Spectra of helium clusters with up to six atoms using soft-core potentials

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In this paper, we investigate small clusters of helium atoms using the hyperspherical harmonic basis. We consider systems with $A = 2,3,4,5,6$ atoms with an interparticle potential which does not present a strong repulsion at short distances. We use an attractive Gaussian potential that reproduces the values of the dimer binding energy, the atom-atom scattering length, and the effective range obtained with one of the widely used He-He interactions, the Aziz and Slaman potential, called LM2M2. In systems with more than two atoms, we consider a repulsive three-body force that, by construction, reproduces the trimer binding energy of the LM2M2 potential. With this model, consisting of the sum of a two- and three-body potential, we have calculated the spectrum of clusters formed by four, five, and six helium atoms. We have found that these systems present two bound states, one deep and one shallow, close to the threshold fixed by the energy of the $(A-1)$-atom system. Universal relations between the energies of the excited state of the A-atom system and the ground-state energy of the $(A-1)$-atom system are extracted, as well as the ratio between the ground state of the A-atom system and the ground-state energy of the trimer.

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I. INTRODUCTION

Systems composed by few helium atoms have been the object of intense investigation from a theoretical and experimental point of view. The existence of the He-He molecule was experimentally established using diffraction experiments [1–4]. Its binding energy E_{2b} 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. On the theoretical side, several He-He potentials have been proposed; in spite of different details and derivations, all of them share the common feature of a sharp repulsion below an interparticle distance of approximately 5 a.u.

Another important characteristic of the He-He interactions is their effective range $r_0 \approx 13$ a.u. Accordingly, the ratio a_0/r_0 is large enough (> 10) to place small helium clusters into the frame of Efimov physics [5,6]. 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; their binding energies scale in a geometrical way and they accumulate at zero energy. The scaling factor, $e^{-2\pi/s_0} \approx 1/515.03$, is universal and depends only on the ratio between particle masses (for three identical bosons $s_0 \approx 1.00624$), not on the details of the two-body interaction (see Ref. [7] for a review). For a finite a_0/r_0 ratio, the number of the Efimov states has been estimated to be $N = (s_0/\pi)\ln|a_0/r_0|$ [6]; for example, the (bosonic) three ^{4}He system presents an excited state just below the atom-dimer threshold that has been identified as an Efimov state.

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. [8–10]). In addition, analysis of the atom-dimer collision in the ultracold regime has also been performed [11–13].

One of the main difficulties in solving the quantum mechanical problem in the case of three helium atoms is the treatment of the strong repulsion at short distances of the He-He potential. Specific algorithms have been developed so far to solve this problem. The Faddeev equation has been opportunely modified [14]. Moreover, the hyperspherical adiabatic (HA) expansion has been extensively used in this case [13] (for a review, see Ref. [15]). 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. [16] the diffusion Monte Carlo method has been used to describe the ground state of He molecules up to 10 atoms, and in Ref. [17] a Monte Carlo technique has been used to construct the lowest adiabatic potential in systems with three and up to 10 helium atoms. On the other hand, description of few-atoms systems using soft-core potentials are currently operated (see, for example, Ref. [18]).

Therefore, the equivalence between hard- or soft-core-potential descriptions needs some clarification. In a recent work [19], an attractive He-He Gaussian potential has been used to investigate the three ^{4}He system. In the absence of direct experimental data, the two-body potential has been designed to reproduce the helium dimer binding energy E_{2b}, the He-He scattering length a_0, and the effective range r_0 of the Aziz and Slaman potential of Ref. [20], called LM2M2. This Gaussian potential can be considered as a regularized-two-body contact term in an effective field theory (EFT) approximation of the physics driven by the LM2M2 potential [21]. It should be noticed that two potentials predicting 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 [21]. The equivalence is lost as the energy is increased, when the details of the potential become more and more important.

Extending the study to the three-body system, differences between the attractive Gaussian and the LM2M2 potentials are immediately observed. For example, the trimer ground-state energies differ by more than 15% (see Table I). A natural way to restore the equivalence between the two potentials is by

the addition of a three-body soft-term force to the Gaussian potential. On the other hand, in an EFT treatment of the three-boson system with large scattering length, a three-body-contact term is required at leading order (LO). Its strength is usually determined by fixing a three-body observable as, for example, one of the trimer bound-state energies. After this choice, cut-off independent results are obtained [22]. Following these ideas, and based on Ref. [19], in the present work we have considered a Gaussian-hypercentral three-body force with the strength fixed to reproduce the LM2M2 ground-state binding energy of the three-atom system. The quality of this description has been studied for different ranges of the three-body force.

Using the two-atom and three-atom systems to fix the model interaction, we have analyzed heavier systems, up to $A = 6$ atoms. The numerical calculations are performed by means of the hyperspherical harmonic (HH) expansion method with the technique developed recently by the authors in Ref. [23]. In this approach, the authors use the HH basis, without a previous symmetrization procedure, to describe bound states in systems up to six particles. The method is based in a particular representation of the Hamiltonian matrix, as a sum of products of sparse matrices, well suited for a numerical implementation. Converged results for different eigenvalues, with the corresponding eigenvectors belonging to different symmetries, have been obtained. In the present paper, we extend the formalism to treat a three-body force. Moreover, as we are dealing with atoms of ^{4}He, only the spectrum corresponding to totally symmetric eigenstates is of interest.

After fixing the strength of the three-body force to correctly describe the LM2M2 three-body ground state $E_{3b}^{(0)} = 126.4$ mK, we have calculated the first three levels of the spectrum with total angular momentum $L = 0$ of the $A = 4,5,6$ systems. In the three cases, we have found that the first two levels are bosonic bound states, one deep, $E_{Ab}^{(0)}$, and one very shallow, $E_{Ab}^{(1)}$, close to the threshold formed by the $A - 1$ system plus one atom. The third state in all cases belongs to a mixed symmetry with an energy above the threshold and therefore not representing a bound state. The appearance of only two bound states in this system is in agreement with previous calculations [17]. This fact has been observed in $A = 4$ and interpreted as a consequence of the Efimov-like spectrum of the $A = 3$ system [24]. It should be noticed that, whereas converged results can be found in the literature for the ground state of the many atom systems, the energy of the excited states is much more difficult to calculate and only rough estimates are available.

