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 $N - 1$ non-interacting 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 $E^{(n,1)}_4$ and $E^{(n,2)}_4$, which are universally linked to the energy $E^{(n)}_3$ of the $n$th Efimov trimer. For infinitely large $^{133}$Cs-$^6$Li and vanishing $^{133}$Cs-$^{133}$Cs scattering lengths, we find $(E^{(1,1)}_4/E^{(1)}_3)^{1/2} \approx 1.51$ and $(E^{(1,2)}_4/E^{(1)}_3)^{1/2} \approx 1.01$. 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].

If there exists an Efimov trimer of size $l_3^{(n)}$ and with energy $E^{(n)}_3$, 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 $E^{(n+1)}_3 = \lambda^{-d} E^{(n)}_3$. Here, $\lambda (\lambda > 1)$ 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, $\lambda$ 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 $\lambda$ takes smaller, and hence more favorable, values for heteronuclear mixtures with infinitely large interspecies $s$-wave scattering length [8]. For $^{133}$Cs-$^{133}$Cs-$^6$Li, e.g., $\lambda$ 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 $E^{(n,1)}_4$ and $E^{(n,2)}_4$ that are universally tied to the $n$th Efimov trimer with energy $E^{(n)}_3$. These four-body states lead to measurable four-atom resonances on the negative scattering length side (at scattering lengths $a^{(n,1)}_4$ and $a^{(n,2)}_4$) 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 $a^{(1,1)}_4 \approx 0.55 a^{(1)}_{3,-}$ and $a^{(1,2)}_4 \approx 0.91 a^{(1)}_{3,-}$. Since $a^{(1,2)}_4$ is close to $a^{(1)}_{3,-}$, 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 $\kappa$ 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 $^{23}$ $^{24}$. 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 $\vec{r}_j$ ($j = 1, \cdots, N - 1$) 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 $r_{jN}$ is equal to $|\vec{r}_j - \vec{r}_N|$. Motivated by our desire to explore the extension of Efimov’s BBX trimer study with large BX and vanishing BB s-wave scattering lengths $^{23}$ $^{26}$ $^{33}$, 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 $R_0 = \sqrt{S}v_0$. 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 $^{10}$ $^{17}$ $^{19}$.

Figure 1 shows the extended Efimov plot for the $C_{S_{N-1}}Li$ system with $N = 3$ and 4 $^{11}$. 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 1). For the lowest two trimers, the ratio deviates from the universal value by 0.8%, indicating that finite-range effects are negligibly small near unitarity. Non-universal 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 $a_{3,-}/a_{3,-}^{(2)} = 5.28(8)$ 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 $a_s \approx 2.6(4)a_{id}^{(1)}$, where $a_{id}^{(1)}$ 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 $1/a_s \leq 1/[13.75(5)a_{id}^{(n)}]$. 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 $n$th 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. Due to 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 $a_{3,-}$ at which the trimer is in resonance with the three-atom threshold and the scattering length $a_{4,-}$ 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 [12] [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 $\kappa$ and larger $N$. Our results for infinitely large $a_s$ are summarized in Table 1. The lowest tetramer becomes less strongly bound with respect to the lowest Efimov trimer with increasing mass ratio and approaches to appear a constant for large $\kappa$. 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 \cite{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 $E^{(1,3)}_4$ 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 7-8 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 $\kappa$. It would be interesting to extend the calculations presented in this paper 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 $4\pi r^2P_{BB}(r)$ (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 $4\pi r^2P_{BX}(r)$ (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 mass ratios, the lengths in Fig. 2 are scaled by the binding momentum $k_3^{(1)}$, where $\hbar k_3^{(1)} = (2\mu E_3^{(1)})^{1/2}$ \cite{44}.

Figures 2(a) and 2(b) show $r^2P_{BB}(r)$ and $r^2P_{BX}(r)$ for the lowest Efimov trimer. Two characteristics are evident. First, $r^2P_{BX}$ is larger at small $r$ than $r^2P_{BB}$. 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 $\kappa$, i.e., the BB pair distribution function becomes narrower with increasing $\kappa$. 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 \cite{24}, as a trimer with a fourth atom “tagged on” (i.e., a “3+1 state”).

