\[
V_\lambda(r) = \lambda \cdot V_{\text{LM2M2}}(r) .
\]

Examples of this strategy exist in the literature [397]. The unitary limit is produced for \( \lambda \approx 0.9743 \) whereas for \( \lambda = 1 \) the values of the LM2M2 are recovered: \( a = 189.41 \, a_0 \), \( E_2 = -1.303 \, \text{mK} \) and the effective range \( r_s = 13.845 \, a_0 \).

Following Ref. [397] we define an attractive two-body Gaussian (TBG) potential

\[
V(r) = V_0 \, e^{-r^2/r_0^2} ,
\]

with range \( r_0 = 10 \, a_0 \) and strength \( V_0 \) fixed to reproduce the values of \( a \) given by \( V_\lambda(r) = \lambda \cdot V_{\text{LM2M2}}(r) \). For example the strength \( V_0 = -1.2343566 \, \text{K} \) corresponds to \( \lambda = 1 \) reproducing the LM2M2 low-energy data, \( E_2 = -1.303 \, \text{mK} \), \( a = 189.42 \, a_0 \), and \( r_s = 13.80 \, a_0 \).

The use of the TBG potential in the three-atom system produces a ground-state-binding energy appreciable deeper than the one calculated with \( V_\lambda(r) \). For example, at \( \lambda = 1 \) the LM2M2 helium-trimer ground-state-binding energy is \( E_3^0 = 126.4 \, \text{mK} \) whereas the one obtained using the two-body-soft-core potential in Eq. (5) is 151.32 mK. Hence, we introduce
a repulsive hypercentral-three-body (H3B) interaction

\[ W(\rho_{123}) = W_0 \, e^{-\rho_{123}/\rho_0}, \]

with the strength \( W_0 \) tuned to reproduce the trimer energy \( E_3^0 \) obtained with \( V_\lambda(r) \) for all the explored values of \( \lambda \). Here \( \rho_{123}^2 = \frac{2}{3}(r_{12}^2 + r_{23}^2 + r_{31}^2) \) is the hyperradius of three particles and \( \rho_0 \) gives the range of the three-body force. Following Ref. [?] we use \( \rho_0 = r_0 \). It should be noticed that the description of the three-boson systems using a two- plus three-body interaction constructed to reproduce the low energy data is equivalent, up to finite range corrections, to a description based on effective field theory (EFT) at leading order [? ].

Varying \( \lambda \) from the unitary limit to \( \lambda = 1.1 \) we obtain a set of values for the ground state binding energy \( E_3^0 \) and first excited state \( E_3^1 \) using the TBG and TBG+H3B potentials in a broad interval of \( a \). We use the results for \( E_3^1 \) at the unitary limit (by means of Eq. (1) with \( n_* = 1 \)) to determine \( \kappa_* = 0.002119 \, a_0^{-1} \) and \( \kappa_* = 0.001899 \, a_0^{-1} \) for the TBG and TBG+H3B, respectively. In Fig. we collect our results for the ratio \( E_3^1/E_2 \) as a function of \( \kappa_* a \) for the TBG potential (full circles) and of the TBG+H3B potential (full squares). We compare the numerical calculations to the predictions of the Efimov’s binding energy Eq. (1), given in the figure by the dashed line. We observe that the numerical results lie on a curve shifted with respect to the dashed line. We can interpret the shift as a consequence of the finite-range character of the numerical results. Accordingly, we can adapt the Efimov’s equation to treat finite-range interactions. Once we fix \( n_* = 1 \), Eq. (1) can be rewritten as follow

\[ \frac{E_3^1}{E_2} = \tan^2 \xi, \quad \kappa_* a = \exp \left[-\Delta(\xi)/2s_0\right]/\cos \xi, \]

where we have introduced finite-range correction by \( \hbar^2/ma^2 \rightarrow E_2 \), in the two-body sector, and by a shift \( \kappa_* a = \kappa_* a + \Gamma \). Our calculations have been made for two different values of \( \kappa_* \), allowing us to infer that in first approximation \( \Gamma \approx \kappa_* r_* \), with \( r_* = 21 \, a_0 \approx 2r_0 \). At the unitary limit, the relative weight of this shift becomes negligible, and Eq. (7) tends to Eq. (1).