To gain insight on the shallow state, we have varied the range of the three-body force (maintaining fixed the three-body ground-state energy) and we have studied the effects of that variation in the $A = 4,5,6$ spectrum. In the range considered, the variation produces small effects in the eigenvalues; however, it is crucial to determine if the shallow state is bound or not with respect to the $A - 1$ threshold. Interestingly, we have observed that when the ranges of the two- and three-body forces have a ratio of about $\sqrt{2}$, the ratio between the shallow- and ground-state energy is $E_{Ab}^{(1)}/E_{A-1b}^{(0)} \approx 1.01$–$1.02$, in agreement with Refs. [25,26]. This analysis confirms previous observations that each Efimov state in the $A = 3$ system produces two bound states in the $A = 4$ system. Furthermore, we have found $E_{4b}^{(0)}/E_{3b}^{(0)} \approx 4.5$, $E_{5b}^{(0)}/E_{3b}^{(0)} \approx 10.5$, and $E_{6b}^{(0)}/E_{3b}^{(0)} \approx 18.5$, which is in agreement with Refs. [26,27].

The paper is organized as follows. In Sec. II, we describe the two- and three-body forces we used in our calculations to reproduce LM2M2 data. In Sec. III, the results for the bound states of the $A = 3,4,5,6$ He clusters are collected, whereas the conclusions are given in the last section. Some technical details of the method have been summarized in the Appendix.

II. SOFT-CORE TWO- AND THREE-BODY HELIUM POTENTIAL

As mentioned in the Introduction, the ^{4}He-^{4}He interaction presents a strong repulsion at short distances, below 5 a.u. This characteristic makes a detailed description of the system with more than four atoms difficult. Accordingly, in the present paper, we have studied small clusters of helium interacting through soft-core two- and three-body potentials, which can be interpreted as regularized two- and three-body contact terms in a LO-EFT approximation of LM2M2.

Following Refs. [10,19], we use the Gaussian two-body potential,

$$V(r) = V_0 e^{-r^2/R^2}, \tag{1}$$

with $V_0 = -1.227$ K and $R = 10.03$ a.u. In the following, we use $\hbar^2/m = 43.281\,307$(a.u.)^{2}K. This parametrization of the two-body potential approximately reproduces the dimer binding energy E_{2b}, the atom-atom scattering length a_0, and the effective range r_0 given by the LM2M2 potential. Specifically, the results for the Gaussian potential are $E_{2b} = -1.296$ mK, $a_0 = 189.95$ a.u., and $r_0 = 13.85$ a.u., to be compared to the corresponding LM2M2 values $E_{2b} = -1.302$ mK, $a_0 = 189.05$ a.u., and $r_0 = 13.84$ a.u. As shown in Ref. [19], the use of the Gaussian potential in the three-atom system produces a ground-state binding energy $E_{3b}^{(0)} = 150.4$ mK, which is appreciably bigger than the LM2M2 helium trimer ground-state binding energy of 126.4 mK. A smaller difference, though still appreciable, is observed in the first excited state (see Table I).

In order to have a closer description to the $A = 3$ system obtained with the LM2M2 potential, we introduce the following three-body interaction:

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

where $\rho_{ijk}^2 = \frac{2}{3}(r_{ij}^2 + r_{jk}^2 + r_{ki}^2)$ is the three-body hyper-radius in terms of the distances of the three interacting particles. Moreover, the strength W_0 is fixed to reproduce the LM2M2 helium trimer binding energy of 126.4 mK. We have studied different cases by varying the range of the three-body force ρ_0 between 4 and 16 a.u. Specific cases with the corresponding results in the $A = 3$ system are shown in Table I. In the first two rows of the table, we report the ground and excited binding energies of the trimer, both for LM2M2 potential and its Gaussian representation. The excess of binding is evident for this last model. Successively, we report, for selected values of W_0 and ρ_0, the binding energies obtained summing to the Gaussian potential the (repulsive) three-body force. By

TABLE I. Ground state $E_{3b}^{(0)}$ and the excited state $E_{3b}^{(1)}$ of the helium trimer calculated with the LM2M2 potential, with its Gaussian representation and with the Gaussian potential plus the three-body potential. In this case the two parameters, the strength W_0 and the range ρ_0, are given.

Potential	$E_{3b}^{(0)}$ (mK)	$E_{3b}^{(1)}$ (mK)
LM2M2 [11]	−126.4	−2.265
Gaussian	−150.4	−2.467
[W_0 (K), ρ_0 (a.u.)]		
(306.9,4)	−126.4	−2.283
(18.314,6)	−126.4	−2.287
(4.0114,8)	−126.4	−2.289
(1.4742,10)	−126.4	−2.292
(0.721,12)	−126.4	−2.295
(0.422,14)	−126.4	−2.299
(0.279,16)	−126.4	−2.302

construction, the ground state has been fixed to the LM2M2 value and, in addition, we can observe that the excited state $E_{3b}^{(1)}$ is now closer to the corresponding LM2M2 result, showing an extremely small variation with ρ_0; the difference between the extremal values obtained for $\rho_0 = 4$ a.u. and $\rho_0 = 16$ a.u. is less than 1%.

It should be noticed that the ranges R of the two-body force and ρ_0 of the three-body force are somehow related. The Gaussian two-body force can be thought as originating from a contact interaction regularized using a Gaussian cutoff with $\Lambda = R^{-1}$ (see, for example, Ref. [7]). This means that configurations, in the $A = 2$ system, in which two atoms have a relative momentum $k > \Lambda$, remain outside the present description or, in other words, details of the interaction for distances below $\sqrt{\langle r^2\rangle} = R/\sqrt{2}$ are not accessible. In the $A > 2$ systems, three atoms interact through the three-body force when they happen to be inside a sphere of radius $\rho_0/\sqrt{2}$ at the same time. It is clear that, as no information is introduced in the two-body system for distances below $R/\sqrt{2}$, from the relation $\rho_{ijk}^2 = \frac{2}{3}(r_{ij}^2 + r_{jk}^2 + r_{ki}^2)$ and putting each distance at the value $R/\sqrt{2}$, we obtain for the three-body range $\rho^2 = R^2$. Since R has been fixed in order to describe two-body quantities, in the description of systems with $A > 3$ atoms, we consider different values of ρ_0 with particular attention at the region $\rho_0 \approx \sqrt{2}R$.

