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Prediction of a weakly bound excited state in the $^4He_2$–^7Li molecule

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A scale-independent approach, valid for weakly bound three-body systems, is used to analyze the existence of excited Thomas–Efimov states in molecular systems with three atoms: a helium dimer together with isotopes of lithium (^{6}Li and ^{7}Li) and sodium (^{23}Na). With the present study and the available data, we can clearly predict that the $^4\mathrm{He}_2-{}^7\mathrm{Li}$ system supports an excited state with binding energy close to 2.31 mK. © *2000 American Institute of Physics.*
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I. INTRODUCTION

Three-body quantum systems have some peculiar effects that had been noticed many years ago. In 1935, Thomas[1] observed that for a nonrelativistic zero-ranged (Dirac-delta) two-boson interaction that supports one bound state, the corresponding ground state for the binding energy of the three-boson state will approach $-\infty$. This is known as the *Thomas collapse*.

Thirty five years later, in 1970, Efimov[2] noted that if the two-body interaction is weakened in such a way that the range of the potential, r_0, is kept fixed, when the two-body binding energy approaches zero ($B_2 \to 0$), the *number of three-body bound states* increases to infinity. This is the well-known Efimov effect. The observation of Efimov can be conveniently generalized in terms of the two-body scattering length (instead of the two-body binding energy), as the two-body system does not need necessarily to be bound: It is well-known that a three-body system can be bound even in the cases where the two-body subsystems are not bound, in what is called *Borromean three-body states*.[3]

The effects observed by Thomas (three-body ground-state collapse) and Efimov (infinite number of excited three-body *finite* energies), apparently very different, were shown to be related by the same scaling mechanism.[4] They are supposed to be model independent, as they are due to the effective interaction at distances outside the range of the potential. The mechanism discussed in Ref. 4 was further explored to classify halo states in nuclei with three-body structures.[5] A universal scaling plot (in dimensionless units), valid in the low energy regime and based on a renormalized zero-ranged theory, was proposed in Ref. 5 to identify Thomas–Efimov states in three-body halo nuclei (Recently, a similar idea was used in Ref. 6 to characterize and classify halo states.) The validity of the approach was also verified in the case of three-atom systems in Ref. 7, where the results of a study of the helium trimer were compared with realistic available calculations.[8–13] A recent independent calculation in halo nuclei, with a realistic two-body interaction, has also confirmed the validity of the scaling mechanism.[14]

As a further motivation, one should notice that in the last three years, a lot of attention was brought to the search of weakly bound Efimov states in atomic systems, considering the possibility of altering (from negative to positive values) the effective scattering length that describes the low-energy atom–atom interaction, by using an external magnetic field.[15] This possibility (of changing the two-body scattering length) can alter in an essential way the balance between the nonlinear first few terms of the mean-field description in the equations that model the Bose–Einstein condensed state in gases.[16] This can certainly open new perspectives for theoretical and experimental investigations related to the many-body behavior of condensed systems.[17] Within the same perspective, the recent interesting experimental proposal suggested by Hegerfeldt and Köhler[18] may also prove to be helpful for the investigation of the weakly bound excited state in helium trimer.

A system of particles with exactly zero two-body binding energy is not easy to be identified in nature. However, the Thomas–Efimov effect is expected to be manifested in weakly bound quantum few-body systems, whenever the size is much larger than the corresponding two-body range, r_0. Most of the recent theoretical studies on Efimov states using realistic interatomic interactions have been concentrated in the ^{4}He trimer,[8,7] where one Efimov state was recognized. The search of Efimov states in such a system was motivated by the remarkable small binding energy of the ^{4}He dimer: $B_{^4\mathrm{He}_2} = 1.31$ mK.

Generalizing the search of Efimov states for atomic systems, Yuan and Lin[19] have also considered different mass arrangements in triatomic molecules. These atomic systems

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will be further discussed in Sec. II, considering the main motivation of the present article: to verify the most favorable systems to allow the existence of Efimov states, using a renormalized zero-ranged (RZR) model. In Secs. III and IV, respectively, we present the basic idea of a scaling function and show how it is constructed using the Faddeev formalism for the RZR model. In the last section we present our main results and conclusions.

