Generalized Efimov Scenario for Heavy-Light Mixtures

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Motivated by recent experimental investigations of Cs-Cs-Li Efimov resonances, this work theoretically investigates the few-body properties of $N-1$ noninteracting identical heavy bosons, which interact with a light impurity through a large s-wave scattering length. For Cs-Cs-Cs-Li, we predict the existence of universal four-body states with energies $E_4^{(n,1)}$ and $E_4^{(n,2)}$, which are universally linked to the energy $E_3^{(n)}$ of the nth Efimov trimer. For infinitely large ^{133}Cs-^{6}Li and vanishing ^{133}Cs-^{133}Cs scattering lengths, we find $(E_4^{(1,1)}/E_3^{(1)})^{1/2} \approx 1.51$ and $(E_4^{(1,2)}/E_3^{(1)})^{1/2} \approx 1.01$. The ^{133}Cs-^{6}Li scattering lengths at which these states merge with the four-atom threshold, the dependence of these energy ratios on the mass ratio between the heavy and light atoms, and selected aspects of the generalized Efimov scenario for $N>4$ are also discussed. Possible implications of our results for ongoing cold atom experiments are presented.

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Continuous and discrete scale invariances underlie many phenomena in physics. The possibly most aesthetically appealing examples are fractals [1], where a given pattern repeats itself as one zooms in. Scale invariance phenomena also emerge in quantum mechanics. A prominent example is the three-body Efimov effect [2,3]. If there exists an Efimov trimer of size $l_3^{(n)}$ and with energy $E_3^{(n)}$ [4], then there should exist another larger and less strongly bound Efimov trimer of size $l_3^{(n+1)} = \lambda l_3^{(n)}$ and with energy $E_3^{(n+1)} = \lambda^{-2} E_3^{(n)}$. Here, λ ($\lambda > 1$) is a scaling factor that depends on the masses and particle statistics of the constituents.

The experimental observation of consecutive three-body resonances is extremely challenging as it requires working in the universal Efimov window. To be in this window, the absolute values of at least two of the three two-body s-wave scattering lengths [5] have to be larger than the other length scales of the underlying two-body potentials and the temperature has to be lower than the energy scale set by the s-wave scattering length. Thus, to observe two consecutive three-atom resonances, exquisite control over the scattering lengths and ultralow temperatures are required. For three identical bosons, λ is approximately equal to 22.7 and two consecutive three-atom resonances in a bosonic system have only been observed recently in ^{133}Cs [6,7].

It is well known that the scaling factor λ takes smaller, and hence more favorable, values for heteronuclear mixtures with infinitely large interspecies s-wave scattering length [3,8–13]. For ^{133}Cs-^{133}Cs-^{6}Li, e.g., λ takes the value 4.877. For notational convenience, we use Cs and Li to refer to the bosonic ^{133}Cs and fermionic ^{6}Li isotopes in what follows. Indeed, recently the Heidelberg [14] and Chicago [15] groups independently reported the experimental observation of, respectively, two and three consecutive Cs-Cs-Li three-atom resonances. The analysis shows that the Cs-Cs interactions play a negligible role at the present precision of the experiments, indicating that the observation of Efimov physics in these heavy-light mixtures is due to the large magnitude of the Cs-Li s-wave scattering length.

The extended Efimov scenario has been studied predominantly for four *identical* bosons with large in absolute value two-body s-wave scattering length [16–22]. In this case, there exist two four-body states with energies $E_4^{(n,1)}$ and $E_4^{(n,2)}$ that are universally tied to the nth Efimov trimer with energy $E_3^{(n)}$. These four-body states lead to measurable four-atom resonances on the negative scattering length side (at scattering lengths $a_{4,-}^{(n,1)}$ and $a_{4,-}^{(n,2)}$) and atom-trimer and dimer-dimer resonances on the positive scattering length side [20–22].

