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Weakly Bound Li He_2 Molecules

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Abstract The results for binding energies of ^{6}Li He_2 and ^{7}Li He_2 systems are presented. They are obtained by solving Faddeev equations in configuration space. It is shown that the excited states in both systems are of the Efimov-type.

1 Introduction

In the last few years an enormous progress was demonstrated in the studying of the Efimov effect [1] in different systems. First of all it concerns ultracold quantum gases trapped by a magnetic field. Being a subject to a magnetic field, certain two-atom systems experience a Feshbach resonance due to Zeeman interaction. In such a case one gets an opportunity to control the atom-atom scattering length, by changing the intensity of the magnetic field. When the two-body scattering length is large compared to the radius of the two-body interaction, the three-body system may have a series of weakly Efimov-type bound states. 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 [1].

In 2006 there was the first observation of Efimov-type resonance in an ultracold gas of cesium atoms [2]. The resonance has to occur in the range of large negative two-body scattering lengths, arising from the coupling of three free atoms to an Efimov trimer. Experimentally, in [2] its signature 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 [3,4]. Although in this experiment only one Efimov resonance was observed, recently the second Efimov level has been measured using the same technique [5]. Starting from the first experiment by R. Grimm's group a lot of other experimental evidence for the Efimov states in three-atomic systems consisting of Li, K, Rb, Cs atoms and its combinations were reported [6–11].

Universality of Efimov effect allows to expect its manifestation in nuclear systems, especially in a halo nuclei. Although the experimental evidence is not yet found, the existence of nuclear Efimov trimer states has been speculated in many isotopes [12]. Of particular interest are the investigations of the isotop of ^{22}C,

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recently studied in [13–15], which has so far the largest detected halo formed by two neutrons [16], and of the isotop ^{62}Ca—the heaviest Borromean nucleus [17]. Studying these systems improves our understanding of nuclear behavior in extreme conditions along the neutron drip line [18].

One of the best theoretically predicted examples of the Efimov three-body system is a naturally existing molecule of the helium trimer where an excited state is of the Efimov nature (see, [19] and refs. therein). Only recently there was the first observation of this long-predicted state of helium trimer using the combination of Coulomb explosion imaging with cluster mass selection by matter wave diffraction [20]. The interaction between two helium atoms is quite small and supports only one bound state with the energy about 1 mK and so a very large scattering length around 100 Å. In addition to the Helium dimer, the He–alkali-atom interactions are even shallower and also support weakly bound states. Thus, in triatomic ^{4}He$_2$–alkali-atom system one can expect the existence of Efimov levels. The $^{6;7}$Li^{4}He$_2$ systems, which are investigated in this work, have the excited states of Efimov-type as will be demonstrated further by the results of the calculations.

2 Method

We solve the Faddeev equations for three interacting atoms using a similar scheme as in our previous investigations of Helium trimer [21]. There, the formalism which consists of a hard-version of the Faddeev differential equations has been described in detail. Since the method employed is mostly the same as detailed in Refs. [21] and [22] we give only a brief outline here.

In the present investigation we assume that LiHe$_2$ molecule has a total angular momentum $L = 0$. Describing the ^{7}Li^{4}He$_2$ three-atomic system we use the standard reduced Jacobi coordinates [23]. We consider the case where the interatomic interactions include a hard core component. Outside the hard core domain they are described by conventional smooth potentials. In the following the ^{4}He atoms are assigned the numbers 1 and 2 while the ^{7}Li atom has the number 3. The identity of the two ^{4}He atoms implies that the corresponding Faddeev components are obtained from each other by a simple rotation of the coordinate space. Thus, we only have two independent Faddeev components, the one associated with the ^{4}He–^{4}He subsystem, and another one associated with a pair of ^{7}Li and ^{4}He atoms. After partial-wave expansion the initial Faddeev equations [23] are reduced to the system of coupled two-dimensional integro-differential equations

$$\left(-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+l(l+1)\left(\frac{1}{x^2}+\frac{1}{y^2}\right)-E\right)f_l^{(\alpha)}(x,y) = \begin{cases} 0, & x<c \\ -V_\alpha(x)\psi_l^{(\alpha)}(x,y), & x>c \end{cases}, \quad \alpha=1,3, \tag{1}$$

and partial boundary conditions

$$f_l^{(\alpha)}(x,y)\Big|_{x=0} = f_l^{(\alpha)}(x,y)\Big|_{y=0} = 0, \quad \psi_l^{(\alpha)}(x,y)\Big|_{x=c} = 0, \quad \alpha=1,3. \tag{2}$$