II. THOMAS–EFIMOV STATES IN THE THREE-BODY MOLECULAR SYSTEM

In Ref. 19, using realistic two-atomic interaction, a search of weakly bound excited three-body states was performed for a set of nine triatomic molecules of the type He–He–X, where $X=$ different isotopes of helium, sodium, and lithium atoms. Considering that the binding energy of the $^4\mathrm{He}-{}^6\mathrm{Li}$ system, $B_{^4\mathrm{He}-{}^6\mathrm{Li}}=0.12$ mK, is much smaller than the energy of the ^{4}He dimer (1.31 mK), and also about 18 times smaller than the binding energy of the $^4\mathrm{He}-{}^7\mathrm{Li}$ ($B_{^4\mathrm{He}-{}^7\mathrm{Li}}=$ 2.16 mK), they select the system $^4\mathrm{He}_2-{}^6\mathrm{Li}$ as the natural candidate to search for at least one Efimov state. However, it turns out quite naturally, from a scaling approach proposed in Ref. 5, that the magnitude of the ratio between the energies of the two-body subsystems and the three-body system is the relevant quantity to be considered in this search. So, the small magnitude of the two-body (binding or virtual) energy is not the only one responsible for the occurrence of Efimov states in the three-body system.

In the present work, applying the approach based on the RZR model defined in Ref. 5, we conclude that, between the three-body molecular systems $^4\mathrm{He}_2-{}^6\mathrm{Li}$ and $^4\mathrm{He}_2-{}^7\mathrm{Li}$ and against the expectation based on the two-body energies,[19] the second is the best candidate to present a weakly bound excited state. As will be shown, with the scaling function and given the ground-state energies, we can also predict the energy of the weakly bound excited state for the $^4\mathrm{He}_2-{}^7\mathrm{Li}$ molecule to be close to 2.31 mK.

The RZR model, applied to low-energy three-body systems, provides a minimum requirement to constrain the existence or not of Efimov states. Using the scaling function, one can relate the energy of the first excited Efimov state with the energy of the ground-state and the energies of the two-body subsystems. In the same way, the second excited Efimov state can also be related with the first Efimov state and the two-body subsystems, and so on. The two-body (binding or virtual) and three-body binding energies become quite naturally the physical two- and three-body scales that parametrize the three-body system in the limit of a renormalized zero-range interaction. As the input energies are fixed in such a renormalized model, the generality of the results is claimed to be model independent. The main physical argument for this universality is related to the unusually large size of the weakly bound three-body system in respect to the interaction range. Consequently, the detailed form of the two-body interaction is not crucial for the determination of the excited states.

The RZR model, discussed for equal mass three-body system in Ref. 20, was successfully applied to study the ^{4}He trimer.[7] An extension of it, considered for the cases where the three-body system can have two distinguished particles, was also applied to study low-energy halo-nuclei systems.[5,21] Here, we consider this version of the model in our search for weakly bound excited states in three-atomic molecular systems. In case of three-body systems with unequal masses, the ratio between the energies of two consecutive Efimov states is very sensitive to the mass asymmetries.[5,7] In the particular case of systems with equal masses, the ratio is close to 500. However, in the other extreme limit of masses, the scaling approach predicts that the ratios between consecutive Efimov energies can be greater than 2000 (for two heavy particles and a light one) or about 140 (for the case of two light particles and a heavy one).