This Letter explores the generalized Efimov scenario for $N-1$ identical heavy bosons and a single light impurity for the case where the magnitude of the heavy-light s-wave scattering length is large compared to all other two-body length scales, including the heavy-heavy s-wave scattering length. For the Cs-Cs-Cs-Li system, we find—as was found for four identical bosons—two tetramer states at unitarity. Moreover, we find that these four-body states become unbound at Cs-Li s-wave scattering lengths $a_{4,-}^{(1,1)} \approx 0.55 a_{3,-}^{(1)}$ and $a_{4,-}^{(1,2)} \approx 0.91 a_{3,-}^{(1)}$. Since $a_{4,-}^{(1,2)}$ is close to $a_{3,-}^{(1)}$, the loss features in the Heidelberg and Chicago experiments [14,15] that were identified as being due to three-body physics could potentially, in the proper temperature and density regime, include a "contamination" from the four-body sector. Our calculations thus suggest that it would be extremely interesting to search for universal four-body physics in Cs-Li mixtures. When the mass ratio κ between the heavy and light atoms is reduced to less than $\approx$13, the energy of the excited tetramer at unitarity lies above that of the trimer. For very large mass ratios, we find—as in the case of the Cs-Cs-Cs-Li system—two tetramers at unitarity.

An intriguing question is how the extended Efimov scenario, if existent, looks for $N > 4$. For N identical bosons, evidence has been presented that there exist five-body and higher-body states that are universally tied to each Efimov trimer [23–25]. While many questions regarding the $N > 4$ extension of the Efimov scenario for identical bosons remain [23,26–28], essentially nothing is known about heteronuclear systems with $N > 4$. We find five- and six-body states for the $B_{N-1}X$ system that are universally tied to the lowest Efimov trimer.

Our model Hamiltonian H,

$$H = -\frac{\hbar^2}{2m_B}\sum_{j=1}^{N-1}\nabla^2_{\vec{r}_j} - \frac{\hbar^2}{2m_X}\nabla^2_{\vec{r}_N} + V_{2b} + V_{3b}, \quad (1)$$

is designed to capture the low-energy properties of N-body droplets. The position vectors of the bosons of mass m_B are denoted by $\vec{r}_j$ ($j = 1, \ldots, N-1$) and the position vector of the impurity of mass m_X is denoted by $\vec{r}_N$. The potential V_{2b} accounts for the pairwise interactions between the bosons and the impurity, $V_{2b} = \sum_{j=1}^{N-1} v_0 \exp[-r_{jN}^2/(2r_0^2)]$, where the depth v_0 ($v_0 < 0$) and the range r_0 are adjusted to reproduce the desired interspecies two-body scattering length a_s and r_{jk} is equal to $|\vec{r}_j - \vec{r}_k|$. Motivated by our desire to explore the extension of Efimov's BBX trimer study with large BX and vanishing BB s-wave scattering lengths [3,8–13], which has been realized experimentally [14,15], to the $N > 3$ sector, we neglect the interactions between the identical heavy bosons.

The potential V_{3b} accounts for a repulsive three-body force for each BBX triple, $V_{3b} = \sum_{j<k}^{N-1} V_0 \exp[-(r_{jk}^2 + r_{jN}^2 + r_{kN}^2)/(2R_0^2)]$ [23,29]. For diverging BX scattering length, the height V_0 and range R_0 of the repulsive three-body interaction are adjusted such that the lowest trimer state is much larger than r_0 and R_0, i.e., such that the wave function of the lowest trimer is insensitive to the details of the model interactions and accurately described by Efimov's zero-range theory [30,31]. Throughout, we use $R_0 = \sqrt{8}r_0$. Having fixed the parameters of the model Hamiltonian by analyzing the properties of the three-body system, the four- and higher-body sectors are explored and found to be universal; i.e., the four- and higher-body observables are found to be largely insensitive to the details of the underlying potential model, provided the N-body ($N > 3$) observables are expressed in terms of the corresponding three-body observables. We emphasize that our model Hamiltonian does not allow us to predict the three-body parameter, which is expected to be determined by the long-range van der Waals tail of the true atom-atom interactions [32–37]. Rather, the model Hamiltonian allows us to predict four- and higher-body properties relative to the three-body properties. The underlying premise is that the four- and higher-body sectors are fully determined by the three-body sector.