Here, x and y stands for reduced Jacobi variables. $\psi_l^{(\alpha)}(x,y)$ are the partial wave functions related to the partial-wave Faddeev amplitudes $f_l^{(\alpha)}(x,y)$ (see, e.g. [22]):

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

The explicit form of the function $h^0_{(\alpha;l)(\beta;l')}(x,y,\eta)$ can be found in Refs. [22,23]. We also use the notation

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

$$\mathsf{c}_{\alpha\beta} = -\left(\frac{\mathrm{m}_\alpha \mathrm{m}_\beta}{(\mathrm{m}_\alpha+\mathrm{m}_\beta)(\mathrm{m}_\beta+\mathrm{m}_\gamma)}\right)^{1/2}, \quad \mathsf{s}_{\alpha\beta} = (-1)^{\beta-\alpha}\,\mathrm{sign}(\beta-\alpha)\left(1-\mathsf{c}_{\alpha\beta}^2\right)^{1/2}.$$

where $\mathsf{c}_{\alpha\beta}$ and $\mathsf{s}_{\alpha\beta}$ stand for the angular coefficients describing the transition from the reduced Jacobi variables associated with a pair β to the ones associated with a pair α. By c in Eqs. (1, 2) we denote the hard-core radius.

This radius was taken the same 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 [21]. By V_1 we denote the interatomic Li–He potential and V_3—the He–He potential adjusted to the corresponding reduced Jacobi coordinates.

The asymptotic boundary condition for a $LiHe_2$ bound state reads as follows (see [22,23])

$$f_l^{(\alpha)}(x, y) = \delta_{l0}\psi_d(x)\exp(\mathrm{i}\sqrt{E-\epsilon_d}\, y)\left[\mathrm{a}_0 + o\left(y^{-1/2}\right)\right] + \frac{\exp(\mathrm{i}\sqrt{E}\rho)}{\sqrt{\rho}}\left[A_l^{(\alpha)}(\theta) + o\left(\rho^{-1/2}\right)\right] \tag{3}$$

as $\rho = \sqrt{x^2+y^2} \to \infty$ and/or $y \to \infty$. The coefficients a_0 and $A_l^{(\alpha)}(\theta)$ describe contributions into $f_l^{(\alpha)}(x, y)$ from (2+1) and (1+1+1) channels respectively. It should be noted that both $E-\epsilon_d$ and E in (3) are negative. This implies that for any $\theta = \arctan(y/x)$ the partial wave Faddeev amplitudes $f_l^{(\alpha)}(x, y)$ decrease exponentially as $\rho \to \infty$. Here we also use the fact that dimers, $^4He_2$ and Li^4He, have a unique bound state and this state only exists for $l = 0$; ϵ_d stands for the correspondent dimer energy while $\psi_d(x)$ denotes the dimer wave function which is assumed to be zero within the core, that is, $\psi_d(x) \equiv 0$ for $x \le c$.

Here we only deal with a finite number of equations (1), assuming $l \le l_{\max}$ where $l_{\max}$ is a certain non-negative integer. As in [21,22] we use a finite-difference approximation of the boundary-value problem (1), (2), (3) in the polar coordinates ρ and θ. The grids are chosen so 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 nodes. The value of the core radius is chosen to be $c = 1$ Å by the argument given in [24]. We also follow the same method for choosing the grid radii ρ_i (and, thus, the grid hyperangles θ_j) as described in [21,24] in details. Atomic mass of isotops are taken from [25].

3 Results and Discussions

Our calculations are based on the semi-empirical LM2M2 potential [26] proposed by Aziz and Slaman for He–He interaction, and the KTTY potential [27] , theoretically derived by Kleinekathöfer, Tang, Toennies and Yiu for Li–He interaction with more accurate coefficients taken from [28,29]. Both of these potentials are widely used in the literature. Calculated values of the binding energy for $^6Li^4He$ is 1.512 mK and for $^7Li^4He$ is 5.622 mK. Such small values of binding energy give indication on possible existence of Efimov states in corresponding He_2–alkali-atom triatomic systems.