Considering the small magnitude of the Efimov excited state energies, the search for such states is not an easy experimental task; it is also tedious to be performed in calculations using realistic interactions if one does not use a convenient scaling. So, it is relevant to take advantage of a given prescription that gives evidence of correlations between the two and three-body binding energies. The RZR model gives such a prescription, as observed in Ref. 7. Such an approach, to identify Efimov states in three-body systems, can be a relevant guide for realistic calculations[19] or for experimental proposals.[18]

III. THE SCALING FUNCTION

In Refs. 5,7 was already presented the basis on which the scaling function is constructed. Here we only give the underlying physical picture for it. Let us suppose we have three bosons (two of them are identical and labeled with α; the third one labeled β) interacting via a short-ranged two-body potential $\lambda V(r)$ with range r_o. Once the form of the potential is known, the two-body binding energies $B_{\alpha\alpha}$ and $B_{\alpha\beta}$ are functions of λ and r_o. A set of these parameters, (λ, r_o), will allow the same constant values of $B_{\alpha\alpha}$ and $B_{\alpha\beta}$. It means that, as $r_o\to 0$, λ has to increase to keep constant the two-body binding energies. Simultaneously, as $r_o\to 0$ the three-body energy B_3 increases as $1/r_o^2$ as observed by Thomas.[1] Thus, one of the scales of the three-body problem, r_o, can be eliminated in favor of the three-body ground-state energy, $B_3^{(0)}$, for example. All the detailed information about the short-range force, beyond the low-energy two-body observables, are retained in only one three-body physical information, in the limit of zero-range interaction. Therefore, in this limit, the three-body problem is quite naturally parametrized by the physical two-body and three-body scales, given by the corresponding energies: $B_{\alpha\alpha}$, $B_{\alpha\beta}$, and B_3. It is reasonable to expect that the three-body low-energy physics would be dominated by these physical scales. In the renormalized zero-range model applied to three-body system, a dimensionless scaling function is defined to express the ratio between two consecutive three-body binding energies, as the $(N+1)$th and the (N)th states. Such scaling function will depend on the mass ratio of the particles and on the ratios of the physical scales of the three-body system: $B_{\alpha\alpha}/B_3^{(N)}$, $B_{\alpha\beta}/B_3^{(N)}$. For simplicity, in our discussion we consider $N=0$, as the scaling function is practically independent of N.[5,7]

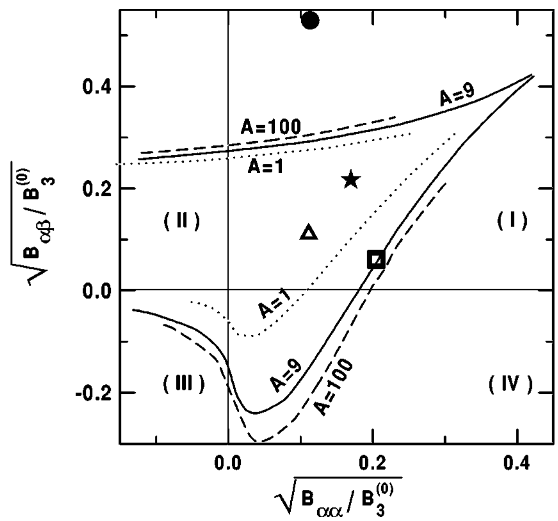

FIG. 1. The scaling approach for the three-body system $\alpha-\alpha-\beta$. The coordinates of the systems with $\alpha\equiv{}^4$He and $\beta={}^4$He, ^{7}Li, ^{6}Li, and ^{23}Na are respectively, represented by a triangle, a star, a square, and a full circle.

The scaling function that related the first excited Efimov state with the ground state is given by

$$\frac{B_3^{(1)}}{B_3^{(0)}}=F\left(\sqrt{\frac{B_{\alpha\alpha}}{B_3^{(0)}}};\sqrt{\frac{B_{\alpha\beta}}{B_3^{(0)}}};A\right), \tag{1}$$

where $A\equiv M_\beta/M_\alpha$ is the dimensionless mass ratio of the α and the β particles. For convenience, we write the arguments of Eq. (1) with square-roots. The two-body subsystems can be bound or virtual, expressed by the corresponding signs of the square-roots, plus and minus, respectively.