Equation (7) can be generalized to states different from the first excited; however, the shift in this case will also depend on the size of the state and will not be negligible at the unitary limit. The corresponding results, obtained by solving Eq. (7) with \( \kappa_* a = \kappa_* a + \kappa_* r_* \), are shown in Fig. (1) as a solid line.
FIG. 1. (Color online) Energy of the first excited state of the trimer as a function of \( \kappa_* a \). The dashed line is the universal prediction of the Efimov law, while the solid line is the translated universal curve. The full circles and full squares are the calculations using the TBG and TBG+H3B potentials respectively.

III. ATOM-DIMER SCATTERING.

To describe atom-dimer scattering below the dimer threshold we calculate \( a_{AD} \) and the s-wave atom-dimer phases \( \delta \) using the TBG and TBG+H3B potentials at different energies. We use the hyperspherical harmonic (HH) method in conjunction with the Kohn variational principle \[?\]. Applications of the method to describe a three-helium system with soft-core interactions as used here can be found in Ref. \[?\]. As an example in Table II the \( a_{AD} \) convergence pattern is given for \( \lambda = 1 \) using the TBG potential. The results for \( a_{AD} \) are studied in terms of the size of the HH basis given by the grand orbital quantum number \( K \) and the quantum number \( m \) of the hyperradial basis (here taken as Laguerre functions \[?\]).
When the TBG+H3B potential is considered the rate of convergence remains the same and the final value is 208 \( a_0 \). It should be noticed that as \( a \) increases, and correspondingly \( |E_2| \) diminishes, is necessary to increase the size of the basis. At the largest value of \( a \) considered, \( a \approx 441 \ a_0 \), we have used a basis with \( m = 60 \) and \( K = 800 \).

| \( m/K \) | 120 | 240 | 360 | 480 |
|-----------|-----|-----|-----|-----|
| 24        | 169.64 | 165.40 | 165.23 | 165.22 |
| 28        | 169.59 | 165.32 | 165.10 | 165.09 |
| 32        | 169.55 | 165.28 | 165.05 | 165.04 |
| 36        | 169.54 | 165.27 | 165.04 | 165.02 |
| 40        | 169.53 | 165.26 | 165.03 | 165.02 |

TABLE I. The atom-dimer scattering length \( a_{AD} \) (in \( a_0 \)) in terms of the number of Laguerre polynomial \( m \) and the grand angular quantum number \( K \).

Defining \( E_2 = \hbar^2/ma_B^2 \), in Fig. 2 we show the results for the ratio \( a_{AD}/a_B \) in terms of the product \( \kappa_s a \). It can be observed that the calculated points, given as full circles (TBG potential) and full squares (TBG+H3B potential), lie on a curve shifted with respect to the dashed line representing Eq. (2) with the parametrization of Ref. [? ]. We can interpret again the shift as produced by the finite-range character of the calculations. Accordingly we can adapt Eq. (2) to describe finite-range interaction as

\[
a_{AD}/a_B = d_1 + d_2 \tan[s_0 \ln(\kappa_s a) + d_3].
\]

(8)

In fact, replacing in the above equation \( \kappa'_s a = \kappa_s a + \kappa_s r_s \), with the same numerical value of \( r_s \) as before, the solid line is obtained in Fig. 2. The values \( d_1 = 1.531 \) \( d_2 = -2.141 \), \( d_3 = 1.100 \) slightly modify the parametrization of Ref. [? ] to better describe the numerical results. This new parametrization is shown as a dotted line in the figure where we can observe an improvement in the description of the results close to the unitary limit.