To solve the time-independent Schrödinger equation for the Hamiltonian given in Eq. (1), we expand the eigenstates in the relative coordinates in terms of explicitly correlated Gaussian basis functions [31,38–40]. The resulting eigenenergies E_N provide, according to the Hylleraas-Undheim-MacDonald theorem, variational upper bounds to the energies of the ground and excited states of the system [31,38,39]. The states considered in this work have vanishing angular momentum and positive parity. Since our implementation provides access only to true bound states and not to resonance states, we are limited to treating N-body states that lie below the ground state of the $(N-1)$-body system; i.e., we have access, provided they exist, to N-body states that are tied to the lowest Efimov trimer and not to those that are tied to energetically higher-lying Efimov trimers.

To validate our approach, we consider the N identical boson system with infinitely large s-wave scattering length [31]. We find $(E_4^{(1,1)}/E_3^{(1)})^{1/2} = 2.127(5)$ and $(E_5^{(1,1)}/E_3^{(1)})^{1/2} = 3.21(5)$, which agrees well with the literature values of 2.147 [19] and 3.22(4) [23]. For the four-body system, the discrepancy can be explained by small finite-range corrections. Moreover, our calculations confirm the existence of an extremely weakly bound excited tetramer [16,17,19].

Figure 1 shows the extended Efimov plot for the $Cs_{N-1}Li$ system with $N = 3$ and 4 [41]. The energies of the dimer, trimer, and tetramer states are shown by dashed, solid, and dotted lines, respectively. The energy ratios between consecutive trimers at unitarity are close to those predicted by the universal zero-range theory (see Table I). For the

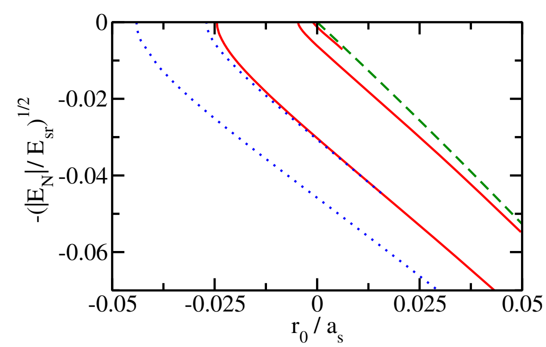

FIG. 1 (color online). Efimov plot for the $B_{N-1}X$ system ($N = 3$ and 4) with $\kappa = 133/6$. The dashed line shows the energy of the BX system. The solid lines show the three lowest energies of the BBX system. The dotted lines show the energies of the two bound states of the $BBBX$ system that are tied to the lowest Efimov trimer. The excited tetramer becomes unbound at $r_0/a_s \approx 0.02$. The calculations are performed for $V_0 = 3.2E_{sr}$, where E_{sr} is equal to $\hbar^2/(2\mu r_0^2)$ and μ denotes the reduced mass, $\mu = m_B m_X/(m_B + m_X)$.

TABLE I. Energies of the $B_{N-1}X$ system with infinitely large interspecies s-wave scattering length for various mass ratios. The second column reports the binding momentum of the lowest trimer state in units of the binding momentum of the short-range energy scale $E_{\rm sr}$. Columns 3–7 report ratios of binding momenta for the systems with $N = 3$–6. For columns 3–6, the energies were extrapolated to the $V_0 \to \infty$ limit. For columns 7–8, we used $V_0 = 3.2E_{\rm sr}$. The symbol "$\cdots$" indicates that no such bound state was found. In the cases where no entry is given, calculations were not performed. For comparison, the last column reports the scaling factor λ calculated from Efimov's zero-range theory.

