Scattering length of the helium-atom–helium-dimer collision

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We present our recent results on the scattering length of ^{4}He-^{4}He$_2$ collisions. These investigations are based on the hard-core version of the Faddeev differential equations. As compared to our previous calculations of the same quantity, a much more refined grid is employed, providing an improvement of about 10%. Our results are compared with other *ab initio* and model calculations.

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I. INTRODUCTION

Weakly bound small ^{4}He clusters have attracted considerable attention in recent years, in particular because of the booming interest in Bose-Einstein condensation of ultracold gases [1,2].

Experimentally, helium dimers have been observed in 1993 by Luo *et al.* [3], and in 1994 by Schöllkopf and Toennies [4]. In the latter investigation the existence of helium trimers has also been demonstrated. Later on, Grisenti *et al.* [5] measured a bond length of 52 ± 4 Å for ^{4}He$_2$, which indicates that this dimer is the largest known diatomic molecular ground state. Based on this measurement, they estimated a scattering length of 104^{+8}_{-18} Å and a dimer energy of $1.1^{+0.3}_{-0.2}$ mK [5]. Further investigations concerning helium trimers and tetramers have been reported in Refs. [6,7], but with no results on size and binding energies.

Many theoretical calculations of these systems were performed for various interatomic potentials [8–11]. Variational, hyperspherical, and Faddeev-type techniques have been employed in this context (see, e.g., Refs. [12–28] and references therein). For the potentials given in Refs. [9,10], it turned out that the helium trimer has two bound states of total angular momentum zero: a ground state of about 126 mK and an excited state of about 2.28 mK. The latter was shown to be of Efimov nature [13,15,21]. In particular, it was demonstrated in Ref. [21] how the Efimov states emerge from the virtual ones when decreasing the strength of the interaction. High accuracy has been achieved in all these calculations.

While the number of papers devoted to the ^{4}He$_3$ bound-state problem is rather large, the number of scattering results is still very limited. Phase shifts of ^{4}He-^{4}He$_2$ elastic scattering at ultralow energies have been calculated for the first time in Refs. [17,18] below and above the three-body threshold. An extension and numerical improvement of these calculations was published in Ref. [24]. To the best of our knowledge, the only alternative *ab initio* calculation of phase shifts below the three-body threshold was performed in Ref. [28]. As shown in Refs. [29,30], a zero-range model formulated in field theoretical terms is able to simulate the scattering situation.

Although it is an ideal quantum mechanical problem, involving three neutral bosons without complications due to spin, isospin or Coulomb forces, the exact treatment of the ^{4}He triatomic system is numerically quite demanding at the scattering threshold. Due to the low energy of the helium dimer, a very large domain in configuration space, with a characteristic size of hundreds of Ångstroms, has to be considered. As a consequence, the accuracy achieved in Refs. [19,24] for the scattering length appeared somewhat limited. To overcome this limitation, we have enlarged in the present investigation the cutoff radius $\rho_{\max}$ from 600 to 900 Å and employed much more refined grids.

II. FORMALISM

Besides the complications related to the large domain in configuration space, the other source of complications is the strong repulsion of the He−He interaction at short distances. This problem, however, was and is overcome in our previous and present investigations by employing the rigorous hard-core version of the Faddeev differential equations developed in Refs. [31,32].

Let us recall the main aspects of the corresponding formalism (for details see Refs. [19,24]). In what follows we restrict ourselves to a total angular momentum $L=0$. In this case one has to solve the two-dimensional integro-differential Faddeev equations

$$\left[-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+l(l+1)\left(\frac{1}{x^2}+\frac{1}{y^2}\right)-E\right]\Phi_l(x,y)=\begin{cases}-V(x)\Psi_l(x,y), & x>c\\ 0, & x<c.\end{cases} \tag{1}$$

Here, x,y stand for the standard Jacobi variables and c for the core range. The angular momentum l corresponds to a dimer subsystem and a complementary atom; for an S-wave three-boson state, l is even ($l=0,2,4,\ldots$). $V(x)$ is the He−He central potential acting outside the core domain. The partial-wave function $\Psi_l(x,y)$ is related to the Faddeev components $\Phi_l(x,y)$ by

$$\Psi_l(x,y) = \Phi_l(x,y) + \sum_{l'} \int_{-1}^{+1} d\eta\, h_{ll'}(x,y,\eta)\Phi_{l'}(x',y'), \tag{2}$$

where

$$x' = \sqrt{\frac{1}{4}x^2 + \frac{3}{4}y^2 - \frac{\sqrt{3}}{2}xy\eta}, \quad y' = \sqrt{\frac{3}{4}x^2 + \frac{1}{4}y^2 + \frac{\sqrt{3}}{2}xy\eta},$$

and $1 \leqslant \eta \leqslant 1$. The explicit form of the function $h_{ll'}$ can be found in Refs. [33,34].