In general, in respect to the energy of the two-body subsystem, $\alpha-\alpha$ and $\alpha-\beta$, we need to examine four theoretical possibilities for the limiting conditions to allow one excited-state energy above the ground-state energy (see Fig. 1): (I) $\alpha-\alpha$ and $\alpha-\beta$ are both bound $(+\ +)$; (II) $\alpha-\alpha$ is virtual and $\alpha-\beta$ is bound $(-\ +)$; (III) $\alpha-\alpha$ and $\alpha-\beta$ are both virtual $(-\ -)$; and (IV) $\alpha-\alpha$ is bound and $\alpha-\beta$ is virtual $(+\ -)$. The critical boundary in the parametric plane, defined by the coordinates $(\sqrt{B_{\alpha\alpha}/B_3^{(0)}},\sqrt{B_{\alpha\beta}/B_3^{(0)}})$, is shown in Fig. 1. The prescription used to determine the critical boundary which allows one Efimov state above a given state, is the following: we solve the equations for the critical conditions in the parametric plane, derived from Eq. (1) in the four possible cases, (I) to (IV). In region (I), where both subsystems are bound, the boundary of the region in which at least one Efimov state can exist is given by

$$F\left(\sqrt{\frac{B_{\alpha\alpha}}{B_3^{(0)}}};\sqrt{\frac{B_{\alpha\beta}}{B_3^{(0)}}};A\right)=\max\left(\frac{B_{\alpha\beta}}{B_3^{(0)}};\frac{B_{\alpha\alpha}}{B_3^{(0)}}\right) . \tag{2}$$

For both two-body subsystems having virtual states, which defines region (III), one has

$$F\left(\sqrt{\frac{B_{\alpha\alpha}}{B_3^{(0)}}};\sqrt{\frac{B_{\alpha\beta}}{B_3^{(0)}}};A\right)=0 . \tag{3}$$

In regions (II) and (IV), where one of the subsystems is bound, the critical boundary is found from

$$F\left(\sqrt{\frac{B_{\alpha\alpha}}{B_3^{(0)}}};\sqrt{\frac{B_{\alpha\beta}}{B_3^{(0)}}};A\right)=\left(\frac{B_{\alpha\alpha}}{B_3^{(0)}}\right)\ \text{or}\ \left(\frac{B_{\alpha\beta}}{B_3^{(0)}}\right) . \tag{4}$$

The above conditions establish the critical boundary for the region in the parametric plane in which Efimov states can occur. A weakly bound excited Efimov state can exist for a system if the corresponding point is inside the region shown in Fig. 1. It is important to observe that the RZR model defines the smallest possible region, as seen in Fig. 1. If ones uses a realistic finite-range interaction, the region can be larger due to range effects. However, as one is more close to the center of the figure, the results of the RZR model approach the ones obtained by using a realistic interaction. This implies that a realistic interaction cannot invalidate the conclusions about existence of Efimov states obtained by using the RZR model. The opposite can be true: one cannot rule out the possibility of having Efimov states in the systems that in the present scaling approach have coordinates outside but near the border of the parametric region defined in Fig. 1.

In order to derive the scaling function, we employ a three-body renormalized zero-range model presented in Ref. 5. In the following we give some details of the formalism.

IV. FADDEEV THREE-BODY EQUATIONS

The scaling function, Eq. (1), is obtained from the numerical solution of the coupled Faddeev integral equations in the zero-range limit of a two-body interaction.[5] To solve the integral equation, a regularization parameter Λ is introduced in the momentum integration, related to the inverse of the interaction range.[2,5] It goes to infinity as the radius of the interaction decreases. In our approach, the limit $\Lambda\to\infty$ is realized while the ratios between each of the two-body energies ($B_{\alpha\alpha}$ and $B_{\alpha\beta}$) and the three-body ground state energy are kept fixed. After partial wave projection, the s-wave $\alpha-\alpha-\beta$ coupled integral equations are given by

$$\chi_{\alpha\alpha}(q)=2\tau_{\alpha\alpha}(q;B_3^{(0)})\int_0^\Lambda dk G_1(q,k;B_3^{(0)})\chi_{\alpha\beta}(k), \tag{5}$$

