Abstract. The helium trimer is studied using two- and three-body soft-core potentials. Realistic helium-helium potentials present an extremely strong short-range repulsion and support a single, very shallow, bound state. The description of systems with more than two helium atoms is difficult due to the very large cancellation between kinetic and potential energy. We analyze the possibility of describing the three helium system in the ultracold regime using a gaussian representation of a widely used realistic potential, the LM2M2 interaction. However, in order to describe correctly the trimer ground state a three-body force has to be added to the gaussian interaction. With this potential model the two bound states of the trimer and the low energy scattering helium-dimer phase shifts obtained with the LM2M2 potential are well reproduced.

1 Introduction

In recent years systems of two- and three-helium atoms have been object of intense investigation from a theoretical and experimental point of view. The existence of the He-He molecule was experimentally established in the nineties using diffraction experiments [1, 2, 3, 4]. Its binding energy has been estimated to be around 1 mK and its scattering length \(a_0\) around 190 a.u. This makes the He-He molecule one of the biggest diatomic molecules. Parallel to these studies, several accurate investigations of the He-He interaction have appeared in the literature. We can mention the potentials called HFDB [5], LM2M2 [6], TTY [7] and the potentials SAPT1 and SAPT2 [8], constructed on a completely \textit{ab initio} calculation made by Korona et al. [9], using infinite order perturbation theory (SAPT) and a very large orbital basis set. In addition, retarded dipole-dipole dispersion interaction is included over the range 0 – 100000 a.u.(SAPT1), or the more appropriate 10-100000 a.u.(SAPT2). Recently, in Refs. [10, 11], He-He interactions including retardation corrections and a non-additive three-body term have also been determined. All these potentials present the common feature of a sharp repulsion below an inter-particle distance of approximately 5 a.u.
Another important characteristic of the He-He interactions is their effective range \( r_0 \), which takes a value of around 13 a.u. Accordingly, the ratio \( a_0/r_0 \) is rather large (\( > 10 \)), which has important consequences in the properties of the three-atom systems. In fact, the (bosonic) three \(^4\)He system presents an excited state just below the atom-dimer threshold that has been identified as an Efimov state \[12\,13\]. As shown by Efimov, when at least two of the two-body subsystems present an infinitely large scattering length (or zero binding energy) an infinite sequence of bound states (called Efimov states) appear in the three-body system. The number of these states has been estimated in Ref. \[13\] to be \( N = (\omega_0/\pi)\ln|a_0/r_0| \), with \( \omega_0 \approx 1.00662378 \) (see Ref. \[14\] and references therein). Triggered by this interesting fact, several investigations of the helium trimer have been produced establishing that its excited state is indeed an Efimov-like state (see for example Refs. \[15\,16\,17\]). In addition, analysis of the atom-dimer collision in the ultracold regime have also been performed \[14\,18\,19\].

Specific algorithms have been developed to solve the quantum mechanical three-body problem. In the particular case of three helium atoms, due to the strong repulsion of the He-He potential, the Faddeev equation has been opportunely modified \[20\]. Also, the hyperspherical adiabatic (HA) expansion has been extensively used in the description of three-body systems (for a review see Ref. \[21\]). However, due to the difficulties in treating the strong repulsion, few calculations exist for systems with more than three helium atoms. For example, in Ref. \[22\] the diffusion Monte Carlo method was used to describe the ground state of He molecules up to 10 atoms. On the other hand, description of few-atoms systems using soft-core potentials are currently operated (see for example Ref. \[23\]). Therefore the question of the equivalence between a description using a hard-core potential or a soft-core one needs some clarification.

Accordingly, in the present work we shall discuss the description of the three \(^4\)He system using an attractive He-He gaussian potential designed to reproduce the helium dimer binding energy, the He-He scattering length \( a_0 \), and the effective range \( r_0 \) of the LM2M2 potential \[5\]. Two potentials having similar values of \( a_0 \) and \( r_0 \) predict similar phase shifts in the low energy limit and, therefore, even if their shape is completely different, they describe in an equivalent way the physical processes in that limit. It is clear that when the energy of the system is increased the details of the potential become more and more important. In a three-body system the relative energy of a two-body subsystem is not fixed and, depending on the particular structure under observation, a certain range of those two-body energies could be of importance in the construction of such a structure. When this range exceeds the region of equivalence of the two potentials, the three-body structures obtained with them could be different. A clear example is the ground state energy of the three-helium system, which takes the value of \(-126.4 \) mK when the LM2M2 potential is used, and \(-150.0 \) mK when using its gaussian representation. It is clear that the lack of repulsion in the gaussian potential allows the atoms to be closer increasing their binding energy.