In summary, this paper 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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**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 $r^2P_{BB}(r)$ while panels (b), (d) and (f) show the scaled pair distribution functions $r^2P_{BX}(r)$. Dotted, solid, and dashed lines are for $\kappa = 8$, 133/6 and 40, respectively. The calculations are performed for $V_{3b} = 3.2E_{3b}$. 

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![Figure 2](image-url)
The Efimov regime for three-body systems can be realized when two of three two-body zero-energy threshold.

The zero-range theory yields values is 0\% 25%. For the purpose of the present work, the difference in the mass ratios is insignificant. See Ref. [31] for details.

The mass ratio for Cs-Li is 22 and plays a role in the three-body sector at unitarity, this means that the correction to the universal 1/R^2 hyperradial potential (R denotes the hyperradius), which scales as r_0/R [V. Efimov, Phys. Rev. Lett. C 47, 1876 (1993)] and plays a role at relatively small hyperradii, gets probed less. This implies that the energetically lowest lying trimer has, for sufficiently large V_0, Efimov character. See Ref. [31] for details.

The repulsive three-body potential “pushes” the amplitude of the lowest trimer state to higher hyperradii. In the three-body sector at unitarity, this means that the correction to the universal 1/R^2 hyperradial potential (R denotes the hyperradius), which scales as r_0/R [V. Efimov, Phys. Rev. Lett. C 47, 1876 (1993)] and plays a role at relatively small hyperradii, gets probed less. This implies that the energetically lowest lying trimer has, for sufficiently large V_0, Efimov character. See Ref. [31] for details.

Note that the three-body potential employed in this paper is parameterized in terms of the sum of the square of the three interparticle distances and not in terms of the hyperradius of the three-body subsystem. For the equal-mass system, the two parameterizations are, except for a scaling factor, equivalent [23].

See to-be-inserted-by-the-editor for details on the comparison with the zero-range theory results, and for details on the basis set expansion approach and other computational aspects.

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The mass ratio for Cs-Li is 22.095, which is 0.3% smaller than the value 133/6 = 22.167 used in the present work. The zero-range theory yields λ = 4.877 and 4.865 for κ = 22.095 and 22.167, respectively. The difference between these λ values is 0.25%. For the purpose of the present paper, the difference in the mass ratios is insignificant.

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^{(c)} - E_3^{(c)}.
Note that the use of the two-body reduced mass $\mu$ is, to some extent, arbitrary; one could alternatively use a three-body reduced mass.
Supplemental material for “Generalized Efimov scenario for heavy-light mixtures”

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The notation employed in this supplemental material follows that introduced in the main text.

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BASIS SET EXPANSION APPROACH

To solve the time-independent Schrödinger equation for the Hamiltonian $H$ given in Eq. (1) of the main text, we employ an explicitly correlated Gaussian basis set [1, 2]. The eigenfunctions $\psi_\beta$ of the Hamiltonian $H$ are expanded in terms of the basis functions $\phi^{(\beta)}_l$,

$$\psi_\beta = \sum_{l=1}^{N_b} c^{(\beta)}_l \phi^{(\beta)}_l,$$

where each of the basis functions $\phi^{(\beta)}_l$,

$$\phi^{(\beta)}_l = S \exp \left[ -\frac{1}{2} \sum_{j=1}^{N-1} \sum_{k>j} \left( \frac{r_{jk}}{\alpha^{(\beta)}_{jk}} \right)^2 \right],$$