κ	$\sqrt{E_3^{(1)}/E_{\rm sr}}$	$\sqrt{E_3^{(2)}/E_3^{(1)}}$	$\sqrt{E_3^{(3)}/E_3^{(2)}}$	$\sqrt{E_4^{(1,1)}/E_3^{(1)}}$	$\sqrt{E_4^{(1,2)}/E_3^{(1)}}$	$\sqrt{E_5^{(1,1)}/E_3^{(1)}}$	$\sqrt{E_6^{(1,1)}/E_3^{(1)}}$	$\lambda = e^{-\pi/s_0}$
8	0.012	12.510(5)		1.647(5)	$\cdots$	2.06(4)		12.4878
12	0.017	8.158(5)		1.58(1)	$\cdots$	1.94(4)		8.1305
16	0.021	6.313(5)		1.544(5)	1.002(1)	1.88(4)		6.2804
133/6	0.024	4.904(5)	4.867(2)	1.510(5)	1.010(5)	1.82(4)	2.03(10)	4.8651
30	0.028	3.998(3)	3.958(3)	1.488(5)	1.026(5)	1.78(4)	1.95(10)	3.9553
40	0.031	3.372(3)	3.330(2)	1.471(5)	1.046(8)	1.75(4)		3.3249
50	0.033	2.996(5)	2.952(4)	1.461(5)	1.067(8)	1.73(4)		2.9470

lowest two trimers, the ratio deviates from the universal value by 0.8%, indicating that finite-range effects are negligibly small near unitarity. Nonuniversal finite-range corrections do, however, play a role when the trimers merge with the three-atom and atom-dimer thresholds. The scattering length ratios where the trimers hit the three-atom threshold are found to be $a_{3,-}^{(2)}/a_{3,-}^{(1)} = 5.28(8)$ and $a_{3,-}^{(3)}/a_{3,-}^{(2)} = 4.95(8)$, which deviate by 8.5% and 1.7%, respectively, from the universal zero-range theory value of 4.865.

For negative and sufficiently large positive interspecies scattering lengths, we find two tetramers that are bound with respect to the lowest trimer. The energies of these tetramers "trace" the energy of the lowest trimer. At unitarity, we find $(E_4^{(1,1)}/E_3^{(1)})^{1/2} = 1.510(5)$ and $(E_4^{(1,2)}/E_3^{(1)})^{1/2} = 1.010(5)$. These values are expected to be fairly close to what the universal zero-range theory would yield. At $a_s \approx 2.6(4)a_{\rm td}^{(1)}$, where $a_{\rm td}^{(1)}$ denotes the scattering length where the lowest trimer energy is equal to that of two dimers, the energy of the excited tetramer is equal to that of the lowest trimer, indicating that the excited tetramer becomes unbound at this scattering length [42].

Qualitatively, the energy spectrum shown in Fig. 1 is similar to that for the N identical boson system, which supports two universal tetramers for $1/a_s \le 1/[13.75(5)a_{\rm td}^{(n)}]$ [19]. In that system, it has been shown that the universal tetramers are not only attached to the lowest Efimov trimer but to each Efimov trimer (for the excited Efimov trimers, the "attached" four-body states correspond to resonance states [19]). We conjecture that this is also true for the B_3X system; i.e., we conjecture that there exist two tetramers with energies $E_4^{(n,1)}$ and $E_4^{(n,2)}$ that are universally tied to the nth Efimov trimer for $1/a_s$ smaller than a critical inverse scattering length. On the positive scattering length side, we restricted our four-body calculations to fairly large a_s. As a_s decreases, the spectrum has been predicted to contain additional four-body states [43], which can be thought of as corresponding to Efimov trimer states consisting of a dimer and two atoms.