The calculations for the $A \geqslant 3$ systems, up to six atoms, are performed using the unsymmetrized HH basis. The method has been recently used to describe up to six nucleons interacting through a central potential [23]. A brief description of the method is given in the Appendix. In this paper we extend the method to deal with the three-body force. Using a particular rotation of the HH basis, it is possible to construct the potential energy as a product of sparse matrices. The Hamiltonian matrix is obtained using the following orthonormal basis:

$$\langle \rho\Omega | m[K]\rangle = \left(\beta^{(\alpha+1)/2}\sqrt{\frac{m!}{(\alpha+m)!}}L_m^{(\alpha)}(\beta\rho)e^{-\beta\rho/2}\right)\mathcal{Y}_{[K]}^{LM}(\Omega_N), \quad (3)$$

where $L_m^{(\alpha)}(\beta\rho)$ is a Laguerre polynomial with $\alpha = 3N-1$ and β a variational nonlinear parameter. The matrix elements of the Hamiltonian are obtained after integrations in the ρ,Ω spaces. They depend on the indices m,m' and $[K],[K']$ as follows:

$$\begin{aligned}\langle m'[K']|H|m[K]\rangle &= -\frac{\hbar^2\beta^2}{m}\left[T_{m'm}^{(1)} - K(K+3N-2)T_{m'm}^{(2)}\right]\delta_{[K'][K]} \\ &+ \sum_{i<j}\left[\sum_{[K''][K''']}\mathcal{B}_{[K][K'']}^{ij,LM}\mathcal{B}_{[K'''][K']}^{ij,LM}V_{[K''][K''']}^{m,m'}\right] \\ &+ \sum_{i<j<k}\left[\sum_{[K''][K''']}\mathcal{D}_{[K][K'']}^{ijk,LM}\mathcal{D}_{[K'''][K']}^{ijk,LM}W_{[K''][K''']}^{m,m'}\right]. \quad (4)\end{aligned}$$

The matrices $T^{(1)}$ and $T^{(2)}$ have an analytical form and are given in Ref. [28]. The matrix elements $V_{[K][K']}^{m,m'}$ and $W_{[K][K']}^{m,m'}$ are obtained after integrating the matrices $V_{12}(\rho)$ and $W(\rho)$ in ρ space (we will call the corresponding matrices V_{12} and W). Introducing the diagonal matrix D such that $\langle [K']|D|[K]\rangle = \delta_{[K],[K']}K(K+3N-2)$, and the identity matrix I in K space, we can rewrite the Hamiltonian schematically as

$$\begin{aligned}H &= -\frac{\hbar^2\beta^2}{m}({}^{(1)}T\otimes I + {}^{(2)}T\otimes D) + \sum_{i<j}\left[\mathcal{B}_{ij}^{LM}\right]^t V_{12}\mathcal{B}_{ij}^{LM} \\ &+ \sum_{i<j<k}\left[\mathcal{D}_{ijk}^{LM}\right]^t W\mathcal{D}_{ijk}^{LM}, \quad (5)\end{aligned}$$

in which the tensor product character of the kinetic energy is explicitly given. A method to diagonalize a matrix of this form is given in Ref. [23].

III. RESULTS FOR $A = 4,5,6$ He CLUSTERS

In this section, we present results for small clusters, up to $A = 6$, formed by atoms of ^{4}He. Despite the differences observed at the level of the three-body system between the Gaussian two-body force and the LM2M2 potential, the computation of the spectrum produced by the Gaussian two-body force only for the $A = 4,5,6$ systems is of interest.

In Table II, we show the $L = 0$ ground state $E_{Ab}^{(0)}$ and the first two excited states $E_{Ab}^{(1)}$ and $E_{Ab}^{(2)}$ for increasing values of the grand-angular momentum K using the unsymmetrized HH basis. The calculations have been performed up to $K = 40$ in $A = 4$, $K = 24$ in $A = 5$, and $K = 22$ in $A = 6$. It is a property of the HH basis that when all states having a fixed value of K are included in the expansion of the wave function, the symmetry of the eigenvectors reflects the symmetries present in the Hamiltonian. Since the Hamiltonian is symmetric under exchange of the particles, the obtained eigenvectors have well-defined particle permutation symmetry. In the present case, the ground state $E_{Ab}^{(0)}$ and first excited state $E_{Ab}^{(1)}$ of the Hamiltonian matrix for $A = 4,5,6$ are symmetric states and belong to the irreducible representation $[\boldsymbol{\lambda}]$ with $\boldsymbol{\lambda} = \boldsymbol{A}$. In all cases, the second excited state $E_{Ab}^{(2)}$ has mixed symmetry and belongs to the irreducible representation $[\boldsymbol{\lambda}\ \mathbf{1}]$ with $\boldsymbol{\lambda} = \boldsymbol{A-1}$. In Table II, we also observe that the ground-state binding energy, $E_{Ab}^{(0)}$, has a very fast convergence in terms of K and can be determined with five digits; this value fixes the threshold of the continuum spectrum in the

TABLE II. $A = 4,5,6$ binding energies of the ground, $E^{(0)}_{Ab}$, and the first two excited states, $E^{(1)}_{Ab}$ and $E^{(2)}_{Ab}$, for increasing values of the grand-angular-quantum number K using the two-body soft-core Gaussian potential. We also report the symmetry of the states; the ground, $E^{(0)}_{Ab}$, and the first-excited, $E^{(1)}_{Ab}$, states are totally symmetric; the second-excited state belongs to a mixed representation.

K	$E^{(0)}_{4b}$(mK) [4]	$E^{(1)}_{4b}$(mK) [4]	$E^{(2)}_{4b}$(mK) [3 1]	$E^{(0)}_{5b}$(mK) [5]	$E^{(1)}_{5b}$(mK) [5]	$E^{(2)}_{5b}$(mK) [4 1]	$E^{(0)}_{6b}$(mK) [6]	$E^{(1)}_{6b}$(mK) [6]	$E^{(2)}_{6b}$(mK) [5 1]
0	725.98	31.688		1913.0	642.84		3773.1	2010.7	
2	725.98	31.688		1913.0	642.84	314.15	3773.1	2010.9	1626.5
4	746.45	77.971		1941.2	746.01	400.95	3807.6	2140.1	1719.3
6	750.15	107.63		1944.1	778.79	516.60	3809.9	2166.2	1840.5
8	751.06	124.48	2.5177	1945.0	802.47	571.03	3810.8	2188.6	1882.5
10	751.28	135.94	29.401	1945.2	813.88	608.58	3810.9	2196.4	1909.0
12	751.35	144.17	50.336	1945.2	820.87	634.25	3810.9	2200.8	1923.4
14	751.37	149.30	66.672	1945.2	824.84	653.19	3810.9	2202.7	1931.9
16	751.37	152.98	79.082	1945.2	827.23	657.59	3810.9	2203.6	1936.5
18	751.38	155.54	89.069	1945.2	828.67	678.86	3810.9	2204.0	1938.7
20	751.38	157.43	97.021	1945.2	829.58	687.87	3810.9	2204.1	1939.7
22	751.38	158.76	103.54	1945.2	830.15	695.23	3810.9	2204.2	1940.0
24	751.38	159.77	108.90	1945.2	830.50	701.29			
26	751.38	160.53	113.38						
28	751.38	161.10	117.16						
30	751.38	161.54	120.37						
32	751.38	161.89	123.13						
34	751.38	162.15	125.52						
36	751.38	162.37	127.60						
38	751.38	162.53	129.42						
40	751.38	162.67	131.02						