depends on $N(N-1)/2$ independent non-linear variational parameters $\alpha^{(\beta)}_{jk}$ that are optimized stochastically. For notational simplicity, the dependence of the $\alpha^{(\beta)}_{jk}$'s on the state index $\beta$ is not indicated explicitly in Eq. (2). $S$ denotes a symmetrizer that ensures that the basis function $\phi^{(\beta)}_l$ is symmetric under the exchange of any two identical bosons. The $c^{(\beta)}_l$ denote linear variational or expansion parameters that are determined by solving the generalized eigenvalue problem $H^{(\beta)} = E^{(\beta)} \Omega^{(\beta)}$, where $H$ and $\Omega$ denote the Hamiltonian and (non-diagonal) overlap matrices, respectively. The vector $\Omega^{(\beta)}$ contains the coefficients $c_1^{(\beta)}, \ldots, c_{N_b}^{(\beta)}$, where $N_b$ denotes the size of the matrix (or equivalently, the size of the basis set). According to the variational principle, the energies $E^{(\beta)}$ are upper bounds to the exact eigenenergies $E_\beta$. Assuming that $E^{(\beta)}_1 \leq E^{(\beta)}_2 \leq \cdots \leq E^{(\beta)}_{N_b}$, one has $E_1 \leq E^{(\beta)}_1, E_2 \leq E^{(\beta)}_2, \cdots$. The matrix elements $H_{ll'}$ and $O_{ll'}$ have closed analytical expressions and the generalized eigenvalue problem is solved using one of ARPACK’s eigenvalue solvers.

The superscript “$(\beta)$” on the right hand side of Eq. (1) indicates that the basis set is constructed for the $\beta$th eigenstate $\psi_\beta$. While one could construct a single basis set that provides a good description of the lowest few eigenstates, our work takes advantage of the fact that the basis set can be optimized separately for each eigenstate. For the BBX system, e.g., the two energetically lowest-lying states differ in size by the scaling factor $\lambda$. This implies that the variational parameters $\alpha^{(\beta)}_{jk}$ that yield an efficient description of the ground state (the state with $\beta = 1$) and of the first excited state (the state with $\beta = 2$) are very different. Another key point of the basis set expansion approach is that the basis set can be systematically improved. Our three-body energies are, except very close to the three-atom break-up threshold, converged to 0.1% or better. Our four-body energies are converged to 1% or better. For the $B_3X$ system at unitarity with $\kappa = 133/6$, e.g., we clearly see that the energy of the first excited four-body state lies below that of the lowest BBX state.

BENCHMARKING OUR APPROACH: $N$ IDENTICAL BOSONS

To validate our approach, we consider $N$ identical bosons of mass $m_B$ with infinitely large $s$-wave scattering length $a_s$ described by the Hamiltonian $H_B$,

$$H_B = \sum_{j=1}^{N} -\frac{\hbar^2}{2m_B} \nabla_{\vec{r}_j}^2 + V_{2b} + V_{3b}. \tag{3}$$

The potential $V_{2b}$ accounts for the interactions between all $N(N-1)/2$ pairs,

$$V_{2b} = \sum_{j=1}^{N-1} \sum_{k>j}^{N} v_0 \exp \left( -\frac{r_{jk}^2}{2r_0^2} \right), \tag{4}$$

where $v_0$ and $r_0$ denote the depth and range of the attractive two-body Gaussian. The depth and range are adjusted such that the free-space two-body system supports one zero-energy bound state. The potential $V_{3b}$ accounts for the interactions between all $N(N-1)(N-2)/6$ triples,

$$V_{3b} = \sum_{j=1}^{N-2} \sum_{k>j}^{N-1} \sum_{l>k}^{N} v_0 \exp \left( -\frac{r_{jk}^2 + r_{kl}^2 + r_{lj}^2}{2R_0^2} \right), \tag{5}$$

