Scattering length calculations via Faddeev approach

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Abstract. The results of calculation for the scattering length for the collision of a ^{4}He atom with a ^{4}He^{7}Li dimer are presented. These investigations are based on the hard-core version of the Faddeev differential equations.

1. Introduction

Weakly bound small atomic clusters attracted considerable attention in recent years especially due to the possibility to observe states of Efimov nature [1]. The interaction between neutral atoms is of the short-range van-der-Waals type and in some cases can almost or just barely support a weakly two-body bound state. In such a cases the scattering length will be much larger than the effective range of the interaction. Efimov discovered that in a three-body system an effective long-range attraction arises, and this attraction may support an infinite number of bound states. The binding energy of these states is arranged in a geometric series with an accumulation point at zero energy threshold. The energies of the Efimov levels are universally related and this relation does not depend on the form of the pair-wise interactions in the three-body system [2].

One of a promising atomic species for observing Efimov states is ^{4}He three-atomic cluster. The interaction between two helium atoms is quite small and supports only one bound state with the energy about 1mK and so a very large scattering length around 100 Å. An excited state of Efimov nature in helium trimer was theoretically predicted (see, [3, 4] and refs. therein). Most recently this has been brilliantly confirmed experimentally using the combination of Coulomb explosion imaging with cluster mass selection by matter-wave diffraction [5].

The implementation of magnetic Feshbach resonances in ultracold atoms experiments gives a possibility to change the scattering length by simply varying the strength of an applied magnetic field. The first observation of Efimov-type resonance in an ultracold gas of cesium atoms has been reported in [6]. Experimentally, in [6] Efimov resonance was observed as a giant three-body recombination loss when the intensity of the magnetic field and so the strength of the two-body interaction was varied. Striking manifestations of the Efimov effect have been predicted for three-body recombination processes in ultracold gases with tunable two-body interactions in [7, 8]. Although in this experiment only one Efimov resonance was observed, recently the second Efimov level has been measured using the same technique [9]. Now it has become possible to study Efimov effect in many other atomic systems [10, 11, 12, 13, 14, 15]. Review of the latest theoretical and experimental advances in Efimov physics can be found in [16].

There is a growing interest in the study of He_2 - Alkali van-der-Waals systems, which are expected to be of Efimov nature. As in case of a ^{4}He dimer, the He - alkali-atom interactions also support a single

weakly bound state. So, in the triatomic $^4He_2Li$ system one can expect the existence of Efimov levels and a large He - HeLi scattering length which is investigated in this work.

2. Method

In describing a three-atomic system we use the standard reduced Jacobi coordinates $\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha$, $\alpha = 1,2,3$, expressed in terms of the position vectors of the atoms $\boldsymbol{r}_\alpha$ and their masses m_α [17]:

$$\begin{aligned} \boldsymbol{x}_\alpha &= \left[\frac{2m_\beta m_\gamma}{m_\beta + m_\gamma}\right]^{1/2} (\boldsymbol{r}_\beta - \boldsymbol{r}_\gamma) \\ \boldsymbol{y}_\alpha &= \left[\frac{2m_\alpha (m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma}\right]^{1/2} \left(\boldsymbol{r}_\alpha - \frac{m_\beta \boldsymbol{r}_\beta + m_\gamma \boldsymbol{r}_\gamma}{m_\beta + m_\gamma}\right), \end{aligned} \tag{1}$$

where (α, β, γ) stand for a cyclic permutation of the atom numbers $(1,2,3)$. The coordinates $\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha$ determine the six-dimensional vector $X \equiv (\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha)$. Relations between them are given by orthogonal transform Jacobi vectors with different α

$$\boldsymbol{x}_\beta = c_{\beta\alpha}\boldsymbol{x}_\alpha + s_{\beta\alpha}\boldsymbol{y}_\alpha, \qquad \boldsymbol{y}_\beta = -s_{\beta\alpha}\boldsymbol{x}_\alpha + c_{\beta\alpha}\boldsymbol{y}_\alpha, \tag{2}$$

where

$$\begin{aligned} c_{\alpha\beta} &= -\left(\frac{m_\alpha m_\beta}{(m_\alpha + m_\beta)(m_\beta + m_\gamma)}\right)^{1/2}, \\ s_{\alpha\beta} &= (-1)^{\beta-\alpha}\,\mathrm{sign}(\beta - \alpha)\left(1 - c_{\alpha\beta}^2\right)^{1/2}. \end{aligned}$$