$A + 1$ system. True bound states in the $A = 4$ systems are those having a binding energy bigger than the trimer binding energy of 150.4 mK and, looking at the table, bound states in the $A = 5,6$ systems appear below the threshold of 751.38 and 1945.2 mK, respectively. Since in all cases the second excited state $E^{(2)}_{Ab}$ is above the threshold, only two bosonic states are bound in the $A = 4,5,6$ systems, one deep and one shallow close to the $A - 1$ threshold. The next bosonic state appears above $E^{(2)}_{Ab}$ and, therefore, it is not bound. This result confirms previous analysis in the four-body sector that the lower Efimov state in the $A = 3$ system produces two bound states: one deep and one shallow. Here, we have extended this observation up to the $A = 6$ system. The convergence of the $E^{(1)}_{Ab}$ is much slower than for the ground state; however, with the extended base used, it has been determined with an accuracy well below 1%.

For this atom-atom potential, the ratio $r_0/a \approx 1/14$ and, therefore, we are not too far from the unitary limit, and we can make predictions for the universal ratios $E^{(1)}_{Ab}/E^{(0)}_{(A-1)b}$ and $E^{(0)}_{Ab}/E^{(0)}_{3b}$. From the table, we can observe that $E^{(1)}_{4b}/E^{(0)}_{3b} = 1.085$, $E^{(1)}_{5b}/E^{(0)}_{4b} = 1.10$, and $E^{(1)}_{6b}/E^{(0)}_{5b} = 1.13$. These results are not so close to the universal ratio of around 1.01, indicating that effective range corrections are important. For the ratios with respect to the trimer ground state, we have $E^{(0)}_{4b}/E^{(0)}_{3b} = 5.01$, $E^{(0)}_{5b}/E^{(0)}_{3b} = 12.97$, and $E^{(0)}_{6b}/E^{(0)}_{3b} = 25.4$. As we will see, these ratios are substantially modified when a three-body force is included.

Now, we consider the model with both two- and three-body interaction. The pattern of convergence for the ground and excited states of the $A = 4,5,6$ helium systems, using the Gaussian two-body potential plus the repulsive three-body potential with $\rho_0 = 14$ a.u., is given in Table III. The maximum grand angular momentum considered is $K = 40$ for $A = 4$, $K = 24$ for $A = 5$, and $K = 22$ for $A = 6$. As in the case in which only the two-body force has been considered, in all of the three cases only two bound states appear: one deep and one shallow very close to the $A - 1$ threshold. The ground state presents a fast convergence with K and the accuracy can be estimated below 0.1 mK. The convergence for the excited state is slower and, for the values of K considered, its accuracy is given at the level of 3 mK. However, from the results, it is well established that, with the value of ρ_0 considered, the excited state, $E^{(1)}_{Ab}$, is bound with respect to the $A - 1$ threshold. In fact, for $A = 4$, the $3 + 1$ threshold appears at 126.4 mK and the upper bound estimate for this state is 129 mK. Its ratio $E^{(1)}_{4b}/E^{(0)}_{3b}$ is 1.020. For $A = 5$, the $4 + 1$ threshold appears at 568.8 mK and the upper bound estimate for the excited state is 575 mK. Its ratio $E^{(1)}_{5b}/E^{(0)}_{4b}$ is 1.011. For $A = 6$, the $5 + 1$ threshold appears at 1326.6 mK and the upper bound estimate for the excited state is 1350 mK. Its ratio $E^{(1)}_{6b}/E^{(0)}_{5b}$ is 1.018. The ratio between the trimer ground state and the ground states of the $A = 4,5,6$ systems are $E^{(0)}_{4b}/E^{(0)}_{3b} = 4.5$, $E^{(0)}_{5b}/E^{(0)}_{3b} = 10.5$, and $E^{(0)}_{5b}/E^{(0)}_{3b} = 18.5$, respectively. These ratios are in good agreement with those given in Refs. [25–27], and represent a substantial improvement with respect to the case in which the three-body force is not included. At the ratio r_0/a under consideration, the use of the two-body soft-core potential alone reduces the Efimov character of ground and first-excited states, which is recovered by including the

TABLE III. $A = 4,5,6$ binding energies of the ground, $E^{(0)}_{Ab}$, and first-excited, $E^{(1)}_{Ab}$, states for increasing values of the grand-angular-quantum number K. The three-body force parameters are $\rho_0 = 14$ a.u. and $W_0 = 0.422$ K. We also report the symmetry of the states; both the ground, $E^{(0)}_{Ab}$, and the first-excited, $E^{(1)}_{Ab}$, states are totally symmetric.

K	$E^{(0)}_{4b}$ (mK) [4]	$E^{(1)}_{4b}$ (mK) [4]	$E^{(0)}_{5b}$ (mK) [5]	$E^{(1)}_{5b}$ (mK) [5]	$E^{(0)}_{6b}$ (mK) [6]	$E^{(1)}_{6b}$ (mK) [6]
0	538.93	4.557	1288.1	365.1	2293.8	1109.9
2	538.93	4.557	1288.1	365.1	2293.8	1109.9
4	561.69	40.29	1319.6	460.4	2331.8	1237.3
6	566.68	67.47	1324.4	497.6	2336.6	1273.0
8	568.21	84.22	1326.1	527.0	2338.4	1307.7
10	568.58	96.04	1326.5	542.7	2338.7	1323.1
12	568.73	105.30	1326.6	554.0	2338.8	1334.4
14	568.77	111.17	1326.6	561.0	2338.9	1340.9
16	568.78	115.58	1326.6	565.9	2338.9	1345.3
18	568.79	118.78	1326.6	569.3	2338.9	1348.2
20	568.79	121.20	1326.6	571.8	2338.9	1350.2
22	568.79	122.98	1326.6	573.6	2338.9	1351.6
24	568.79	124.38	1326.6	574.9		
26	568.79	125.47				
28	568.79	126.33				
30	568.79	127.02				
32	568.79	127.57				
34	568.79	128.02				
36	568.79	128.40				
38	568.79	128.70				
40	568.79	128.96				
Ref. [16]	558.4		1302.2		2319.4	
Ref. [17]	559.7	132.6	1309.3	597.1	2329.4	1346.7

three-body force. It is interesting to compare the results obtained using the soft-core representation of the LM2M2 potential with the results of Refs. [16,17] (quoted in Table III) obtained using the original LM2M2 interaction. For the ground state, the agreement is around 2% for $A = 4,5$ and around 1% for $A = 6$. The agreement is worst for the excited state; however, the results from Ref. [17] are obtained using approximate solutions of the adiabatic hyperspherical equations.