$$\chi_{\alpha\beta}(q)=\tau_{\alpha\beta}(q;B_3^{(0)})\int_0^\Lambda dk[G_1(k,q;B_3^{(0)})\chi_{\alpha\alpha}(k) + AG_2(q,k;B_3^{(0)})\chi_{\alpha\beta}(k)], \tag{6}$$

$$\tau_{\alpha\alpha}(q;E)\equiv\frac{1}{\pi}\left[\sqrt{E+\frac{A+2}{4A}q^2}\mp\sqrt{B_{\alpha\alpha}}\right]^{-1}, \tag{7}$$

$$\tau_{\alpha\beta}(q;E)\equiv\frac{1}{\pi}\left(\frac{A+1}{2A}\right)^{3/2}\times\left[\sqrt{E+\frac{A+2}{2(A+1)}q^2}\mp\sqrt{B_{\alpha\beta}}\right]^{-1}, \tag{8}$$

$$G_1(q,k;E)\equiv\log\frac{2A(E+k^2+qk)+q^2(A+1)}{2A(E+k^2-qk)+q^2(A+1)}, \tag{9}$$

$$G_2(q,k;E)\equiv\log\frac{2(AE+qk)+(q^2+k^2)(A+1)}{2(AE-qk)+(q^2+k^2)(A+1)}. \tag{10}$$

The plus and minus signs in Eqs. (7) and (8) refer to virtual and bound two-body subsystems, respectively. We made the assumption that the range of the $\alpha-\alpha$ and $\alpha-\beta$ interactions are about the same, considering that the three-body model is renormalized[20] and only needs one three-body observable to be fixed, together with the two-body low-energy physical information. We solve Eqs. (5)–(10) in units such that $\Lambda=1$. The corresponding dimensionless quantities are: $\epsilon_3^{(0)} \equiv B_3^{(0)}/\Lambda^2$, $\kappa_{\alpha\alpha}\equiv\pm\sqrt{B_{\alpha\alpha}}/\Lambda$, $\kappa_{\alpha\beta}\equiv\pm\sqrt{B_{\alpha\beta}}/\Lambda$. The two-body observables can be written in terms of the three-body binding energy $B_3^{(0)}$, by replacing Λ, such that $\kappa_{\alpha\alpha}/\sqrt{\epsilon_3^{(0)}}=\pm\sqrt{B_{\alpha\alpha}/B_3^{(0)}}$ and $\kappa_{\alpha\beta}/\sqrt{\epsilon_3^{(0)}}=\pm\sqrt{B_{\alpha\beta}/B_3^{(0)}}$. The Thomas effect occurs for $\Lambda\rightarrow\infty$ with the energies of the two-body systems kept fixed, whereas the Efimov states arise when $B_{\alpha\alpha}$ and $B_{\alpha\beta}\rightarrow 0$ with Λ kept fixed. The results for the RZR model appear when the cutoff is written as a function of $B_3^{(0)}$; thus, the three-body observables naturally scale with $B_3^{(0)}$. Finally, the scaling function, Eq. (1), is obtained when the numerical results of the excited state energies as a function of the two-body energies are rescaled by $B_3^{(0)}$.

V. RESULTS AND DISCUSSION

Our analysis has considered a few particular three-body molecular systems, in which the three-body ground-state energy and the corresponding energies of the two-body subsystem is known and given in Ref. 19: ^{4}He trimer, $^4He_2-{}^6Li$, $^4He_2-{}^7Li$, and $^4He_2-{}^{23}Na$. In Ref. 19, the authors have considered realistic two-body interactions with finite nonzero ranges; their results for the ground-state energies are appropriate for our purpose of predicting excited Efimov states using the scaling approach.