In the following the Helium atoms are assigned the numbers 1 and 3 while the Lithium atom has the number 2. Since two atoms of ^4He are identical bosons the corresponding Faddeev component $F_2(\boldsymbol{x}_2, \boldsymbol{y}_2)$ is invariant under the permutation of the 1 and 3 particles

$$F_2(-\boldsymbol{x}_2, \boldsymbol{y}_2) = F_2(\boldsymbol{x}_2, \boldsymbol{y}_2). \tag{3}$$

The identity of the two ^4He atoms also implies that the Faddeev components $F_1(\boldsymbol{x}_1, \boldsymbol{y}_1)$ and $F_3(\boldsymbol{x}_3, \boldsymbol{y}_3)$ are obtained from each other by a simple rotation of the coordinate space. Thus, we only have two independent Faddeev components: $F_2(\boldsymbol{x}, \boldsymbol{y})$, which is associated with the ^4He–^4He subsystem, and $F_1(\boldsymbol{x}, \boldsymbol{y})$ - associated with a pair of Li and ^4He atoms. The resulting hard-core Faddeev equations read

$$(-\Delta_{\boldsymbol{x}_\alpha} - \Delta_{\boldsymbol{y}_\alpha} - E) F_\alpha(\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha) = \begin{cases} 0, & |\boldsymbol{x}_\alpha| < c \\ -V_\alpha(\boldsymbol{x}_\alpha)\Psi^{(\alpha)}(\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha), & |\boldsymbol{x}_\alpha| > c \end{cases}, \tag{4}$$

$$\Psi^{(\alpha)}(\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha)\Big|_{|\boldsymbol{x}_\alpha| = c} = 0, \qquad \alpha = 1,2, \tag{5}$$

where $\Psi^{(1)}$ and $\Psi^{(2)}$ denote the total wave function $\Psi(X)$ of the Li^4He_2-system written in terms of the Faddeev components F_1 and F_2 in coordinates $\boldsymbol{x}_1, \boldsymbol{y}_1$, and $\boldsymbol{x}_2, \boldsymbol{y}_2$, respectively (see [18, 19]). By c we denote the hard-core radius. This radius was taken the same (in coordinates $\boldsymbol{x}_\alpha$) for all three inter-atomic interaction potentials and was chosen in such a way that any further decrease of it does not affect the trimer ground-state energy. A detailed description of the Faddeev differential equations in the hard-core model in case of symmetric helium trimer can be found in [18]. By V_1 we denote the interatomic Li–He potential and V_2 - the He–He potential adjusted to the corresponding reduced Jacobi coordinates $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, respectively.

In the present investigation, we apply the above formalism to the ^{7}Li^{4}He$_2$ three-atomic systems with total angular momentum $L=0$. Expanding the functions F_1 and F_2 in a series of bispherical harmonics we have

$$F_\alpha(\boldsymbol{x},\boldsymbol{y}) = \sum_l \frac{f_l^{(\alpha)}(x,y)}{xy} \mathscr{Y}_{ll0}(\widehat{x},\widehat{y}), \quad \alpha = 1,2, \tag{6}$$

where $x=|\boldsymbol{x}|$, $y=|\boldsymbol{y}|$, $\widehat{x}=\boldsymbol{x}/x$, and $\widehat{y}=\boldsymbol{y}/y$. As a result the equations (4) and boundary conditions (5) are transformed to the following partial integro-differential equations

$$\begin{aligned}\left(-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+l(l+1)\left(\frac{1}{x^2}+\frac{1}{y^2}\right)-E\right) f_l^{(\alpha)}(x,y) \\ = \left\{\begin{array}{ll} 0, & x<c \\ -V_\alpha(x)\psi_l^{(\alpha)}(x,y), & x>c \end{array}\right., \qquad \alpha=1,2,\end{aligned} \tag{7}$$

and partial boundary conditions

$$\psi_l^{(\alpha)}(x,y)\Big|_{x=c} = 0, \qquad \alpha=1,2. \tag{8}$$

The partial wave functions $\psi_l^{(\alpha)}$, $\alpha=1,2$, read as follows

$$\psi_l^{(\alpha)}(x,y) \;=\; f_l^{(\alpha)}(x,y) + \sum_{l',\beta\neq\alpha} \int_0^1 d\eta\, h^0_{(\alpha;ll0)(\beta;l'l'0)}(x,y,\eta) f_{l'}^{(\beta)}(x_{\beta\alpha}(\eta), y_{\beta\alpha}(\eta))$$

