Universal Four-Body States in Heavy-Light Mixtures with a Positive Scattering Length

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Universal four-body states in heavy-light mixtures with positive scattering length

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The number of four-body states known to behave universally is small. This work adds a new class of four-body states to this relatively short list. We predict the existence of a universal four-body bound state for heavy-light mixtures consisting of three identical heavy fermions and a fourth distinguishable lighter particle with mass ratio $\kappa \gtrsim 9.5$ and short-range interspecies interaction characterized by a positive s-wave scattering length. The structural properties of these universal states are discussed and finite-range effects are analyzed. The bound states can be experimentally realized and probed utilizing ultracold atom mixtures.

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Universality plays an important role in nearly all areas of physics and allows one to connect phenomena governed by vastly different energy and length scales. A simple class of universal states consists of two-body bound states whose size is much larger than any other length scale in the problem. Prominent examples include diatomic Feshbach molecules [1], which are nowadays created routinely in cold atom laboratories around the world, and di-mesons such as the charmonium resonance near 3870 MeV [2]. The former have a binding energy of order 10^{-10} eV while the latter have a binding energy of order 0.5×10^{6} eV. Yet, once expressed in terms of the two-body s-wave scattering length a_s, the binding energy can be written, to a very good approximation, as $E_2^{\rm ZR} \approx -\hbar^2/(2\mu a_s^2)$ in both cases; here, μ is the reduced mass of the constituents.

Although the concept of universality has been extended successfully to three- and higher-body systems [3–22], the list of examples, particularly for few-body systems consisting of more than $n = 3$ constituents, is still comparatively small. Most notably, three- and four-body physics has been investigated in the context of Efimov physics. The three-body Efimov effect [5], i.e., the existence of infinitely many geometrically spaced three-body bound states, can occur when the s-wave scattering length is much larger than the range of the two-body potential. This at first sight purely academic scenario can be realized in cold atom experiments by tuning the s-wave scattering length in the vicinity of a Fano-Feshbach resonance through application of an external magnetic or optical field [1, 12]. In the four-body sector, Efimov physics can occur via two different routes, as a true four-body Efimov effect [22] or as four-body states universally tied to three-body Efimov states [6, 8, 9]. In either case, the description of the Efimov scenario requires two parameters, the s-wave scattering length and a higher-body parameter [5].

This Letter reports on a new class of universal four-body states, predicted to exist—just as Efimov states—in three spatial dimensions that are fully determined by the two-body s-wave scattering length a_s. As such, they are fundamentally different from Efimov states, which depend on two parameters. The universal four-body bound states exist in heavy-light mixtures that consist of three identical heavy fermions and a fourth distinguishable particle, which interacts with the heavy particles through a short-range two-body potential with positive s-wave scattering length a_s. We find that the four-body bound states exist for mass ratios κ larger than $\kappa_{c,4} \approx 9.5$. For effectively two- or one-dimensional confinement, the universal tetramers are expected to be more strongly bound than in three spatial dimensions. In fact, universal tetramers under quasi-two-dimensional confinement have very recently been predicted to exist for $\kappa \gtrsim 5$ [21]. Just as the three-body bound states for positive a_s are connected to Efimov states (which exist, in the zero-range limit, for $\kappa > 13.607$) [17–20, 23, 24], the universal four-body states predicted here are expected to be connected to four-body Efimov states, which have been predicted to exist for $13.384 < \kappa < 13.607$ [22]. The different classes of states can be described in a unified framework within the hyperspherical coordinate or effective field theory formulations. We analyze the dependence of the binding energy on the range of the underlying two-body interaction potential and interpret our findings employing hyperspherical coordinates. The universal four-body bound states discussed here are not only interesting from the few-body point of view but also have important implications for the many-body phase diagram of heavy-light mixtures [25–28] that can be realized with cold atoms [29–32], electrons [33] and quarks.