We employed the Eqs. (1, 2) and the bound-state asymptotic boundary condition (3) to calculate the binding energy of the trimer Li^4He_2. The three-body interaction is expected to be small as in the case of helium trimer [30] and we do not take it into account. Our results for the $^{6;7}Li^4He_2$ trimers binding energies, as well as the results obtained by other authors, are presented in Table 1. The results show that used potential models support two bound states. The energy of excited state is very close to the LiHe two-body threshold. However, as it is seen from the Table 1, different methods demonstrate a large discrepancy between the results. In contrast to our calculation, the hyperradial Shrödinger equation has been solved by other authors. The third column contains the results obtained by Wu et al. [31] using the mapping method within the frame of the hyperspherical coordinates [32]. The next two columns are the results of calculations by Suno et al. [33] using the Gaussian expansion method and the adiabatic hyperspherical representation respectively, although with different He–He potentals. They employed the He–He potential suggested by Jeziorska et al. [36]. The two methods are found to differ from each other, but authors in [33] mentioned that the adiabatic hyperspherical representation is less accurate. The next column is the results of calculations by Suno and Esry [34,35] by the adiabatic hyperspherical method. They also employed the He–He potential from [36], but different potential for Li–He interaction proposed by Cvetko et al. [40]. The seventh column contains the results obtained by Baccarelli et al. [37] with the same potential as in [35], but using a different computation method. The column VIII presents one of the first results obtained by Yuan and Lin [38], using the adiabatic hyperspherical method which gives an upper bound to the ground state. In the last column is the prediction of the bound state energies made by Delfino et al. [39] using the scaling ideas and zero-range model calculations. We can see from the Table 1 that all calcultations predict the existence of two states in both $^6Li^4He_2$ and $^7Li^4He_2$systems. The energy of the excited state is close to the two-body LiHe threshold which is lower then He_2. The binding

Table 1 Comparison of the bound state energies (in mK) obtained for a grid with $N_\rho = N_\theta = 800$, ρ_{max} up to 1000 Å and $l_{max} = 4$ with other calculations

E (mK)	Present	[31]	[33]	[33]	[35]	[37]	[38]	[39]
He–He potential	LM2M2	LM2M2	Jeziorska	Jeziorska	LM2M2	LM2M2	KTTY	
He–Li potental	KTTY	KTTY	KTTY	KTTY	Cvetko	Cvetko	KTTY	
$\lvert E_{^7Li^4He_2}\rvert$	50.89	78.73	76.32	81.29	64.26	73.3	45.7	45.7
$\lvert E^*_{^7Li^4He_2}\rvert$	5.625	5.685	5.51	5.67	3.01	12.2		2.31
$\lvert E_{^6Li^4He_2}\rvert$	35.45			58.88		51.9	31.4	31.4
$\lvert E^*_{^6Li^4He_2}\rvert$	1.719			2.09		7.9		–

energies are very sensitive to the methods and the potential models used as it was aslo mentioned in [31,35]. However, the bound-state energy for the nonsymmetrical helium trimer $^3He^4He_2$ obtained using adiabatic hyperspherical approach [41] agrees fairly well with our previous calculations of this system [22]. For the potentials used, the difference in these systems is in the larger value of the binding energy of the ^{7}LiHe dimer than the He_2 dimer. It means that the system $^7LiHe_2$ is not so close to the universal regime as in case of the helium trimer and it could be the reason of the discrepancy.

The excited state of $^7LiHe_2$ demonstrates a Efimov-type behavior. To study the Efimov properties we multiplied the original Li–He potential by a factor λ. An increase of the coupling constant λ makes potential more attractive. In this case the Efimov levels should become weaker and disappear with further increase of λ. Namely this situation is observed for the excited state energy of $^7LiHe_2$ in contrast to the ground state energy whose absolute value increases continuously with increasing attraction. The difference between the dimer energy of ^{7}LiHe (the lowest two-body threshold) and the energy of the $^7LiHe_2$ trimer excited state increases with potential weakening up to the moment when the energy of the ^{7}LiHe dimer become less than the energy of He_2. Further decrease of the coupling constant weakens only the Li–He potential and although the LiHe dimer energy is approaching zero, the He–He two-body threshold remain the same. So the difference between the He_2 dimer energy and the energy of the $^7LiHe_2$ trimer excited state becomes smaller and the excited state disappears with a further decrease of λ. As it was shown for helium trimer, the Efimov level transforms into a virtual state [42] . It would be interesting to see what happens in the case of the $LiHe_2$ system and it is a subject of our further investigations.

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