The overall agreement for $A = 4,5,6$ between LM2M2 and the soft potential gives a further indication that at the LO in an EFT approach to the Efimov physics, there is no need for a four-body force; this is only a side observation which is not at all conclusive for the lack of a systematic study as a function of the cutoff.

Moreover, in the four panels of Fig. 1, we analyze modifications to the spectrum of the systems we have considered when different values of W_0 and ρ_0 are used. The results for $A = 3$ can be extracted from Table II; the $A = 3$ ground state is stable by construction, and small variations are observed for $E^{(1)}_{3b}$. As shown in Fig. 1(a), $E^{(1)}_{3b}$ is always below the 2+1 threshold. For $A = 4$, see Fig. 1(b) the excited state $E^{(1)}_{4b}$ is above the 3+1 threshold, and therefore not bounded for values of $\rho_0 < 7$ a.u. For $A = 5$, Fig. 1(c), and $A = 6$, Fig. 1(d), the corresponding excited states are above the 4+1 and 5+1 thresholds for values of $\rho_0 < 12$ a.u. and $\rho_0 < 10$ a.u., respectively. For $A = 5,6$, the results for the bound state present a bump with the smaller binding energy around $\rho_0 = 10$ a.u. To sum up, the most sensitive property of the spectrum as a function of ρ_0 is, for $A = 4,5,6$, if the $E^{(1)}_{Ab}$ is above or below threshold. As previously discussed, a reasonable choice is $\rho_0 = 14$ a.u., and around this value all the excited states are bound.

Finally, in Table IV, the results for the universal ratios are shown for values of $\rho_0 = 12,14,16$ a.u.; we observe that small variations of ρ_0 do not drastically change these values. It should be noticed that in the present analysis the unitary limit is not completely reached, since the ratio between the two-body effective range and scattering length is $r_0/a \approx 1/14$. An analysis of the universal ratios as a function of a is in progress.

IV. CONCLUSIONS

In this paper, we have attacked two different problems. From one side, we have studied the possibility of calculating bound and excited states in a bosonic (atomic) system up to $A = 6$ using the unsymmetrized HH expansion and considering soft two- and three-body forces. On the other hand, the model has been constructed to approximate the description of small helium clusters taking as a reference the results of the LM2M2 potential. These two problems are related, since the LM2M2 presents a strong repulsion at short distances. Therefore, the possibility of using a soft-core representation of the original potential has been analyzed in detail. In Ref. [19], bound states and low-energy scattering states of the trimer have been analyzed using the soft-core representation of the LM2M2. The results obtained in that work were encouraging in the sense that they were found to be in close agreement to those obtained using the original potential.

Here, we have extended the analysis to bigger systems. Therefore, the description of such systems with sufficient

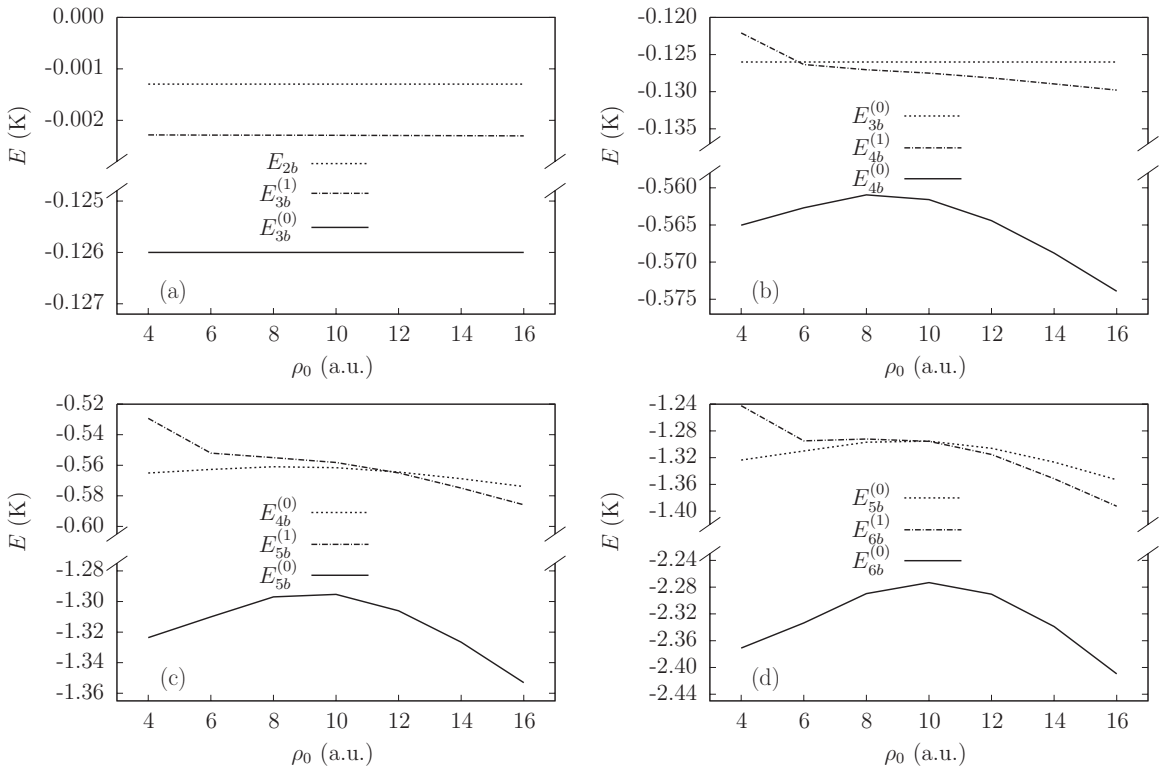


FIG. 1. Ground- and excited-state energies of the $A = 2,3,4,5,6$ systems as a function of ρ_0. In panel (a), we report the ground- and excited-state energy of the $A = 3$ system together with the ground-state energy of $A = 2$; for all of the values of ρ_0 we have considered, the excited $A = 3$ state is bounded. In panel (b), we report the ground- and excited-state energy of the $A = 4$ system together with the ground-state energy of $A = 3$; the excited $A = 4$ state is bounded for $\rho_0 > 7$. In panel (c), we report the ground- and excited-state energy of the $A = 5$ system together with the ground-state energy of $A = 4$; the excited $A = 5$ state is bounded for $\rho_0 > 12$. In panel (d), we report the ground- and excited-state energy of the $A = 6$ system together with the ground-state energy of $A = 5$; the excited $A = 6$ state is bounded for $\rho_0 > 10$.