We find that the scattering lengths where the four-body states merge with the four-atom threshold are given by $a_{4,-}^{(1,1)} \approx 0.55a_{3,-}^{(1)}$ and $a_{4,-}^{(1,2)} \approx 0.91a_{3,-}^{(1)}$ for the ground and excited tetramers, respectively. Because of finite-range effects, these ratios are expected to differ somewhat from those values that the universal zero-range theory would predict. The fact that the excited tetramer is very weakly bound with respect to the trimer implies that the scattering length $a_{3,-}^{(1)}$ at which the trimer is in resonance with the three-atom threshold and the scattering length $a_{4,-}^{(1,2)}$ at which the excited tetramer is in resonance with the four-atom threshold are quite close. Taking the value of $a_{3,-}^{(1)} = -337(9)a_0$ $[-320(10)a_0]$ from the Chicago [15] [Heidelberg [14]] experiment, this yields $a_{4,-}^{(1,1)} \approx -187a_0$ $[-178a_0]$ and $a_{4,-}^{(1,2)} \approx -305a_0$ $[-290a_0]$. Our results suggest that the analysis of the experimental data could be impacted by the existence of the excited tetramer discussed in the present work. Future work should disentangle the zero- and finite-range effects, and possibly build van der Waals universality into the model Hamiltonian. Moreover, finite temperature effects need to be investigated carefully.

We now discuss extensions of Fig. 1 to other mass ratios κ and larger N. Our results for infinitely large a_s are summarized in Table I. The lowest tetramer becomes less strongly bound with respect to the lowest Efimov trimer with increasing mass ratio and appears to approach a constant for large κ. The ratio $(E_4^{(1,2)}/E_3^{(1)})^{1/2}$ at unitarity increases from 1.002(1) for $\kappa = 16$ to 1.067(8) for $\kappa = 50$. Our results disagree with a recent study that reported that $BBBX$ systems with mass ratios $\kappa = 30$ and 50 support a single tetramer state tied to each Efimov trimer [43]. The reason for this disagreement is not clear. We find that the excited tetramer appears at $\kappa \approx 13$. For $\kappa = 12$ and 8, we find an excited tetramer that is bound relative to the lowest trimer for negative scattering lengths away from unitarity but not at unitarity. This shows that the excited tetramer ceases to exist at different a_s for $\kappa = 8$ to 133/6. We did not investigate what happens to the excited tetramer for $\kappa = 30$–50 on the positive scattering length side. For $\kappa = 50$ and infinitely large interspecies scattering length, we searched for a second excited tetramer with energy $E_4^{(1,3)}$ that is bound with respect to the lowest Efimov trimer but did not find one. The energies of the lowest $N = 5$ and 6 states (see columns 7 and 8 of Table I) behave similar to the energy of the lowest tetramer; i.e., the binding of the lowest pentamer relative to the lowest tetramer and the binding of the lowest $N = 6$ state relative to the lowest pentamer decrease with increasing κ. It would be interesting to extend the calculations presented in this Letter to larger N.

Figure 2 shows the pair distribution functions for the $B_{N-1}X$ systems ($N = 3$ and 4) with $\kappa = 8$ (dotted line), 133/6 (solid line) and 40 (dashed line) for infinitely large BX and vanishing BB scattering lengths. The scaled pair distribution function $4\pi r^2 P_{BB}(r)$ (left column of Fig. 2) tells one the likelihood to find two identical bosons at a distance r from each other while the scaled pair distribution function $4\pi r^2 P_{BX}(r)$ (right column of Fig. 2) tells one the likelihood to find a B atom at a distance r from the X atom. To facilitate the comparison between systems with different