The $^4He_3$ atomic system was extensively studied by several authors,[8–13] strongly supporting the existence of at least one weakly bound excited state. The present scaling approach was previously applied to this particular molecule,[7] with a result that is in very good agreement with realistic calculations. One should note, from the ^{4}He trimer studies,[8–13] that the ground state is extremely sensitive to the potential well region, and that the Efimov excited states are also very sensitive to certain features of the long-range part of the potential. However, in Ref. 7, it was definitely clarified that such apparent independent sensitivities (of the ground and Efimov state energies) disappear once the ratio of the dimer binding energy to the helium trimer ground-state energy is kept fixed.[7] This leads us to conclude that other details (beyond the dimer and trimer ground-state energies) presented in the realistic interactions that have been used are quite irrelevant to the existence of Efimov states. These features validate a universal scaling function, relating the trimer ground-state, the dimer, and the weakly bound excited three-body energy state. As the scaling limit works in the ^{4}He trimer case, this suggests its application to study other similar systems, including the case where two kinds of atoms are mixed. The conditions for the validity of the approach are that the atoms should have a very shallow and short-ranged two-body interaction, with the binding energy close to zero. These are indeed the cases we are considering. The main relevant data we need to take into account in the present study of the occurrence of weakly bound excited states are given in Table I. In this table, we also present the corresponding numerical results obtained with the scaling approach for the molecular systems under consideration.

TABLE I. Results for the molecular systems $\alpha-\alpha-\beta$ identified in the first column. The ground-state energies and the corresponding energies of the two-body subsystems are given in the second, third, and forth columns, taken from Ref. 19. In the fifth and sixth columns we give the corresponding coordinates of the points represented in Fig. 1. In the last column, we have the predictions obtained with the scaling function for the weakly bound excited state energies: ^{4}He trimer was obtained in Ref. 7, and $^4He_2-{}^7Li$ is given by Fig. 2.

Molecule α-α-β	$B_3^{(0)}$ (mK)	$B_{\alpha\alpha}$ (mK)	$B_{\alpha\beta}$ (mK)	$\sqrt{\frac{B_{\alpha\alpha}}{B_3^{(0)}}}$	$\sqrt{\frac{B_{\alpha\beta}}{B_3^{(0)}}}$	$B_3^{(1)}$ (mK)
$^4He_3$	106.0	1.31	1.31	0.111	0.111	2.05
$^4He_2-{}^6Li$	31.4	1.31	0.12	0.204	0.0618	⋯
$^4He_2-{}^7Li$	45.7	1.31	2.16	0.169	0.217	2.31
$^4He_2-{}^{23}Na$	103.1	1.31	28.98	0.113	0.530	⋯

The data and results given in Table I are related to the results shown in Figs. 1 and 2. In these figures, the coordinates are dimensionless variables that depend on the energies of the two- and three-body system. In Fig. 1 we have the critical boundary that constrains the weakly bound excited states, as previously discussed. In Fig. 2, we show the calculated scaling function for the system $^4He_2-{}^7Li$, that was obtained in the same way as the scaling function for the helium trimer in Ref. 7.

The first important point to notice, is that the existence of Efimov state is not directly connected to the two-body binding energy alone, but rather to the ratio of binding energies shown in columns 5 and 6 of Table I. Through common knowledge, one could naively expect that the $^4He_2-{}^6Li$ molecule is the favorite one to search for an Efimov state, since it presents the smallest values for the two-atom binding energies displayed in Table I. Surprisingly this is not the case, as the representative point (0.204, 0.0618) lies outside the region defined by the critical curve of the $^4He_2-{}^6Li$