In order to make the description with the gaussian potential closer to the one obtained when using the LM2M2 potential, we shall include a three-body force of short-range character, such that its strength will be fixed to reproduce
the ground state binding energy of the system. The quality of this description will be judged by comparing the binding energy of the excited Efimov state and the low energy helium-dimer phase shifts to those obtained with the LM2M2 potential. As we will see, both descriptions are in extremely good agreement showing that it is possible to replace the potential presenting a sharp repulsion by opportune designed two- and three-body soft-core potentials to explore the low-energy regime.

The numerical calculations will be performed by means of the hyperspherical adiabatic expansion method as a tool to obtain three-body wave functions [21], and the recently introduced integral relations in order to extract the phase shifts in 1+2 reactions [24, 25]. A brief summary of these two methods will be given in the next section. In section 3 we give the details of the soft-core gaussian He-He interaction, and discuss the results obtained for the three-4He system when such interaction is used. As we shall show, the use of the integral relations will permit to extract accurate phase shifts without requiring a correct description of the asymptotic part of the three-body wave function. The role played by the inclusion of the short-range three-body force is investigated in section 4. We close the paper with the summary and the conclusions.

2 Scattering states using the HA expansion

2.1 Phase shifts and integral relations

Scattering states are usually investigated by determining the asymptotic part of the scattering wave function, from which the phase shifts (or the $\mathcal{K}$-matrix) are extracted. However, even for processes involving only three particles, the calculation of the large distance part of the wave function is a delicate issue. Very often a proper description of this asymptotic part requires an extremely large basis set, which makes the problem sometimes unaffordable.

In Refs. [24, 25] a new method intended to extract phase shifts for 1+N reactions was presented. This method, which is derived from the Kohn Variational Principle, is a generalization to more than two particles of the integral relations shown in [26, 27], and it permits to extract phase shifts from the internal part of the wave functions. In other words, knowledge of the large distance asymptotics is not needed, and therefore accurate calculations can be performed by use of a basis of a much smaller size. Here we summarize the method for 1+2 reactions where only the elastic channel is open, although it can be generalized to multichannel processes [28].

Let us consider a process where a particle hits a bound dimer (1+2 reaction), and let us assume that the incident energy is below the threshold for breakup of the two-body bound target. This is a three-body process that can be described through the usual Jacobi coordinates $x$ and $y$ [21], where for convenience the $x$-coordinate is chosen between the two particles forming the dimer. The three-body wave function $\Psi$ describing the corresponding three-body system is given by the solution of the Schrödinger equation:

$$\left( \mathcal{H} - E \right) \Psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + V - E \right) \Psi = 0,$$  (1)
where $m$ is the normalization mass used to describe the Jacobi coordinates [21].

$V$ represents the sum of the interactions between each pair of particles, and $E$ is the three-body energy.

For our particular case, where the energy of projectile is below the threshold for breakup of the dimer, the asymptotics of the three-body wave function takes the form:

$$\Psi \rightarrow AF + BG = A \left(F + \frac{B}{A} G\right), \quad (2)$$

where

$$F = \sqrt{k_y j_y(k_y y)} \left[\psi^{j_x} \otimes [Y_{\ell_y}(\Omega_y) \otimes \chi_{s_y}]^{J_M}\right],$$

$$G = \sqrt{k_y \eta_y(k_y y)} \left[\psi^{j_x} \otimes [Y_{\ell_y}(\Omega_y) \otimes \chi_{s_y}]^{J_M}\right], \quad (3)$$

where $j_y$ and $\eta_y$ are the regular and irregular spherical Bessel functions, $\ell_y$ is the relative angular momentum between projectile and target, $\psi^{j_x}(x)$ is the wave function of the bound dimer with angular momentum $j_x$, and $\chi_{s_y}$ is the spin function of the projectile. The quantum numbers $\ell_y$ and $s_y$ couple to $j_y$, which couples to $j_x$ to the total angular momentum $J$ of the three-body system with projection $M$. Finally, the momentum $k_y$ is given by $\sqrt{2m(E - E_{2b})/\hbar^2}$, where $E_{2b}$ is the binding energy of the dimer.