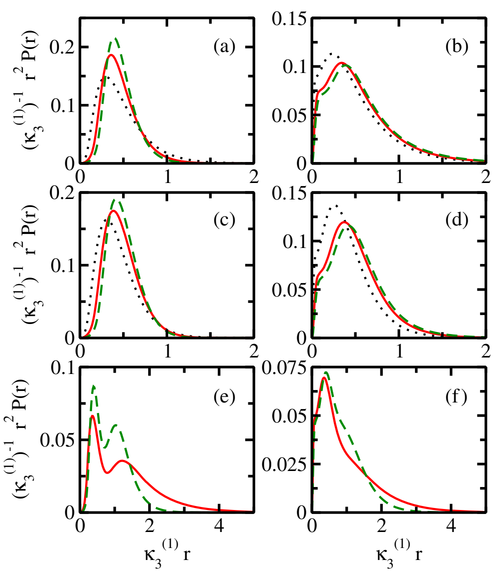

FIG. 2 (color online). Pair distribution functions for infinitely large BX and vanishing BB scattering lengths for (a) and (b) the lowest trimer, (c) and (d) the lowest tetramer, and (e) and (f) the first excited tetramer. Panels (a), (c), and (e) show the scaled pair distribution functions $r^2 P_{BB}(r)$ while panels (b), (d), and (f) show the scaled pair distribution functions $r^2 P_{BX}(r)$. Dotted, solid, and dashed lines are for $\kappa = 8$, 133/6, and 40, respectively. The calculations are performed for $V_{3b} = 3.2 E_{\mathrm{sr}}$.

mass ratios, the lengths in Fig. 2 are scaled by the binding momentum $\kappa_3^{(1)}$, where $\hbar\kappa_3^{(1)} = (2\mu|E_3^{(1)}|)^{1/2}$ [44].

Figures 2(a) and 2(b) show $r^2 P_{BB}(r)$ and $r^2 P_{BX}(r)$ for the lowest Efimov trimer. Two characteristics are evident. First, $r^2 P_{BX}$ is larger at small r than $r^2 P_{BB}$. This is not surprising, as the B atoms do not interact and are held together through the light impurity. Second, the B atoms become slightly more localized with increasing mass ratio κ; i.e., the BB pair distribution function becomes narrower with increasing κ. Figures 2(c)–2(f) show the scaled pair distribution functions for the $BBBX$ system. The scaled pair distribution functions for the lowest tetramer [Figs. 2(c)–2(d)] behave similarly to those for the lowest trimer. For the excited tetramer [Figs. 2(e)–2(f)], the scaled pair distribution functions exhibit a double-peak structure (BB distance) or "shoulder" at large distances (BX distance), indicating that the excited tetramer can be roughly thought of, like the excited tetramer in the four identical boson system [24], as a trimer with a fourth atom "tagged on" (i.e., a "3+1 state").

In summary, this Letter presented results for the extended Efimov scenario for heteronuclear $B_{N-1}X$ mixtures. It was found that the number of universal four-body bound states that are tied to the Efimov trimers depends on the mass ratio and scattering length. Structural properties of the four-body system were analyzed and extensions to the five- and six-body sector were presented. The results presented constitute an important contribution to the understanding of universal low-energy phenomena across the fields of atomic, nuclear, and particle physics. Our calculations present the first comprehensive study of the extension of the generalized Efimov scenario to heteronuclear mixtures and are directly relevant to on-going cold atom experiments on ultracold Cs-Li mixtures. Concretely, an estimate of the four-atom resonance positions was given.

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[41] The mass ratio for Cs-Li is 22.095, which is 0.3% smaller than the value $133/6 \approx 22.167$ used in the present work. The zero-range theory yields $\lambda = 4.877$ and 4.865 for $\kappa =$ 22.095 and 22.167, respectively. The difference between these λ values is 0.25%. For the purpose of the present Letter, the difference in the mass ratios is insignificant.
[42] The scattering length at which the energy of the excited tetramer crosses the energy of the lowest trimer is expected to be sensitive to finite-range effects, i.e., a precise determination of the critical scattering length value requires precise knowledge of the energy difference $E_4^{(n,2)} - E_3^{(n)}$.
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