where $v_0$ and $R_0$ denote the depth and range of the repulsive three-body Gaussian. Our calculations use $R_0 = \sqrt{8}r_0$. As discussed in Ref. [3], the repulsive three-body potential serves to eliminate deeply-bound non-universal states in the $N = 3$ sector. In essence, the three-body potential “cuts off” the short-range portion of the effective hyperradial potential curve that is
governed by the two-body effective range and deviates from the effective three-body hyperradial Efimov potential curve. Using this model, the ratio of the binding momenta of the two energetically lowest-lying three-body states is \((E_3^{(1)}/E_3^{(2)})^{1/2} = 22.99\) for \(V_0 = 0\), takes a minimum value of \((E_3^{(3)}/E_3^{(2)})^{1/2} = 21.48\) for \(V_0 \approx 0.3E_{sr}\), and approaches \((E_3^{(1)}/E_3^{(2)})^{1/2} = 22.71\) as \(V_0 \to \infty\). For \(V_0 \geq E_{sr}\), the ratio \(E_3^{(1)}/E_3^{(2)}\) lies within 0.08% of the universal zero-range value of 22.694. The small difference of the binding momentum ratios for the finite-range Hamiltonian \(H_B\) and for the zero-range model can be attributed to the fact that both \(V_{2b}\) and \(V_{3b}\) have a finite range.

The four identical boson system with infinitely large s-wave scattering length has been benchmarked most precisely by Deltuva [4] using a momentum space representation that allows for the treatment of bound and resonance states. It was shown that the four-body energies \(E_4^{(n,1)}\) and \(E_4^{(n,2)}\) approach the ratios \((E_4^{(n,1)}/E_4^{(n,2)})^{1/2} = 2.147\) and \((E_4^{(n,2)}/E_4^{(n,1)})^{1/2} = 1.0011\), respectively, for sufficiently large \(n\) [4]. For the Hamiltonian given in Eq. 4 with \(V_0 = 4.8E_{sr}\), we find (see also the main text) that the binding momentum ratio of the lowest four-body state and the lowest three-body state is \((E_4^{(1,1)}/E_3^{(1)})^{1/2} = 2.127(5)\). For this \(V_0\), the lowest three-body energy is \(-2.64 \times 10^{-4}E_{sr}\), i.e., the three-body system is large compared to both \(r_0\) and \(R_0\) and thus, to a good approximation, independent of \(r_0\) and \(R_0\). We also find a weakly-bound excited four-body state with the binding momentum ratio \((E_4^{(1,2)}/E_3^{(1)})^{1/2} \geq 1.0004\) that is tied to the lowest three-body state. Although the variational principle does not apply to energy ratios, we can assign the “≥” sign since the energy of the lowest three-body state has a significantly smaller basis set error than the energy of the excited four-body state.

**HEAVY-LIGHT (2,1) SYSTEM AT UNITARITY**

To validate our calculations for the (2,1) system with unequal masses, we consider the case where the interspecies s-wave scattering length is infinitely large and the intraspecies two-body potential is set to zero. In the limit of zero-range interactions, the hyperangular and hyperradial degrees of freedom separate, and the hyperradial density \(P_{hyper}(R)\) can be calculated analytically [5] (see the solid line in Fig. 1 for \(\kappa = 133/6\)). Here, the hyperradius \(R\) is defined through

\[
\mu R^2 = 2 \sum_{j=1}^{2} m_B (\vec{r}_j - \vec{r}_{cm})^2 + m_X (\vec{r}_3 - \vec{r}_{cm})^2,
\]

where \(\vec{r}_{cm}\) denotes the center-of-mass vector of the B2X system. For comparison, squares and circles show the hyperradial densities for the energetically lowest-lying and second lowest-lying states obtained from our basis set expansion calculations for the Hamiltonian \(H\) [see Eq. (1) of the main text]. To make this figure, the lengths have been scaled by the three-body parameter \(\kappa_3\).