The functions $\Phi_l(x,y)$ satisfy the boundary conditions

$$\Phi_l(x,y)_{x=0} = \Phi_l(x,y)_{y=0} = 0. \tag{3}$$

Moreover, in the hard-core model they are required to satisfy the condition

$$\Phi_l(c,y) + \sum_{l'} \int_{-1}^{+1} d\eta\, h_{ll'}(c,y,\eta)\Phi_{l'}(x',y') = 0. \tag{4}$$

This guarantees the wave function $\Psi_l(x,y)$ to be zero not only at the core boundary $x=c$, but also inside the core domains.

The asymptotic boundary condition for the partial-wave Faddeev components of the two-fragment scattering states reads, as $\rho \to \infty$ and/or $y \to \infty$,

$$\Phi_l(x,y;p) = \delta_{l0}\psi_d(x)\{\sin(py) + \exp(ipy)[a_0(p) + o(y^{-1/2})]\} + \frac{\exp(i\sqrt{E}\rho)}{\sqrt{\rho}}[A_l(\theta) + o(\rho^{-1/2})]. \tag{5}$$

Here, $\psi_d(x)$ is the dimer wave function, E stands for the scattering energy given by $E=\varepsilon_d+p^2$ with ε_d the dimer energy, and p for the relative momentum conjugate to the variable y. The variables $\rho=\sqrt{x^2+y^2}$ and $\theta=\arctan(y/x)$ are the hyperradius and hyperangle, respectively. The coefficient $a_0(p)$ is nothing but the elastic scattering amplitude, while the functions $A_l(\theta)$ provide us, at $E>0$, with the corresponding partial-wave Faddeev breakup amplitudes. The ^{4}He–^{4}He$_2$ scattering length ℓ_{sc} is given by

$$\ell_{sc} = -\frac{\sqrt{3}}{2}\lim_{p\to 0}\frac{a_0(p)}{p}. \tag{6}$$

Here, we only deal with a finite number of equations (1)–(4), assuming $l \leqslant l_{max}$, where l_{max} is a certain fixed even number. As in Refs. [19,24] we use a finite-difference approximation of the boundary-value problem (1)–(5) in the polar coordinates ρ and θ. The grids are chosen such that the points of intersection of the arcs $\rho=\rho_i$, $i=1,2,\ldots,N_\rho$ and the rays $\theta=\theta_j$, $j=1,2,\ldots,N_\theta$, with the core boundary $x=c$ constitute the knots. The value of the core radius is chosen to be $c=1$ Å by the argument given in Ref. [24]. We also follow the same method for choosing the grid radii ρ_i (and thus the grid hyperangles θ_j), as described in Refs. [19,24].

III. RESULTS

Our calculations are based on the semiempirical HFD-B [8] and LM2M2 [9] potentials by Aziz and co-workers, and the more recent, purely theoretically derived TTY [10] potential by Tang, Toennies, and Yiu. For the explicit form of these polarization potentials, we refer to the appendix of Ref. [24]. As in our previous calculations, we choose $\hbar^2/m = 12.12$ K Å^2, where m stands for the mass of the ^{4}He atom. The ^{4}He dimer binding energies and ^{4}He–^{4}He scattering lengths obtained with the HFD-B, LM2M2, and TTY potentials are shown in Table I. Note that the inverse of the wave number $\varkappa^{(2)}=\sqrt{|\varepsilon_d|}$ lies rather close to the corresponding scattering length.

TABLE I. Dimer energy ε_d, wave length $1/\varkappa^{(2)}$, and ^{4}He–^{4}He scattering length $\ell_{sc}^{(2)}$ for the potentials used, as compared to the experimental values of Ref. [5].

	ε_d (mK)	$\ell_{sc}^{(2)}$(Å)	Potential	ε_d (mK)	$1/\varkappa^{(2)}$ (Å)	$\ell_{sc}^{(2)}$ (Å)
			LM2M2	−1.30348	96.43	100.23
Expt.	$1.1^{+0.3}_{-0.2}$	104^{+8}_{-18}	TTY	−1.30962	96.20	100.01
			HFD-B	−1.68541	84.80	88.50

Unlike the trimer binding energies, the ^{4}He–^{4}He$_2$ scattering length is much more sensitive to the grid parameters. To investigate this sensitivity, we take increasing values of the cutoff hyperradius ρ_{max}, and simultaneously increase the dimension of the grid $N=N_\theta=N_\rho$. Surely, in such an analysis we can restrict ourselves to $l_{max}=0$. The results obtained for the TTY potential are given in Table II and Fig. 1. Inspection of this figure shows that, when increasing the dimension N of the grid, convergence of the ^{4}He-^{4}He$_2$ scattering length ℓ_{sc} is essentially achieved, however, with different limiting values of ℓ_{sc} for different choices of ρ_{max}. This concerns, in particular, the transition from $\rho_{max}=600$ Å to $\rho_{max}=700$ Å, while the transition to 800 Å or even 900 Å has practically no effect.

Bearing this in mind, we feel justified to choose $\rho_{max}=700$ Å when going over from $l_{max}=0$ to $l_{max}=2$ and 4. The corresponding results are presented in Table III. There we also show our previous results [24] where, due to lack of computer facilities, we had to restrict ourselves to $\rho_{max}=460$ Å and $N=605$. We see that an improvement of about 10% is achieved in the present calculations, as already indicated by the trends in Fig. 1.