accuracy is crucial. To this end, we have used a method recently developed in Ref. [23] in which the HH basis is used without symmetrization of the basis states. The basis is complete and, when all basis elements are included up to a certain maximum value of the grand angular momentum K, the eigenvectors reflect the symmetries present in the Hamiltonian. In the particular case here considered, the eigenvectors have well-defined symmetry under particle permutation and they can be organized as belonging to the different irreducible representations of the group of permutations of A objects, S_A. This simple fact has allowed us to make an important statement regarding the number of bosonic bound states present in the systems under study. After the direct diagonalization of the A-body system, we have analyzed the first three states for increasing values of K. We have considered a very extended basis: up to $K = 40$ for the $A = 4$ system and $K = 24$ ($K = 22$) for the $A = 5$ ($A = 6$) system. This allowed us to obtain converged results for the first eigenvalues of the spectrum.

TABLE IV. Ratios $E^{(0)}_{Ab}/E^{(0)}_{3b}$ and $E^{(1)}_{Ab}/E^{(0)}_{(A-1)b}$ as a function of the three-body cutoff ρ_0.

ρ_0 (a.u.)	$E^{(0)}_{4b}/E^{(0)}_{3b}$	$E^{(1)}_{4b}/E^{(0)}_{3b}$	$E^{(0)}_{5b}/E^{(0)}_{3b}$	$E^{(1)}_{5b}/E^{(0)}_{4b}$	$E^{(0)}_{6b}/E^{(0)}_{3b}$	$E^{(1)}_{6b}/E^{(0)}_{5b}$
12	4.47	1.01	10.33	1.001	18.12	1.005
14	4.50	1.02	10.50	1.011	18.50	1.018
16	4.54	1.03	10.70	1.021	19.06	1.029

The first two were symmetric states having eigenvalues with energy below the continuum threshold (fixed by the lowest bound state in the $A - 1$ system) and therefore they represent true bound states. The third state was found to belong to a mixed symmetry and is above the threshold. This was the case for all the systems considered ($A = 4,5,6$) and it means that the next bosonic state has an energy above the mixed state and therefore it is not bound. Therefore, we have unambiguously determined that these systems present only two bound states.

The two bosonic bound states have been studied for different values of the three-body potential rage ρ_0. This analysis is given in Fig. 1, where the position of the excited state moves from unbound to bound as ρ_0 increases. The particular case $\rho_0 \approx \sqrt{2}R$ is explicitly given in Table II, showing that in fact the excited state is slightly bound. Moreover, since the He-He potential predicts a large two-body scattering length, we have studied the universal ratios $E^{(0)}_{Ab}/E^{(0)}_{3b}$ and $E^{(1)}_{Ab}/E^{(0)}_{(A-1)b}$. These ratios have been studied in detail in the $A = 4$ case (see Refs. [24–26]). Estimates have also been obtained for bigger systems [27]. Our calculations, obtained for one particular value of the ratio r_0/a, are in agreement with those references on the universal character of these states in $A > 3$ systems. An analysis of the universal ratios as $a \to \infty$ is at present underway.

Finally, we would like to discuss the quality of the description using the two- and three-body soft-core-potential model. We observe a substantial good agreement, at the level

of 2% or better, for the ground states of the A-atom systems in comparison to the results of the LM2M2 potential given by Lewerenz [16]. The excited states have been calculated in Ref. [17], though using a reduced Hilbert space. Comparing to those results, we observe an agreement around 5%. From this analysis, we can conclude that a four-body force will have effects beyond this level of accuracy. A deeper analysis in this subject is in progress.

APPENDIX

Following Refs. [23,28], we present a brief overview of the properties of the HH basis and its implementation without generating basis elements with well-defined permutational symmetry. This approach allows us to avoid the complications of symmetry-adapted-basis construction, and to easily treat permutational-symmetry-breaking terms [23,29]

We start with the following definition of the Jacobi coordinates for an equal mass A-body system with Cartesian coordinates $\mathbf{r}_1 \ldots \mathbf{r}_A$,

$$\mathbf{x}_{N-j+1} = \sqrt{\frac{2j}{j+1}}(\mathbf{r}_{j+1} - \mathbf{X}_j), \quad j = 1, \ldots, N. \tag{A1}$$

For a given set of Jacobi coordinates $\mathbf{x}_1, \ldots, \mathbf{x}_N$, we can introduce the hyper-radius ρ,

$$\begin{aligned}\rho &= \left(\sum_{i=1}^{N} x_i^2\right)^{1/2} = \left(2\sum_{i=1}^{A}(\mathbf{r}_i - \mathbf{X})^2\right)^{1/2} \\ &= \left(\frac{2}{A}\sum_{j>i}^{A}(\mathbf{r}_j - \mathbf{r}_i)^2\right)^{1/2},\end{aligned} \tag{A2}$$

the hyperangular coordinates Ω_N,

$$\Omega_N = (\hat{\boldsymbol{x}}_1, \ldots, \hat{\boldsymbol{x}}_N, \phi_2, \ldots, \phi_N), \tag{A3}$$

with the hyperangles ϕ_i defined via

$$\begin{aligned} x_N &= \rho\, \cos\phi_N \\ x_{N-1} &= \rho\, \sin\phi_N \cos\phi_{N-1} \\ &\vdots \\ x_i &= \rho\, \sin\phi_N \cdots \sin\phi_{i+1} \cos\phi_i \\ &\vdots \\ x_2 &= \rho\, \sin\phi_N \cdots \sin\phi_3 \cos\phi_2 \\ x_1 &= \rho\, \sin\phi_N \cdots \sin\phi_3 \sin\phi_2. \end{aligned} \tag{A4}$$