where (cf. [17])

$$\begin{aligned} & h^L_{(\alpha;l\lambda L)(\beta;l'\lambda' L)}(x,y,\eta) = \\ & \quad \frac{xy}{x_{\beta\alpha}(\eta)y_{\beta\alpha}(\eta)} (-1)^{l+L} \frac{(2\lambda+1)(2l+1)}{2^{\lambda+l}} \left[(2\lambda)!(2l)!(2\lambda'+1)(2l'+1)\right]^{1/2} \\ & \quad \times \sum_{k=0}^{k_{max}} (-1)^k (2k+1) P_k(\eta) \sum_{\substack{\lambda_1+\lambda_2=\lambda,\\ l_1+l_2=l}} \frac{y^{\lambda_1+l_1} x^{\lambda_2+l_2}}{[y_{\beta\alpha}(\eta)]^\lambda [x_{\beta\alpha}(\eta)]^l} (-1)^{\lambda_1} \mathsf{c}_{\beta\alpha}{}^{\lambda_1+l_2} \mathsf{s}_{\beta\alpha}{}^{\lambda_2+l_1} \\ & \quad \times [(2\lambda_1)!(2l_1)!(2\lambda_2)!(2l_2)!]^{-1/2} \sum_{\lambda''l''} (2\lambda''+1)(2l''+1) \begin{pmatrix} \lambda_1 & l_1 & \lambda'' \\ 0 & 0 & 0 \end{pmatrix} \\ & \quad \times \begin{pmatrix} \lambda_2 & l_2 & l'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} k & \lambda'' & \lambda' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} k & l'' & l' \\ 0 & 0 & 0 \end{pmatrix} \\ & \quad \times \begin{Bmatrix} l' & \lambda' & L \\ \lambda'' & l'' & k \end{Bmatrix} \begin{Bmatrix} \lambda_1 & \lambda_2 & \lambda \\ l_1 & l_2 & l \\ \lambda'' & l'' & L \end{Bmatrix}, \\ & \quad k_{max} = \frac{1}{2}(l+\lambda+l'+\lambda'). \end{aligned} \tag{9}$$

Here $P_k(\eta)$ is the Legendre polynomial of order k. The standard notation for the 3-j, 6-j, and 9-j Wigner symbols are used. We also use the notation

$$x_{\beta\alpha}(\eta) = \sqrt{\mathsf{c}_{\beta\alpha}^2 x^2 + 2\mathsf{c}_{\beta\alpha}\mathsf{s}_{\beta\alpha} xy\eta + \mathsf{s}_{\beta\alpha}^2 y}, \quad y_{\beta\alpha}(\eta) = \sqrt{\mathsf{s}_{\beta\alpha}^2 x - 2\mathsf{c}_{\beta\alpha}\mathsf{s}_{\beta\alpha} xy\eta + \mathsf{c}_{\beta\alpha}^2 y}.$$

The asymptotic boundary condition for the partial-wave Faddeev components of the scattering wave function for $\rho = \sqrt{x^2+y^2} \to \infty$ and/or $y \to \infty$ reads as follows (cf. [20])

$$\begin{aligned} f_l^{(\alpha)}(x,y,p) &= \delta_{l0}\psi_d^{(\alpha)}(x)\left\{sin(py)+\exp(\mathrm{i}py)\left[\mathrm{a}_0^{(\alpha)}(p)+o\left(y^{-1/2}\right)\right]\right\} \\ &+\frac{\exp(\mathrm{i}\sqrt{E}\rho)}{\sqrt{\rho}}\left[A_l^{(\alpha)}(E,\theta)+o\left(\rho^{-1/2}\right)\right] \end{aligned}, \tag{10}$$