![FIG. 1: (Color online) Hyperradial density \(P_{hyper}(R)\) for the B2X system with infinitely large interspecies s-wave scattering length and \(\kappa = 133/6\). The squares and circles show the hyperradial densities for the ground and first excited state of the finite-range model Hamiltonian with \(V_0 = 3.2E_{sr}\) and \(R_0 = \sqrt{3}r_0\). The solid line shows the hyperradial density for the zero-range model Hamiltonian. For all three curves, dimensionless units are used (see the text for details).](image-url)

For the circles and the solid line, \(\kappa_3\) is defined through \(\hbar^2 \kappa_3^2/(2\mu) = |E_3^{(2)}|\), where \(E_3^{(2)}\) is the energy of the first excited state of the finite-range model Hamiltonian. For the squares, we define \(\kappa_3\) through \(\hbar^2 \kappa_3^2/(2\mu) = \lambda^2 |E_3^{(2)}|\), where \(\lambda\) is obtained by solving the hyperangular portion of the zero-range model Hamiltonian. As shown in Table I of the main text, this zero-range scaling factor is very close to the scaling factor obtained from the spacing between the two lowest three-body energies of the finite-range model Hamiltonian. The good agreement for \(\kappa_3 R \gtrsim 0.5\) between the hyperradial density for the zero-range model and the hyperradial densities of the finite-range Hamiltonian with two- and three-body interactions demonstrates that the model Hamiltonian employed in our work captures the Efimov physics in the three-body sector accurately.

Varying \(V_0\) changes the three-body parameter. The scaled hyperradial densities and energy ratios, however, are, to a good approximation, unchanged for \(V_0 \gtrsim E_{sr}\) and agree well with those for the zero-range model. As an example, Fig. 2 shows the binding momentum ratio \((E_3^{(1)}/E_3^{(2)})^{1/2}\) as a function of \(V_0\) for infinitely large interspecies s-wave scattering length and \(\kappa = 133/6\). As can be seen, the binding momentum ratio is approximately independent of \(V_0\) for \(V_0 \gtrsim E_{sr}\). In the large \(V_0\) limit, the binding momentum ratio is close but not identical to the binding momentum ratio predicted by the zero-range theory. The small deviation can be attributed to the weak breaking of the discrete scale invariance of the
model Hamiltonian by the finite-range two- and three-body interactions.

**HEAVY-LIGHT (3,1) SYSTEM**

Symbols in Figs. 3(a) and 3(b) show the binding momentum ratios \((E_3^{(1)}/E_3^{(2)})^{1/2}\) as a function of \(V_0\) for the B_2X system with infinitely large interspecies s-wave scattering length and \(\kappa = 133/6\). For these calculations, we used \(R_0 = \sqrt{8}r_0\). The dotted line shows the binding momentum ratio for the zero-range model.

To further test the robustness of our results against changes of the parameters in the model Hamiltonian, we considered a 1.5 times larger range of the repulsive three-body potential while keeping the two-body range \(r_0\) unchanged. The resulting change in the observables was found to be quite small. In addition, we varied the functional form of \(V_3\), i.e., we considered a repulsive three-body potential that is parameterized in terms of the hyperradii of the B_2X subsystems as opposed to the sum of the squares of the interparticle distances. The key difference between this alternative parametrization and the parametrization employed earlier is that this alternative three-body potential does, for the B_2X system, not depend on the hyperangles; note, however, that this alternative \(V_3\) does depend on the hyperangles for \(N \geq 4\). For this three-body potential, the four-body states are bound a bit more weakly relative to the lowest three-body state than for the three-body potential used in the main text. At unitarity, we obtain \((E_4^{(1,1)}/E_3^{(1)})^{1/2} = 1.47(2)\) and \((E_4^{(1,2)}/E_3^{(1)})^{1/2} \geq 1.004\). For the scattering lengths at which the four-body system becomes unbound, we find \(a_4^{(1,1)} \approx 0.57a_3^{(1)}\) and \(a_4^{(1,2)} \approx 0.92a_3^{(1)}\). For comparison, the corresponding values reported in the main text are 0.55 and 0.91, respectively. The mass ratio at which the excited four-body state ceases to exist at unitarity changes from approximately 13 (this is the value reported in the main text) to 17 for the alternative three-body potential. These calculations suggest that the generalized Efimov scenario discussed in the main text is fairly robust with respect to changes in the model Hamiltonian.

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