The explicit expression for the HH functions, having well-defined values of LM, is

$$\begin{aligned}\mathcal{Y}^{LM}_{[K]}(\Omega_N) = &\left[\prod_{j=2}^{N} \mathcal{P}_{K_j}^{\alpha_{l_j},\alpha_{K_{j-1}}}(\phi_j)\right][Y_{l_1}(\hat{\mathbf{x}}_1) \otimes Y_{l_2}(\hat{\mathbf{x}}_2)|_{L_2} \cdots \\ &\otimes Y_{l_{N-1}}(\hat{\mathbf{x}}_{N-1})|_{L_{N-1}} \otimes Y_{l_N}(\hat{\mathbf{x}}_N)]_{LM},\end{aligned} \tag{A5}$$

with the indicated coupling scheme. The hyperspherical polynomial is

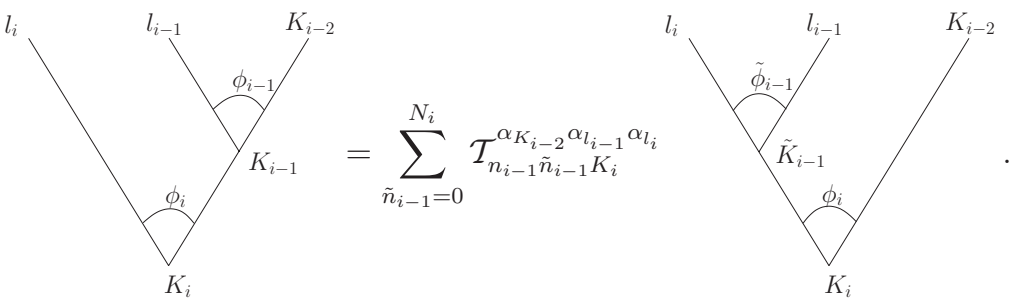
$$\begin{aligned}\mathcal{P}_{K_j}^{\alpha_{l_j},\alpha_{K_{j-1}}}(\phi_j) = &\mathcal{N}^{\alpha_{l_j},\alpha_{K_j}}_{n_j\,\alpha_{K_{j-1}},\alpha_{l_j}}(\cos\phi_j)^{l_j}(\sin\phi_j)^{K_{j-1}} \\ &\times P^{\alpha_{K_{j-1}},\alpha_{l_j}}_{n_j}(\cos 2\phi_j).\end{aligned} \tag{A6}$$

The set of quantum numbers $[K]$ includes the $n_2 \ldots n_N$ indices of the Jacobi polynomials, the $l_1 \ldots l_N$ angular momenta of the particles, and the intermediate couplings $L_2 \ldots L_{N-1}$. The K_j quantum numbers are defined as

$$K_j = \sum_{i=1}^{j}(l_i + 2n_i), \quad n_1 = 0, \quad K \equiv K_N, \tag{A7}$$

$K \equiv K_N$ is known as the grand angular momentum, and $\mathcal{N}_n^{\alpha\beta}$ is a normalization factor. For the definition of the α_a, where a can be either an angular momentum l_j or a quantum number K_j, one needs to introduce the hyperspherical-binary-tree structure [30]. For example, the tree of Fig. 2 corresponds to the choice of hyperangles given by Eq. (A4), in which the coefficients specialize to $\alpha_{K_j} = K_j + 3j/2 - 1$ and $\alpha_{l_j} = l_j + 1/2$.

Hyperspherical functions constructed using different hyperspherical-coordinate definitions can be related using the $\mathcal{T}$ coefficients [31,32]. Schematically, these coefficients relate the following tree structures:



(A8)

Here $K_i = K_{i-1} + l_i + 2n_i = \tilde{K}_{i-1} + l_i + 2\tilde{n}_i$. The explicit definition of the coefficients is given in Ref. [23]. Let us call $\mathcal{Y}^{LM}_{[K]}(\Omega^i_N)$ the HH basis element constructed in terms of a set of Jacobi coordinates in which the ith and $(i+1)$th Jacobi vectors result from the transposition between particles $j, j+1$,

$$\begin{aligned}\mathbf{x}'_i &= -\frac{1}{j}\mathbf{x}_i + \frac{\sqrt{(j+1)^2 - 2(j+1)}}{j}\mathbf{x}_{i+1} \\ \mathbf{x}'_{i+1} &= \frac{\sqrt{(j+1)^2 - 2(j+1)}}{j}\mathbf{x}_i + \frac{1}{j}\mathbf{x}_{i+1},\end{aligned} \tag{A9}$$

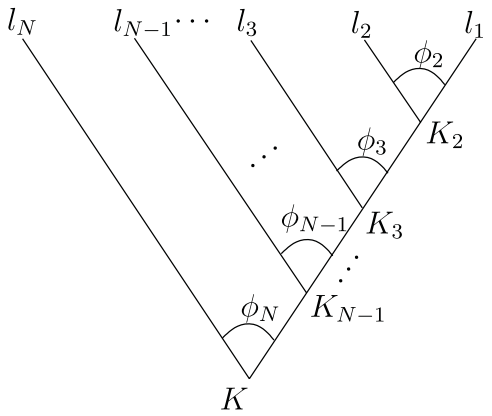


FIG. 2. Hyperspherical tree corresponding to Eq. (A4).

with all the other vectors equal to the original ones (transposed basis). The coefficients

$$\mathcal{A}^{i,LM}_{[K][K']} = \int d\Omega_N \left[\mathcal{Y}^{LM}_{[K]}(\Omega_N)\right]^* \mathcal{Y}^{LM}_{[K']}(\Omega^i_N) \tag{A10}$$

are the matrix elements of a matrix $\mathcal{A}^{LM}_i$ that allows us to express the transposed HH basis elements in terms of the reference basis. The coefficients $\mathcal{A}^{i,LM}_{[K][K']}$ form a very sparse matrix and they can be calculated analytically using the $\mathcal{T}$-coupling coefficients and the Raynal-Revai matrix elements [23]. A generic rotation between the reference HH basis and a basis in which the last Jacobi vector is defined as $\mathbf{x}'_N = \mathbf{r}_j - \mathbf{r}_i$ can be constructed as successive products of the $\mathcal{A}^{k,LM}_{[K][K']}$ coefficients. Defining $\mathcal{Y}^{LM}_{[K]}(\Omega^{ij}_N)$, the HH basis element constructed in terms of a set of Jacobi coordinates in which the Nth Jacobi vector is defined $\mathbf{x}'_N = \mathbf{r}_j - \mathbf{r}_i$, this coefficient can be given in the following form:

$$\begin{aligned}\mathcal{B}^{ij,LM}_{[K][K']} &= \int d\Omega \left[\mathcal{Y}^{LM}_{[K]}(\Omega_N)\right]^* \mathcal{Y}^{LM}_{[K]}(\Omega^{ij}_N) \\ &= \left[\mathcal{A}^{LM}_{i_1}\cdots\mathcal{A}^{LM}_{i_n}\right]_{[K][K']}. \end{aligned}\tag{A11}$$

The particular values of the indices $i_1,\ldots,i_n$, labeling the matrices $\mathcal{A}^{LM}_{i_1},\ldots,\mathcal{A}^{LM}_{i_n}$, depend on the pair (i,j). The matrix

$$\mathcal{B}^{LM}_{ij} = \mathcal{A}^{LM}_{i_1}\cdots\mathcal{A}^{LM}_{i_n} \tag{A12}$$

is written as a product of the sparse matrices $\mathcal{A}^{LM}_i$.