From Eq.(2) we can immediately identify:

$$\tan \delta = -\frac{B}{A}, \quad (4)$$

and the coefficients $A$ and $B$ are given by [24, 25]

$$B = -\frac{2m}{\hbar^2} \left[\langle F|\mathcal{H} - E|\Psi \rangle - \langle \Psi|\mathcal{H} - E|F \rangle\right], \quad (5)$$

$$A = -\frac{2m}{\hbar^2} \left[\langle \Psi|\mathcal{H} - E|G \rangle - \langle G|\mathcal{H} - E|\Psi \rangle\right], \quad (6)$$

where we have made used of the normalization condition:

$$-\frac{2m}{\hbar^2} \left[\langle F|\mathcal{H} - E|G \rangle - \langle G|\mathcal{H} - E|F \rangle\right] = 1. \quad (7)$$

When $\Psi$ is the exact solution of the Schrödinger equation (1), it is then obvious that $A$ and $B$ are given by:

$$B = \frac{2m}{\hbar^2} \langle \Psi|\mathcal{H} - E|F \rangle \quad (8)$$

$$A = -\frac{2m}{\hbar^2} \langle \Psi|\mathcal{H} - E|G \rangle. \quad (9)$$

In Refs. [24, 25, 28] it is proved that, thanks to the Kohn Variational Principle, when a trial three-body wave function $\Psi^t$ is used, the two expressions above are still valid up to second order in $\delta\Psi = \Psi - \Psi^t$. This fact permits to extract a second order approximation of the phase shifts according to Eq.(4).
It is important to have in mind that the Bessel function $\eta \ell y$ contained in $G$, Eq.(3), is not regular at the origin. This technical problem is solved by replacing in the expressions above the function $G$ by $G(1 - e^{-\gamma y})\ell y$, where $\gamma$ is a non-linear parameter. The results are stable with $\gamma$ in a range of values around $1/r_0$ where $r_0$ is the range of the interactions.

As already mentioned, a crucial point is that the integral relations in Eqs.(8) and (9) depend only on the short-range structure of the scattering wave function $\Psi_t$. This is because $F$ and $G$ are asymptotically solutions of $(H - E)F, G = 0$. As a consequence, it is not necessary to compute the trial three-body wave function $\Psi_t$ at very large distances, and the numerical problem is enormously simplified.

In a general multichannel process the coefficients $A$ and $B$ are actually $n_0 \times n_0$ matrices, with $n_0$ being the number of open channels, and the corresponding $K$-matrix is given by $A^{-1} B$ [28].

2.2 The hyperspherical adiabatic expansion method

When describing 1+2 reactions, a particularly convenient choice for the three-body trial wave function $\Psi_t$ is the one obtained by use of the adiabatic expansion method. In this method the wave functions are described by means of the hyperspherical coordinates, which contain a radial coordinate, the hyperradius $\rho$, and five hyperangles $\{\alpha, \Omega_x, \Omega_y\}$. The hyperradius is defined from the Jacobi coordinates as $\rho^2 = x^2 + y^2$, while the hyperangle $\alpha$ is given by $\tan \alpha = x/y$, and $\Omega_x$ and $\Omega_y$ describe the directions of $x$ and $y$, respectively.

The key of the method is that the hyperangular coordinates vary much faster than $\rho$, in such a way that it is possible to solve first the angular part of the Schrödinger (or Faddeev [21]) equation for a set of frozen values of $\rho$. This amounts to solve the eigenvalue problem:

$$ \left[ \hat{G}^2 + \frac{2m\rho^2}{\hbar^2} V(\rho, \Omega) \right] \Phi_n(\rho, \Omega) = \lambda_n(\rho) \Phi_n(\rho, \Omega), \tag{10} $$

where $\hat{G}$ is the grand-angular operator whose eigenfunctions are the hyperspherical harmonics.

The three-body wave function is then expanded in terms of the basis formed by the complete set of angular functions $\{\Phi_n(\rho, \Omega)\}$, in such a way that:

$$ \Psi(x, y) = \frac{1}{\rho^{5/2}} \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\rho, \Omega), \tag{11} $$

and the radial functions $f_n(\rho)$ are obtained after solving the coupled set of radial equations [21]:

$$ \left( -\frac{\partial^2}{\partial \rho^2} + \frac{\lambda_n(\rho) + \frac{15}{\rho^2}}{Q_{nn}} - \frac{2m(E - W_{3b}(\rho))}{\hbar^2} \right) f_n(\rho) = \sum_{n \neq n'} \left( 2P_{nn'} \frac{\partial}{\partial \rho} + Q_{nn'} \right) f_{n'}(\rho), \tag{12} $$
where the coupling terms $P_{nn'}$ and $Q_{nn'}$ are given by:

$$P_{nn'}(\rho) = \left\langle \Phi_n(\rho, \Omega) \frac{\partial}{\partial \rho} \phi_{n'}(\rho, \Omega) \right\rangle_\Omega,$$

$$Q_{nn'}(\rho) = \left\langle \Phi_n(\rho, \Omega) \frac{\partial^2}{\partial \rho^2} \phi_{n'}(\rho, \Omega) \right\rangle_\Omega. \quad (13)$$