Table III also contains the fairly recent results by Blume and Greene [23] and Roudnev [28]. The treatment of [23] is based on a combination of the Monte Carlo method and the

TABLE II. The ^{4}He–^{4}He$_2$ scattering length ℓ_{sc}(Å) for $\ell_{max}=0$ in case of the TTY potential as a function of the grid parameters ρ_{max} and $N=N_\rho=N_\theta$.

ρ_{max}	N					
	1005	1505	2005	2505	3005	3505
600	162.33	159.80	158.91	158.61	158.31	
700	164.13	159.99	158.57	157.99	157.65	157.48
800	167.15	160.98	158.90	158.03	157.46	
900	171.19	162.52	159.66	158.40	157.66	

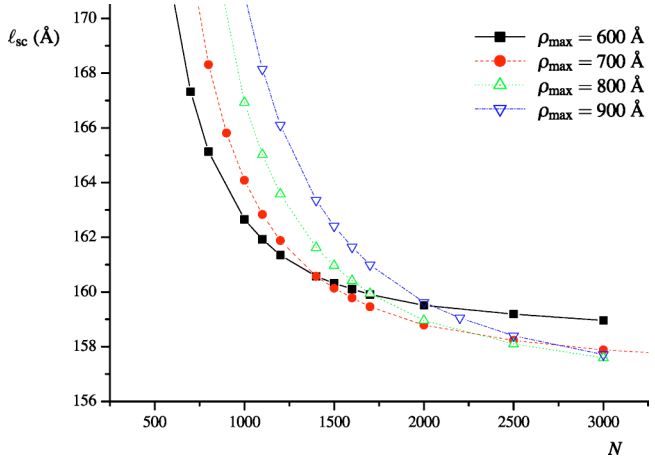

FIG. 1. The ^{4}He–^{4}He$_2$ scattering length ℓ_{sc} for $l_{max}=0$ in the case of the TTY potential as a function of the grid dimension $N \equiv N_\rho = N_\theta$.

hyperspherical adiabatic approach. The one of Ref. [28] employs the three-dimensional Faddeev differential equations in the total angular momentum representation. Our results agree rather well with these alternative calculations.

This gives already a good hint on the quality of our present investigations. A direct confirmation is obtained by extrapolating the curves in Fig. 1. According to this figure, convergence of ℓ_{sc} as a function of N is essentially, but not fully, achieved. A certain improvement, thus, is still to be expected when going to higher N. In order to estimate this effect we approximate the curves of Fig. 1 by a function of the form

$$\ell_{sc}(N) = \alpha + \frac{\beta}{N - \gamma}. \tag{7}$$

Clearly, $\ell_{sc}(\infty) = \alpha$. The constants α, β, and γ are fixed by the values of ℓ_{sc} at $N=1005$, 2005, and 3005. In this way we get the corresponding optimal scattering lengths $\ell_{sc}(\infty)=157.5$, 156.4, 155.4, and 154.8 Å for $\rho_{max}=600$, 700, 800, and 900 Å, respectively. Comparing with Table II shows that the differences between these asymptotic values and the ones for $N=3005$ lie between 1 and 3 Å.

For $l_{max}=4$, $\rho_{max}=700$ Å and the LM2M2 potential, the scattering length has been calculated for $N=1005$, 1505, and 2005. Employing again the extrapolation formula (7) with α, β, γ being chosen according to these values, we find $\ell_{sc}(\infty)=117.0$ Å. The difference between the scattering length obtained for $N=2005$ and the extrapolated value is therefore 1.7 Å. A direct calculation for higher N should lead to a modification rather close to this result. Following this argument, we conclude that the true value of ℓ_{sc} for the LM2M2 and TTY potentials lies between 115 and 116 Å.

TABLE III. The ^{4}He–^{4}He$_2$ scattering length ℓ_{sc}(Å) obtained for a grid with $N_\rho = N_\theta = 2005$ and $\rho_{max}=700$ Å.

Potential	l_{max}	This work	Ref. [24]	Ref. [23]	Ref. [28]	Ref. [35]	Ref. [30]
	0	158.2	168				
LM2M2	2	122.9	134				
	4	118.7	131	126	115.4	114.25	113.1
	0	158.6	168				
TTY	2	123.2	134				
	4	118.9	131		115.8		114.5
	0	159.6	168				
HFD-B	2	128.4	138				
	4	124.7	135		121.9		120.2

For completeness, we mention that besides the above *ab initio* calculations there are also model calculations, the results of which are given in the last two columns of Table III. The calculations of Ref. [35] are based on employing a Yamaguchi potential that leads to an easily solvable one-dimensional integral equation in momentum space. The approach of Ref. [30] (see also Ref. [29] and references therein) represents intrinsically a zero-range model with a cutoff introduced to make the resulting one-dimensional Skornyakov-Ter-Martirosian equation [36] well defined. The cutoff parameter in Refs. [29,30] as well as the range parameter of the Yamaguchi potential in Ref. [35] are adjusted to the three-body binding energy obtained in the *ab initio* calculations. In other words, these approaches are characterized by a remarkable simplicity, but rely essentially on results of the *ab initio* three-body calculations.

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