We consider now the potential energy of an A-body system constructed in terms of two-body interactions:

$$V = \sum_{i<j} V(i,j). \tag{A13}$$

In terms of the HH basis, it reads

$$\sum_{ij} V_{ij}(\rho) = \sum_{ij} \left[\mathcal{B}^{LM}_{ij}\right]^t V_{12}(\rho) \mathcal{B}^{LM}_{ij}, \tag{A14}$$

where the matrix elements of the matrix $V_{12}(\rho)$ are defined as

$$\begin{aligned} V^{(1,2)}_{[K][K']}(\rho) &= \left\langle \mathcal{Y}^{LM}_{[K]}(\Omega_N)\right| V(1,2) \left|\mathcal{Y}^{LM}_{[K']}(\Omega_N)\right\rangle \\ &= \delta_{l_1,l'_1}\cdots\delta_{l_N,l'_N}\delta_{L_2,L'_2}\cdots\delta_{L_N,L'_N}\delta_{K_2,K'_2}\cdots\delta_{K_N,K'_N} \\ &\quad\times \int d\phi_N (\cos\phi_N \sin\phi_N)^2 \mathcal{P}^{\alpha_{l_N},\alpha_{K_{N-1}}}_{K_N}(\phi_N) \\ &\quad\times V(\rho\cos\phi_N)\mathcal{P}^{\alpha_{l_N},\alpha_{K_{N-1}}}_{K'_N}(\phi_N). \end{aligned}\tag{A15}$$

Each term of the sum in Eq. (A14) results in a product of sparse matrices, a property which allows an efficient implementation of matrix-vector product. This procedure can be easily extended to spin-dependent potentials [33].

We now consider a three-body force depending on the hyper-radius ρ_{ijk} of a triplet of particles $\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k$,

$$V^{(3)} = \sum_{i<j<k} W(\rho_{ijk}). \tag{A16}$$

The term in which $i,j,k \equiv 1,2,3$ verifies $\rho^2_{123} = x^2_N + x^2_{N-1}$. It can be calculated on a hyperspherical-basis set relative to a nonstandard hyperspherical tree with the branches attached to leaves x_N and x_{N-1} going to the same node. The transition between the two hyperspherical sets is given by the $\mathcal{T}$ coefficients

$$\mathcal{Y}^{LM}_{[K]}(\Omega_N) = \sum_{\tilde{n}_{N-1}} \mathcal{T}^{\alpha_{K_{N-2}}\alpha_{l_{N-1}}\alpha_{l_N}}_{n_{N-1}\tilde{n}_{N-1}K} \mathcal{Y}^{LM}_{[\tilde{K}]}(\tilde{\Omega}_N), \tag{A17}$$

where all the variables with the tilde refer to the nonstandard tree. With this choice, we simply have

$$\rho_{123} = \rho\,\cos\phi_N, \tag{A18}$$

and the fixed-ρ matrix elements read

$$\begin{aligned} &\left\langle \mathcal{Y}^{LM}_{[\tilde{K}']}(\tilde{\Omega}_N)\right| W(\rho) \left|\mathcal{Y}^{LM}_{[\tilde{K}]}(\tilde{\Omega}_N)\right\rangle \\ &\quad= \delta_{l'_1,l_1}\cdots\delta_{l'_N,l_N}\delta_{L'_2,L_2}\cdots\delta_{L',L}\delta_{M',M}\delta_{\tilde{K}'_2,\tilde{K}_2}\cdots\delta_{\tilde{K}'_{N-1},\tilde{K}_{N-1}} \\ &\qquad\times \int (\cos\phi_N)^4 (\sin\phi_N)^{3N-8} d\phi_N \mathcal{P}^{\alpha_{\tilde{K}_{N-1}},\alpha_{K_{N-2}}}_{K'}(\phi_N) \\ &\qquad\times \mathcal{P}^{\alpha_{\tilde{K}_{N-1}},\alpha_{K_{N-2}}}_{K}(\phi_N) W(\rho\,\cos\phi_N). \end{aligned}\tag{A19}$$

The three-body force matrix $W(\rho)$ is extremely sparse, and it is diagonal on all quantum numbers but the grand-angular momentum. Finally, the matrix $W(\rho)$ in the standard basis is obtained by means of the $\mathcal{T}$ coefficients,

$$\begin{aligned} &\left\langle \mathcal{Y}^{LM}_{[K']}(\Omega_N)\right| W(\rho) \left|\mathcal{Y}^{LM}_{[K]}(\Omega_N)\right\rangle \\ &\quad= \sum_{\tilde{n}_{N-1}} \mathcal{T}^{\alpha_{K_{N-2}}\alpha_{l_{N-1}}\alpha_{l_N}}_{n'_{N-1}\tilde{n}_{N-1}K'} \mathcal{T}^{\alpha_{K_{N-2}}\alpha_{l_{N-1}}\alpha_{l_N}}_{n_{N-1}\tilde{n}_{N-1}K} \\ &\qquad\times \left\langle \mathcal{Y}^{LM}_{[\tilde{K}']}(\tilde{\Omega}_N)\right| W(\rho_{123}) \left|\mathcal{Y}^{LM}_{[\tilde{K}]}(\tilde{\Omega}_N)\right\rangle. \end{aligned}\tag{A20}$$

In order to calculate the other terms of the three-body force, we use the matrices $\mathcal{A}^{LM}_p$, defined in Eq. (A10), that transpose particles; with a suitable product of these sparse matrices,

$$\mathcal{D}^{LM}_{ijk} = \mathcal{A}^{LM}_{p_1}\cdots\mathcal{A}^{LM}_{p_m}, \tag{A21}$$

we can permute the particles in such a way that $\mathbf{x}_N = \mathbf{r}_i - \mathbf{r}_j$, $\mathbf{x}_{N-1} = 2/\sqrt{3}[\mathbf{r}_k - (\mathbf{r}_i + \mathbf{r}_j)/2]$, $\rho^2_{ijk} = x^2_{N-1} + x^2_N$, and the total three-body force reads

$$V^{(3)} = \sum_{i<j<k} \left[\mathcal{D}^{LM}_{ijk}\right]^t W(\rho) \mathcal{D}^{LM}_{ijk}. \tag{A22}$$

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