where $p = \sqrt{E-\varepsilon_d^{(\alpha)}}$ is the momentum conjugate to the coordinate y and E is the scattering energy. $\varepsilon_d^{(\alpha)}$ stands for the correspondent dimer energy while $\psi_d^{(\alpha)}(x)$ denotes the dimer wave function which is assumed to be zero within the core, that is, $\psi_d^{(\alpha)}(x) \equiv 0$ for $x \le c$. The coefficient $\mathrm{a}_0^{(\alpha)}(p)$ is the elastic scattering amplitude and $A_l^{(\alpha)}(E,\theta)$ are the corresponding partial-wave Faddeev breakup amplitudes. The ^{4}He – ^{4}He^{7}Li scattering length $\ell_{\rm sc}$ is given by

$$\ell_{\rm sc} = -\sqrt{\frac{m_1+m_2+m_3}{2m_1(m_2+m_3)}}\lim_{p\to 0}\frac{\mathrm{a}_0^{(1)}(p)}{p}. \tag{11}$$

Here we only deal with a finite number of equations (7), assuming $l \le l_{\max}$ where $l_{\max}$ is a certain non-negative integer. As in [18, 19] we use a finite-difference approximation of the boundary-value problem (7), (8), (10) 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 [19]. We also follow the same method for choosing the grid radii ρ_i (and, thus, the grid hyperangles θ_j) as described in [18, 19] in details. Atomic masses of the isotopes are taken from [21].

3. Results and Discussion

Our calculations are based on the semi-empirical LM2M2 [22] potential by Aziz and Slaman for He-He interaction, and the theoretically derived KTTY [23] potential by Kleinekathöfer, Tang, Toennies and Yiu for Li-He interaction with more accurate coefficients taken from [24]. Both of these potentials are widely used in the literature and presented in Fig. 1 as well as all other He - Alkali atom KTTY potentials from [24]. It is clearly seen that He-Alkali atom potentials become much shallower and wider with increasing mass of alkali atom. Calculated values of the binding energy for correspondent dimers are presented in Table 1. All He-Alkali dimers are weakly bound and in the case of HeLi and HeCs systems, the binding energy is of the same order as in helium dimer. It gives an indication on possible existence of Efimov states in correspondent He_2 - Alkali atom triatomic systems. Indeed, in calculations [25, 26, 27, 28, 29] the excited state with the energy very close to the LiHe threshold has been found. However, different methods demonstrate a large discrepancy between the results (see Table 1 of [28] or Table II of [29]). The energy levels of He_2Li trimer are found to be very sensitive to the details of the numerical methods and the interaction potentials. We can conclude that this triatomic system is much more complicated for investigation than the helium trimer studied previously [3, 4].

The scattering length calculations are very sensitive to the grid parameters. To investigate this sensitivity we calculate the scattering length with increasing cutoff hyperradius ρ_{max} up to 500 Å and increasing grid numbers $N \equiv N_\rho = N_\theta$ up to 2500. The value of l_{max} has been increased up to 4. The results for the ^{4}He -^{4}He^{7}Li scattering length $\ell_{\rm sc}$ as a function of the grid dimension N are presented in Fig.2. Convergence of the scattering length value is essentially achieved for $N \sim 2500$. Increasing values of the cutoff hyperradius ρ_{max} from 250 Å to 500 Å change the value of $\ell_{\rm sc}$ by 2%. Taking into account partial angular momentum $l_{max} = 2$ increase the scattering length by 10% while $l_{max} = 4$ gives only 2% . As a result, we found that the ^{4}He -^{4}He^{7}Li scattering length for the LM2M2 and KTTY potentials is negative and equals -267 Å for the largest grid that we could achieve. The large value of the scattering