The shifted formula can be used to determine the ratio \( a_*/a_- \), where \( a_- \) is the scattering length at which the three-body states disappear into the three-atom continuum, and \( a_* \) is the scattering length at which the three-body states disappear into the atom-dimer continuum. For the potential models used in this work the values of \( a_- \) are given in Ref. [? ] whereas the values of \( a_* \) can be extracted by equating the argument of the tangent in Eq. (8) to

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\[ -\pi/2. \] Using these inputs we obtain \( a_*/a_- \approx -0.32 \) for both \( \kappa_* = 0.002119 \ a_0^{-1} \) and \( \kappa_* = 0.001899 \ a_0^{-1} \). The zero-range universal formulas Eq. (1) and Eq. (2) predict \( a_*/a_- = -1.07 \), but recent experimental results give lower values for this ratio \[ ? \]. The difference is given by finite-range effects \[ ? \], which in our case are encoded in the shift.

![Graph](image)

**FIG. 2.** (Color online) Universal plot for \( a_{AD}/a_B \) in terms of \( \kappa_* a \). Open circles and open squares correspond to TBG and TBG+H3B potentials respectively. The dashed line corresponds to Eq. (2), whereas the solid line corresponds to Eq. (8). The dotted line shows the present parametrization of Eq. (8).

It is interesting to see that the finite-range corrections cancel in the description of the scattering length as a function of the trimer energy. This is shown in Fig. 3 in which the present calculations and the zero-range universal theory, Eqs. (1) and (2), are in close agreement.

We now present results for atom-dimer scattering at energies below the dimer breakup threshold for different values of \( a \). We adapt Eq. (3) to finite-range interactions by con-
FIG. 3. (Color online) The ratio \( a_{AD}/a_B \) as a function of \( E_3^1/E_2 \). Open circles and open squares correspond to TBG and TBG+H3B potentials respectively. The dashed line corresponds to Eq. (2) with the parametrization of Ref. [? ], whereas the dotted line shows the present parametrization of Eq. (8).

\[
\kappa_\ast = 2.119 \times 10^{-3} \ a_0^{-1} \quad \kappa_\ast = 1.899 \times 10^{-3} \ a_0^{-1}
\]

sidering \( ka_B \cot \delta \) as a function of the dimensionless center of mass energy \((ka)^2\) and using \( \kappa'_a = \kappa_a + \kappa_r \) in the argument of the logarithm function.

\[
ka_B \cot \delta = c_1(ka) + c_2(ka) \cot [s_0 \ln(\kappa'_a) + \phi(ka)]. \tag{9}
\]

In Fig. 4 we show our results (given as full squares) at different values of \( \kappa'_a \). In the figure we can observe very different patterns. For the smallest values of \( \kappa'_a \) the behavior is almost linear in all the energy range. Starting at values of \( \kappa'_a \approx 0.4 \) a curvature appears close to zero energy, pointing out to an emergent pole structure that becomes evident at larger values of \( \kappa'_a \). Specifically, the pole appears when \( a_{AD} \) changes sign (see Fig. 2) or, as given in Eq. (9), when the argument of the cotangent function becomes zero (or \( n\pi \)). The shadow plot in the first row of Fig. 4 corresponds to the case \( \lambda = 1 \) and describe \(^4\text{He}^-\text{He}_2\) scattering (full
FIG. 4. (Color online) The effective range function at different values of $\kappa^*a$ as a function of $(ka)^2$. The square points are our calculations; the triangle points are the calculations for real $^4\text{He} - ^4\text{He}_2$ scattering. The full circles, for $\kappa^*a = 0.543055$, correspond to neutron-deuteron scattering in the doublet channel. The solid curves have been calculated using the translated-universal formula for the different values of $\kappa^*a$.

The shadow plot in the second row corresponds to nucleon-deuteron scattering as discussed below. The solid curves are obtained using the finite-range-adapted Eq. (9) with the parametrization of Ref. [? ]. We can observe a noticeable agreement along the whole range of values.
IV. NUCLEON-DEUTERON SCATTERING.