It is important to note that the coupled equations (12) are actually a set of radial Schrödinger-like equations with effective radial potentials:

$$V_{eff}(\rho) = \frac{\hbar^2}{2m} \left( \frac{\lambda_n(\rho) + \frac{15}{4}}{\rho^2} - Q_{nn}(\rho) \right), \quad (14)$$

which contain the eigenvalues $\lambda_n(\rho)$ of the angular part (10).

The great advantage of using the hyperspherical adiabatic expansion method is that each adiabatic term in the expansion (11) is associated to a very specific asymptotic structure. In particular, if the three-body system contains one or more bound two-body subsystems, we have that for each of them one of the angular eigenvalues goes asymptotically as $\lambda_n(\rho) \rightarrow 2mE_{2b}\rho^2/\hbar^2$ [21], which means that its effective potential partner (14) goes asymptotically to the binding energy $E_{2b} (<0)$ of the corresponding bound two-body subsystem. Furthermore, it can be proved, see for instance [21], that the angular eigenfunction $\Phi_n(\rho, \Omega)$ associated to the eigenvalue $\lambda_n(\rho)$ corresponds asymptotically to a bound two-body state (the one with binding energy $E_{2b}$), and the third particle in the continuum.

Summarizing, when using the hyperspherical adiabatic expansion method, all the possible elastic, inelastic, or rearrangement channels in a 1+2 reaction (or in general in a 1+$N$ reaction) are easily identified. In fact, they are associated to some specific adiabatic terms. This means that for each incoming channel, only a reduced amount of adiabatic terms in the expansion (11) behave asymptotically as (2) and (3). All the others vanish asymptotically, and therefore the size of the K-matrix describing the full process is also small. Only breakup processes are described by infinitely many adiabatic terms, but this situation will not be considered in this work.

Another important point concerning three-body calculations is that when only pairwise interactions are included, the binding energies obtained for bound three-body states typically do not match with the experimental values. The case of the halo nuclei $^6$He or $^{11}$Li are well known examples [29]. The reason for this behavior lies in the fact that three-body correlations, particle polarizations, and in general all those effects that go beyond pure two-body correlations, are not taken into account. To solve this problem, the usual way is to fine tune the binding energies by including an effective hypercentral three-body potential, which has been denoted by $W_{3b}(\rho)$ in the radial Eqs.(12). Since this potential is intended to account for the effects beyond two-body correlations, it should play a role only when all the three particles are close of each other. This implies that the potential has to be of short-range character.

Application of the hyperspherical adiabatic expansion method has proved to be very efficient for the description of bound states. The convergence of the
expansion in Eq.(11) is rather fast, and usually no more than about seven or eight terms are more than enough to get an accurate wave function. However, when describing scattering states, the convergence of the phase shifts extracted from the asymptotic part of the wave function slows down dramatically [30]. Even more, extrapolation of the computed phase shifts in terms of the number of adiabatic channels included in the calculation could lead to a quite inaccurate value. Nevertheless, as shown in [24, 25], this problem disappears when the phase shift is obtained through the integral relations (8) and (9). In this case, since they are obtained from the internal part of the wave function, the convergence is as fast as for bound states. Thanks to this, the hyperspherical adiabatic expansion method appears as a very efficient way of computing the trial three-body wave function to be used in the integral relations. The convergence of the computed phase shift is fast, the size of the basis required in the calculations remains within affordable limits, and the clean distinction between the different open channels provided by the adiabatic approximation can then be exploited.