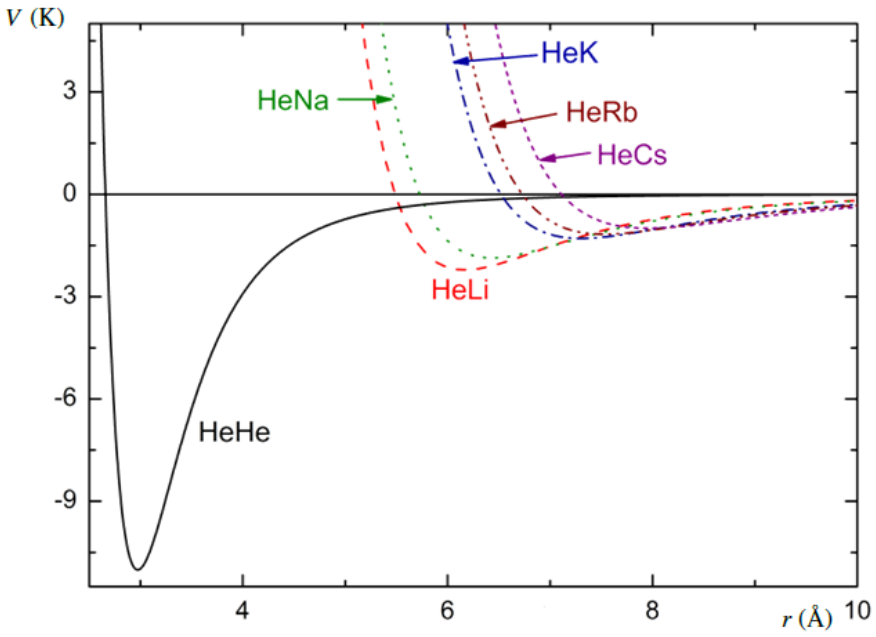

Figure 1. The He–He LM2M2 potential and He - Alkali atoms KTTY potentials V (in K) as a function of the interatomic distance r (in Å).

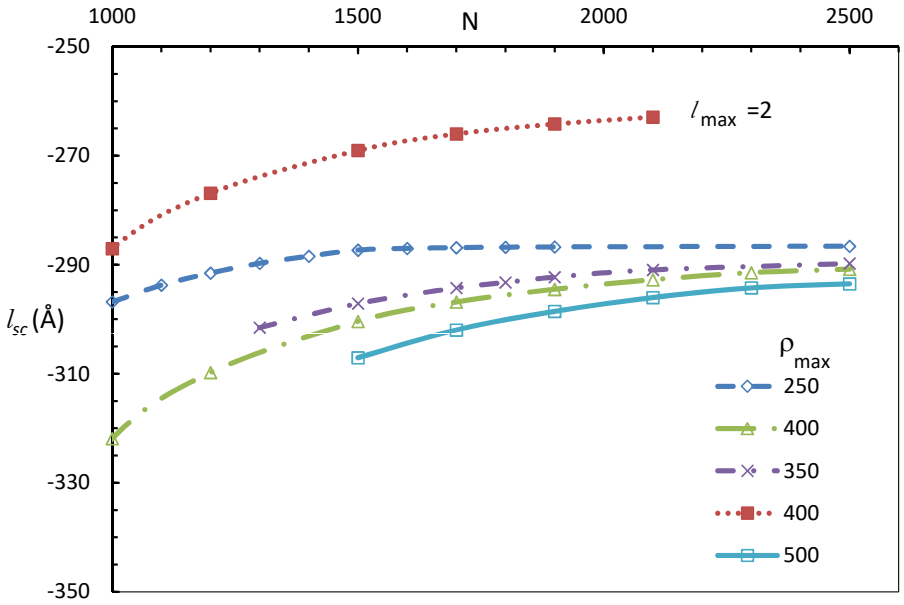

Figure 2. The ^{4}He -^{4}He^{7}Li scattering length ℓ_{sc}(Å) as a function of the grid dimension $N \equiv N_\rho = N_\theta$. The curves presented are distinguished by the value of the cutoff hyperradius. The upper curve shows the results obtained for $l_{max} = 2$, other curves correspond to $l_{max} = 0$.

Table 1. Absolute values of dimer energies $|\varepsilon_d|$ (in mK) for He-He and ^{4}He−Alkali atom for the potentials used.

Dimer	$\lvert\varepsilon_d\rvert$ (mK)	Dimer	$\lvert\varepsilon_d\rvert$ (mK)
^{4}He^{3}He	–	^{4}He^{23}Na	28.97
^{4}He^{4}He	1.310	^{4}He^{39}K	11.20
^{4}He^{6}Li	1.512	^{4}He^{85}Rb	10.27
^{4}He^{7}Li	5.617	^{4}He^{133}Cs	4.945

length supports the assumption that ^{4}He$_2$^{7}Li is the system of Efimov type. The negative sign means that this system is more likely to have the virtual state than the excited state. However, it could also mean that asymptotic behavior at used cutoff hyperradius $\sim$ 500 Å has not yet started. Studying of this fact requires further investigation.

In conclusion, the results of calculation of the scattering length for the collision of a ^{4}He atom on a ^{4}He^{7}Li dimer are presented. Its large value indicates that ^{4}He$_2$^{7}Li system is of Efimov type.

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