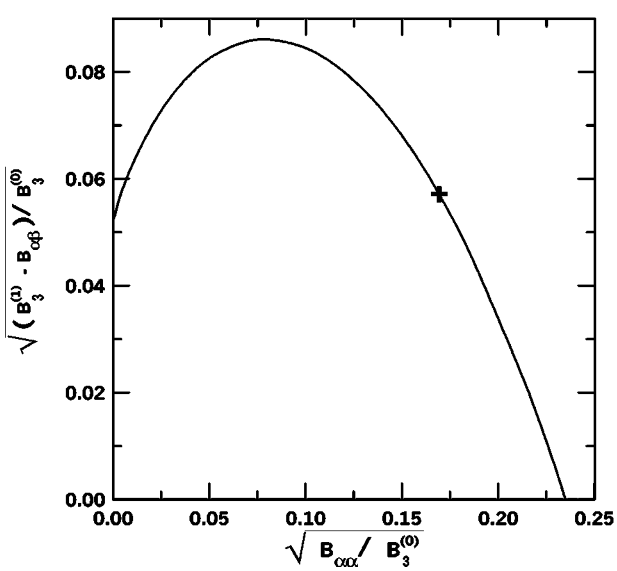

FIG. 2. Plot of the scaling limit showing the coordinates related to the system $^4He_2-{}^7Li$. The cross indicates that the energy of the excited state is $B_3^{(1)}=2.31$ mK, considering the data given in Table I.

molecule system (the mass ratio in this case is $A=1.5$). The $^4He_2-^7Li$ molecule (with $A=1.75$) has the coordinates of its representative point in the parametric space given by (0.169, 0.217) (see Table I). This point is inside the region where the occurrence of at least one Efimov state is possible (see Fig. 1). Again, we stress here the role played by the three-body scale (ground-state energy) in determining the Efimov state. The possibility of Efimov state in $^4He_2-^6Li$ molecule cannot be completely excluded if range effects expand the corresponding region. However, the occurrence of Efimov state in the case of $^4He_2-^{23}Na$ ($A=5.75$) can be more easily excluded. As we can see in Fig. 1, its representative point (0.113, 0.530) is outside and far from the border of the corresponding parametric region.

From the set of molecules we have considered, the existence of one Efimov state is concrete only in two cases: ^4He trimer and $^4He_2-^7Li$. In the same way the scaling function in Ref. 7 was used to predict the Efimov energy of the ^4He trimer, we can also consider the corresponding scaling function for the system $^4He_2-^7Li$. The scaling function is calculated for $\sqrt{B_{^4He^7Li}/B_3^{(0)}}=0.217$ (see Table I), while we vary the ratio $\sqrt{B_{^4He^4He}/B_3^{(0)}}$ to show the analytical form of such function. The result is given in Fig. 2, where it is shown the plot of $\sqrt{(B_3^{(1)}-B_{^4He^7Li})/B_3^{(0)}}$ is shown against $\sqrt{B_{^4He_2}/B_3^{(0)}}$. The coordinates that will give us the Efimov state energy is indicated on this curve by the symbol + and corresponds to $\sqrt{B_{^4He_2}/B_3^{(0)}}=0.169$. The predicted energy of the Efimov state, $B_3^{(1)}$, is obtained from $\sqrt{(B_3^{(1)}-B_{^4He^7Li})/B_3^{(0)}}=0.057$, implying $B_3^{(1)}=2.31$ mK.

In summary, using the scaling function derived from a RZR model,[5] we can predict an excited weakly bound state for the molecular $^4He_2-^7Li$ system. As shown in Table I, considering the three-body molecular system analyzed in Ref. 19 that has two-body sub-systems bound, one can expect one Thomas–Efimov state only in the ^4He trimer and in the $^4He_2-^7Li$ system. The weakly bound excited state in helium trimer, first predicted in Ref. 8, was proven to be a good test for the predictive power of the scaling approach in Ref. 7 (essentially the same result was obtained). Amongst the systems $^4He_2-^6Li$ and $^4He_2-^7Li$, the scaling approach eliminates the naive expectation that the first system is more favorable to have Efimov states. Even considering that the energy of the subsystem $^4He-^6Li$ (0.12 mK) is about 18 times smaller than the energy of the subsystem $^4He-^7Li$ (2.16 mK), the system $^4He_2-^7Li$ is more favorable to allow one weakly bound excited state. This is not surprising using the scaling approach, as the relevant quantities to be characterized are dimensionless ratios of physical observables, where the three-body ground-state energy is the natural scale for the three-body system.

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