3 The helium trimer using a two-body gaussian potential

3.1 The He-He interaction

As mentioned in the introduction, in this work we shall describe the $^4$He-$^4$He interaction by means of gaussian soft-core potential. Following [17], its form is chosen as

$$V_{2b}(r) = -1.227 e^{-r^2/10.03^2},$$

(15)

where $r$ is given in a.u. and the strength is in K. This potential leads to a bound $0^+$ $^4$He$_2$ dimer with binding energy $E_{2b} = -1.2959$ mK, scattering length $a_0 = 189.947$ a.u., and effective range $r_0 = 13.846$ a.u.. This potential was built to provide a good agreement with the more realistic and sophisticated hard-core LM2M2 potential [6], in particular for the binding energy of the Helium dimer and He-He scattering at low energy. The corresponding LM2M2 values are $E_{2b} = -1.302$ mK, $a_0 = 189.054$ a.u. and $r_0 = 13.843$ a.u..

In order to investigate the energy range where the equivalence of the two potentials holds, we define the effective range function as

$$K(E) = k \cot \delta,$$

(16)

where $k^2 = M_{He}E/\hbar^2$ ($M_{He}$ is the mass of the He-atom and $E$ is the two-body center of mass energy), and $\delta$ is the $s$-wave helium-helium phase shift. For low energy values this function is known to take the form:

$$K(E \rightarrow 0) \rightarrow -\frac{1}{a_0} + \frac{1}{2} r_0 k^2.$$

(17)

In Fig. 3 the phase shifts of the LM2M2 (triangles) and gaussian (circles) potentials are given in the form of the effective range function (16) as a function of the two-body energy $E$. As a reference the straight line of the low energy representation of $K(E)$, Eq.(17), is also displayed. From the figure we can see that the phase shifts of both potentials follow the low energy limit of $K(E)$ up to 0.2 K approximately. Above this value the phase shifts do not follow the straight line and above 0.4 K they start to be different for both potentials.
3.2 The Helium trimer

In this section we investigate elastic He-He$_2$ collisions at energies below the dimer break-up threshold. The energy range of interest is thus $E_{2b} < E < 0$, where $E_{2b}$ is the binding energy of the dimer.

We compute the atom-diatom phase shifts by means of the integral relations given in Eqs. (8) and (9), and which permit to obtain the phase shift as given in (4). The advantage of using this approach is that the accuracy of the result depends only on the internal part of the wave-function, and knowledge of its asymptotic behaviour is not necessary. To illustrate this point the continuum wave functions for the He-He$_2$ system are obtained by imposing a simple box boundary condition to the coupled set of hyperradial equations (12), that is $f_n(\rho) = 0$ for $\rho \geq \rho_{max}$, where $\rho_{max}$ determines the size of the box. In other words, we solve the Eqs. (12) by putting an infinite wall in all the effective adiabatic potentials (13) at $\rho_{max}$.

A direct consequence of imposing a box boundary condition is that the continuum spectrum of the system is discretized. Only three-body energies associated to wave functions that are zero at the wall of the box are allowed. The energies of the discretized spectrum change in values when $\rho_{max}$ is changed, and increase in number and density as $\rho_{max}$ increases. This is contrary to what happens to a bound state, whose wave function always vanishes at the wall of the box provided that the box is big enough to hold it.

In order to study the convergence of the phase shift calculation in function of the size of the box, we have chosen four values of $\rho_{max}$, namely 420.976 a.u., 1619.436 a.u, 2916.698 a.u, and 4221.912 a.u., which all give rise to a discrete continuum state with a three-body energy of $-7959$ mK. This corresponds to

Figure 1. The effective range function of the LM2M2 potential (triangles) and its gaussian representation (circles) as a function of the two-body center of mass energy. The low energy limit of the effective range function is given as a solid line.
an incident energy for the $^4$He projectile of 0.5 mK. In Table 1 the negative spectrum in the energy region $E_{2b} < E < 0$ of the different boxes is shown. For ease of reference, the boxes are numbered according to their increasing size. The two smaller boxes present only one negative eigenvalue, whereas the third box has three and the fourth box has four. In the two larger boxes the selected eigenvalue of $-0.7959$ mK is the second one.

Table 1. Negative eigenvalues (in mK) above $E_{2b}$ obtained for the four different boxes

| box | 1        | 2        | 3        | 4        |
|-----|----------|----------|----------|----------|
| $\rho_{max}$ [a.u.] | 420.976  | 1619.436 | 2916.698 | 4221.912 |
|      | -0.795891| -0.795891| -0.178999| -0.409160|
|      | -0.795891| -0.795891| -1.171742| -1.074084|
|      |          |          | -1.240771|          |

Fig. 2 shows the first three hyperradial wave functions $f_n(\rho)$ ($n = 1, 2, 3$) obtained by solving the system (12) at energy $E = -0.7959$ mK for each of the four boundary conditions discussed above, namely, “box 1” (thick solid curve), “box 2” (dotted curve), “box 3” (dashed curve), and “box 4” (thin solid curve). As we can see, all the hyperradial wave functions perfectly overlap, except in proximity of their respective $\rho_{max}$ value, where they begin to bend in order to reach zero all of them at $\rho_{max}$.