The universal effective range function has been determined using the TBG and the TBG+H3B potentials describing an atomic three-helium system. The universal character of the function allow us to apply it to describe a very different system: nucleon-deuteron \((n - d)\) scattering. Many efforts have been given in the past to understand the peculiar form of the \(n - d\) effective range function at low energies (see Refs. [? ? ? ]). However, Efimov showed that this process can be described with the universal formula of Eq.(3) [? ]. Accordingly we would like to apply Eq.(9) to perform a quantitatively description of \(n - d\) scattering at low energies. To this aim we use the results of Ref. [? ] in which \(n - d\) scattering has been described using a spin dependent central potential. In that reference they obtained \(a_{nd} = 0.71\) fm for the \(n - d\) scattering length, and the effective range function has been parametrized as

\[
k \cot \delta = \frac{-1/a_{nd} + rs k^2/2}{1 + E_{c.m.}/E_p}
\]

with \(E_p = -160\) keV and \(rs \approx -127\) fm. It should be noticed that this particular parametrization of the effective range function can be simple related to Eq.(9) in the low energy limit. Accordingly, from the values of \(E_p\) and \(a_{nd}\) it is possible to determine the corresponding values of \(a\) and \(\kappa' a\) by using the universal function \(\phi\) and Eq. (8). We obtain \(a = 4.075\) fm and \(\kappa' a = 0.5779\). The pole appears in the negative region similar to what happens in Fig. 4 at intermediate \(\kappa' a\) values. The shadow panel of the second row in Fig. 4 shows a comparison of the universal function (solid line) to the \(n - d\) scattering results of Ref. [? ] (full circles). We observe a noticeable agreement. It should be noticed that the spin dependent potential used in Ref [? ] reproduces the singlet \((^1a_{np} \approx -20\) fm) and triplet \((^3a_{np} \approx 5\) fm) \(n - p\) scattering lengths. Accordingly, the three-nucleon systems has a symmetric plus a mixed symmetry component. The value of \(a\) extracted from the universal function, which is close to \(^3a_{np}\), can be considered an effective value in an equivalent three-boson system with the given \(a_{nd}\) and the corresponding effective range function. A more deeper analysis extending the model to spin dependent interactions is at present underway.

This study could be of interest in light neutron halo systems in which a low energy neutron can impact on a loosely bound n-core system. For example, specific applications of Eq.(3) recently appears in low energy \(n - ^{19}\text{C}\) scattering [? ]. We expect that the use of Eq.(3) will be useful in further studies of such systems.
V. CONCLUSIONS

In this work we have analyzed the low energy behavior of a three-boson system in which the interaction between two bosons produces a large scattering length. Following Ref. [? ], we have used the three-helium system as a reference system and, in the spirit of EFT at LO, we have constructed an attractive two-body interaction plus a repulsive three-body interaction devised to reproduce the two-body scattering length and three-body binding energy of the LM2M2 interaction. From our numerical results we have shown that, when finite range interactions are used, the zero-range universal formula has to be adapted introducing a shifted three-body parameter $\kappa'_a = \kappa_a + \kappa r_s$. This is a particular type of range corrections and the numerical value of $r_s \approx 2r_0$, in the case of the helium system, has been extracted from our calculations. We have proposed and solved Eq.(7) to describe the spectrum of a three-boson system. This equation can be considered an extension of Eq.(1) for finite range interactions; they are characterized by two parameters, the effective range $r_s$ (in the relation between $E_2$ and $a$) and the shift $r_*$, that are somehow connected. Their relation is at present subject of investigation.

In the case of atom-dimer scattering we have proposed Eqs.(8) and (9) introducing the shifted parameter $\kappa'_a$. In order to describe our numerical results we have used the parametrization of Ref. [? ], which, without the inclusion of the shift, can not quantitatively describe the very complicated structure of the effective range function. Interestingly, the value of $r_*$ necessary to describe the results is the same for $E_3$, for $a_{AD}$ and for the effective range function. This type of correction can be compared to the range corrections obtained in very recent works [? ? ].

As a second application we have used Eq.(9) to describe low energy $n - d$ scattering. The values of $\kappa'_a$ and $a$ entering in the equation have been determined from the pole energy $E_p$ and the doublet scattering length $a_{nd}$ given in Ref. [? ]. A quantitative agreement between a direct application of Eq.(9) and the calculations on the $n - d$ system has been found. This analysis connects the universal behavior of atomic systems having large two-body scattering length to nuclear systems. Work in progress includes the extension of the present analysis to energies above the dimer breakup, in particular the description of the recombination rate at threshold, and the extension to include spin and isospin degrees of freedom in order to consider nuclear systems.