Once the radial wave functions for the “box 1”, “box 2”, “box 3”, and “box 4” calculations have been obtained, it is possible to compute the corresponding atom-diatom phase shift by using the integral relations. When the calculation is performed, we obtain for the four cases a phase shift value of $-47.19$ degrees (“box 1”), $-40.20$ degrees (“box 2”), $-40.54$ degrees (“box 3”), and $-40.54$ degrees (“box 4”). These results have been obtained using 30 adiabatic terms in the expansion (11), which are more than enough to get a converged result. The same result is actually obtained when about half of the adiabatic terms are considered. As we can see, the first two boxes used are too small, since the three-body wave function is set equal to zero at $\rho$ values where it still contributes to the integrands of the relations (8) and (9). For a sufficiently large box the phase shift stabilizes at a value of $-40.54$ degrees. This value agrees with the result of Ref. [28], where the same reaction with the same incident energy and the same gaussian two-body potential is investigated, but with a three-body wave function showing the correct asymptotic behavior. These results confirm and justify our approach. In fact, we notice that as expected, by using the integral relations, an accurate phase shift can be extracted by a wave-function which is accurate in the internal region, but which is completely inaccurate in the external asymptotic region. In fact, in our calculation the asymptotic part is simply chosen equal to zero.
The helium trimer with soft-core potentials

Figure 2. (Color online) Three first radial wave functions for the He-He\(_2\) system at a three-body energy of \(-0.7959\) mK, which corresponds to an incident energy of the \(^4\)He projectile of 0.5 mK. They have been computed imposing a box boundary condition. The wave functions have been obtained with four different values of \(\rho_{\text{max}}\) (see text) such that all of them give rise to the same selected discretized continuum state. The thick solid, dotted, dashed, and thin solid curves are the radial wave functions corresponding to the boxes 1, 2, 3, and 4, respectively.

4 Hypercentral three-body force

A significant difference between the gaussian potential [15] and the LM2M2 potential appears in the description of the helium trimer bound states. Table 2 presents the binding energy for the two helium trimer bound states, \(E_0\) and \(E_1\), as well as the atom-diatom scattering length \(a_0\). The gaussian potential leads to two bound states of energies \(-150.0\) mK and \(-2.467\) mK. The LM2M2 potential also supports two bound states, but with energies \(-126.4\) mK and \(-2.265\) mK. The gaussian potential thus significantly overbounds the two states. This phenomenon can be easily understood as, lacking the hard core, it leads to more compact structures where the three particles are closer to each other. Though smaller, the
difference in the binding energy of the shallow excited state is also appreciable. It should be noticed that the structure of this state corresponds to a two-atom bound structure with the third atom orbiting far away. If the attraction of the two-body potential is increased the two-atom bound structure reduces its size and the third atom evaporates. This is the mechanism from which the Efimov-like states disappear from the spectrum when the two-body potential results more attractive. Finally, there is also a noticeable difference in the atom-diatom scattering length $a_0$ calculated with the LM2M2 potential (from Ref. [14]) and with the gaussian potential.

Table 2. The ground state $E_0$, the excited state $E_1$, and the helium-dimer scattering length $a_0$ calculated with the LM2M2 potential and with its gaussian representation. In the last four rows, the results of the gaussian potential plus the three-body forces are given.

| Potential       | $E_0$ [mK] | $E_1$ [mK] | $a_0$ [a.u.] |
|-----------------|------------|------------|--------------|
| LM2M2 [14]      | −126.4     | −2.265     | 217.3        |
| gaussian        | −150.0     | −2.467     | 165.9        |
| $(W_0$ [K], $\rho_0$ [a.u.]) |            |            |              |
| (306.9, 4)      | −126.4     | −2.283     | 211.7        |
| (18.314, 6)     | −126.4     | −2.287     | 210.6        |
| (4.0114, 8)     | −126.4     | −2.289     | 210.0        |
| (1.4742, 10)    | −126.4     | −2.292     | 209.2        |

Similarly to what done in standard nuclear three-body calculations, where the disagreement between computed and experimental binding energies is corrected by the inclusion of an effective three-body force, here we shall investigate the possibility of correcting the discrepancy between the binding energies shown in Table 2 by adding an analogous three-body force to the gaussian potential in the description of the helium trimer. We require that the range of the effective three-body potential $W_{3b}$ be of the order of the size of the trimer in its ground state. Therefore this force will help to fix the proper scale in the three-body system given by the physics (not observed) included in the repulsion of the original LM2M2 potential. We propose the following simple two-parameter hyperradial three-body force

$$W(\rho) = W_0 e^{-\rho^2/\rho_0^2}.$$  \hspace{1cm} (18)

We analyze four different values for $\rho_0$, namely, 4, 6, 8 and 10 a.u.. For each $\rho_0$, the strength of the force $W_0$ has been fixed to reproduce the value of $-126.4$ mK given by the LM2M2 potential for the trimer ground state. This results in four different pairs $(W_0, \rho_0)$. The corresponding calculated values for $E_0$, $E_1$ and $a_0$ are given in the last rows of Table 2. The results for $E_1$ and $a_0$ are predictions and, as we can observe from the table, the inclusion of the three body force brings them much closer to the values of the LM2M2 potential in all four cases.

The analysis can be extended to the description of atom-diatom scattering states below the breakup threshold in three atoms. Using the technique described in the previous sections, the s-wave phase shift $\delta_0$ has been calculated for different
values of the incident center of mass energy $E_i = E - E_{2b}$, where $E$ is the total (negative) energy of the system and $E_{2b}$ is the dimer energy. The results are shown in Fig. 3 where they are compared to the calculations in Refs. [19, 31, 18], which are given by the solid line, solid squares and dashed line, respectively. The results for the gaussian potential with and without the three-body force are represented the solid circles and solid triangles, respectively. In fact, the phase shifts obtained using the four parametrizations overlap and they are practically indistinguishable. As we can see, inclusion of the effective hypercentral three-body force leads to results very close to the ones in Refs. [19, 18]. We can therefore conclude that the gaussian potential, constructed to reproduce the low energy spectrum of the two-helium system given by a realistic potential as the LM2M2 selected in the present analysis, plus a three-body force, constructed to reproduce the LM2M2 trimer ground state, reproduces the low energy spectrum of the three-helium system.

5 Conclusions

In this paper we have discussed the possibility of describing the helium trimer system using a soft-core interaction. The potential, selected of a gaussian type with two parameters, has been constructed in order to reproduce the low-energy He-He scattering as calculated using the LM2M2 potential. We have shown (see
Fig. 1 that approximately above 0.4 K the equivalence breaks down as the details of the internal part of the interaction become important. When the study is extended to the three-body system, similar problems arise, and in fact at a much earlier stage, since already the description of the ground three-body state is significantly different between the two potentials. Using the LM2M2 potential the trimer binding energy is around $-126$ mK whereas using its gaussian representation an energy of $-150$ mK is obtained. It is clear that the short range physics embedded in the repulsive part of the LM2M2 potential is missing in the attractive gaussian potential. The question addressed in this work is if the inclusion of a repulsive short-range three-body force can recover those aspects of the dynamics not present in the soft-core potential. To this aim a repulsive gaussian hyperradial three-body force has been parametrized in order to reproduce the LM2M2 trimer energy. Four different ranges, from 4 a.u. to 10 a.u., have been considered taking into account the fact that the repulsive part of the $^4$He-$^4$He interaction has a range $r_p \approx 5$ a.u. and the hyperradius corresponding to a configuration of an equilateral triangle of side $r_p$ is $\sqrt{3}r_p$. For each value used for the range the corresponding strength has been fixed and, as it can be observed from Table 2, the LM2M2 trimer energy has been reproduced. Furthermore we can observe a much better description of the first excited state whose energy results to be almost constant for the four different parametrizations used. A difference of about 0.01 mK is observed between the largest and the shorter ranges. Interestingly, also the atom-dimer scattering length is much better described when the hypercentral potential is included. With the four parametrizations a value of around 211 a.u. has been obtained, which is only 3% lower than the LM2M2 value.

The atom-dimer phase shifts have been studied with the soft-core potential with and without the inclusion of the three-body term. When this term is included we have found that the phase shifts, using the four parametrizations, are almost identical. Moreover they agree very well with the LM2M2 phase shifts calculated in Refs. [31, 18] and with the phase shifts given in Ref. [19] using a different He-He potential. However this is not the case when only the gaussian two-body potential is used. Therefore we can conclude that it is justified to use soft-core potentials to describe three helium atoms in the ultracold regime using a potential model that includes a short-range three-body term constructed to fix the ground state energy at the correct level.

As mentioned in the Introduction, it is very difficult to get an accurate description for systems with more than three helium atoms using potentials presenting a strong short-range repulsion. Ref. [22] remains an isolate example of an study in which ground state energies of He molecules, up to 10 atoms, are computed using the diffusion Monte Carlo algorithm. No information about excited states are given in the literature. On the other hand, the possibility of using soft-core potentials in the description of these systems will allow the use of methods that at present cannot be applied. Accordingly this study has to be considered as a first step in this direction. Studies at higher energies in the three-body system and in systems with more than three atoms are at present in progress and they will serve to support the use of soft-core potentials in particular energy regimes.
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References

1. F. Luo, C. F. Giese and W. R. Gentry, J. Chem. Phys. 104, 1151 (1996)
2. W. Schoellkopf and J. P. Toennies, J. Chem. Phys. 104, 1155 (1995)
3. W. Schollkopf and J. P. Toennies, Science 266, 1345 (1994)
4. R. Grisenti, W. Schoellkopf, J. P. Toennies, G. C. Hegerfeldt, T. Kohler and M. Stoll, Phys. Rev. Lett. 85, 2284 (2000)
5. R. A. Aziz, F. R. W. McCourt and C. C. K. Wong, Molecular Physics 61, 1487 (1987)
6. R. A. Aziz and M. J. Slaman, J. Chem. Phys. 94, 8047 (1991)
7. K. T. Tang, J. P. Toennies and C. L. Yiu, Phys. Rev. Lett. 74, 1956 (1995)
8. A. R. Janzen and R. A. Aziz, J. Chem. Phys. 107, 914 (1997)
9. T. Korona, H. L. Williams, R. Bukowski, B. Jeziorski and K. Szalewicz, J. Chem. Phys. 106, 5109 (1997)
10. M. Jeziorska et al., J. Chem. Phys. 127, 124303 (2007)
11. W. Cencek et al., J. Phys. Chem. A111, 11311 (2007)
12. V. Efimov, Phys. Lett. 33B, 563 (1970)
13. V. Efimov, Sov. J. Nucl. Phys. 12, 589 (1971)
14. E.A. Kolganova, A.K. Motovilov, and W. Sandhas, Phys. Part. and Nucl. 40, 206 (2009)
15. B. D. Esry, C. D. Lin and Chris H. Greene, Phys. Rev. A 54 394 (1996)
16. P. Barletta and A. Kievsky, Phys. Rev. A64, 042514 (2001)
17. E. Nielsen, D.V. Fedorov, and A.S. Jensen, J. Phys. B31, 4085 (1998).
18. A. K. Motovilov, W. Sandhas, S. A. Sofianos, E. A. Kolganova, Eur. Phys. J. D 13, 33 (2001)
19. H. Suno and B.D. Esry, Phys. Rev A 78, 062701 (2008).
20. E. A. Kolganova, A. K. Motovilov, and S. A. Sofianos, J. Phys. B31, 1279 (1998)
21. E. Nielsen, D.V. Fedorov, A.S. Jensen, and E. Garrido, Phys. Rep. 347, 373 (2001)

22. M. Lewerenz, J. Chem. Phys. 106, 4596 (1997)

23. J. von Stecher and Chris H. Greene, Phys. Rev. A 80, 022504 (2009)

24. P. Barletta, C. Romero-Redondo, A. Kievsky, M. Viviani, and E. Garrido, Phys. Rev. Lett. 103, 090402 (2009).

25. A. Kievsky, M. Viviani, P. Barletta, C. Romero-Redondo, and E. Garrido, Phys. Rev. C81, 034002 (2010).

26. F.E. Harris, Phys. Rev. Lett. 19, 173 (1967).

27. A.R. Holt and B. Santoso, J. Phys. B5, 497 (1972).

28. C. Romero-Redondo, E. Garrido, P. Barletta, A. Kievsky, M. Viviani, Phys. Rev. A, in press

29. M.V. Zhukov, B.V. Danilin, D.V. Fedorov, J.M. Bang, I.J. Thompson, and J.S. Vaagen, Phys. Rep. 231, 131 (1995).

30. P. Barletta and A. Kievsky, Few-body Syst. 45, 25 (2009).

31. V. Roudnev, Chem. Phys. Lett. 367, 95 (2003).