Our starting point is the non-relativistic Hamiltonian H in free space for $n-1$ identical heavy fermions of mass M and a single distinguishable light particle of mass m,

$$H = \sum_{j=1}^{n-1} \frac{-\hbar^2}{2M}\nabla^2_{\vec{r}_j} + \frac{-\hbar^2}{2m}\nabla^2_{\vec{r}_n} + \sum_{j=1}^{n-1} V_{\rm tb}(r_{jn}), \qquad (1)$$

where $V_{\rm tb}(r_{jn}) = -V_0 \exp\left[-r_{jn}^2/(2r_0^2)\right]$. Here, $\vec{r}_j$ denotes the position vector of the jth particle and r_{jk} the interparticle distance, $r_{jk} = |\vec{r}_j - \vec{r}_k|$. The interaction between the heavy and light particles is described by the

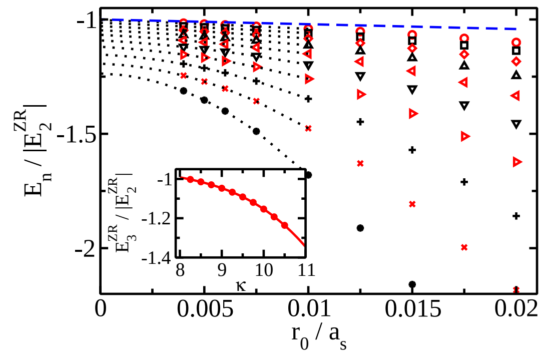

FIG. 1: (Color online) Scaled energies as a function of r_0/a_s. The dashed line shows $E_2/|E_2^{\mathrm{ZR}}|$. The symbols show $E_3/|E_2^{\mathrm{ZR}}|$ for $\kappa = 8.25 - 10.5$ (top to bottom), in steps of 0.25; E_3 is determined by the stochastic variational approach. Dotted lines show three-parameter fits. Inset: Symbols show $E_3^{\mathrm{ZR}}/|E_2^{\mathrm{ZR}}|$ as a function of κ. The solid line shows a four-parameter fit.

Gaussian potential V_{tb} with depth V_0 and range r_0. We are interested in the regime where the two-body free-space s-wave scattering length a_s is positive and $r_0 \ll a_s$. Throughout, we express lengths in units of a_s and energies in units of $|E_2^{\mathrm{ZR}}|$, where E_2^{ZR} denotes the relative s-wave energy of the two-body system with zero-range interactions (realized when $r_0 \to 0$), $E_2^{\mathrm{ZR}} = -\hbar^2/(2\mu a_s^2)$ with $\mu = Mm/(M+m)$. For a given r_0/a_s, we adjust the depth V_0 such that the two-body potential supports a single s-wave bound state.

To determine the eigenstates and eigenenergies of H, we expand the relative wave function in terms of explicitly correlated Gaussians [34]. To construct basis functions with good total relative angular momentum L, projection quantum number M_L ($M_L = 0$), and parity Π, we employ the global vector approach [35, 36]. The parameters of the explicitly correlated Gaussian basis functions are optimized semi-stochastically. According to the generalized Ritz variational principle [34], the approach yields variational upper bounds for the eigenenergies of the ground and excited states.

We first consider the $n = 3$ system with $L^{\Pi} = 1^-$ symmetry. Employing zero-range s-wave interactions, a universal trimer state has been predicted to exist for $\kappa_{c,3} \gtrsim 8.173$ [20]. A second universal trimer state has been predicted to be supported for $\kappa_{c,3}^* \gtrsim 12.917$ [20]. Symbols in Fig. 1 show the relative energy E_3 of the energetically lowest-lying three-body state with 1^- symmetry, calculated by the stochastic variational approach and scaled by $|E_2^{\mathrm{ZR}}|$, as a function of r_0/a_s for various mass ratios κ ($\kappa = M/m$). The trimer energy becomes more negative with increasing κ for a fixed r_0/a_s. Moreover, the trimer energies approach the zero-range limit from below, with the range dependence becoming larger with increasing κ. For comparison, the dashed line shows the quantity $E_2/|E_2^{\mathrm{ZR}}|$; here, E_2 denotes the relative two-body energy. Due to the scaling chosen, the dimer energy is independent of the mass ratio. The dependence of the dimer energy on r_0 is smaller than that of the trimer energy. Dotted lines in Fig. 1 show three-parameter fits to the three-body energies with $r_0/a_s \leq 0.01$ [37]. The symbols in the inset of Fig. 1 show the extrapolated zero-range energies E_3^{ZR}, scaled by $|E_2^{\mathrm{ZR}}|$, as a function of the mass ratio κ. The solid line shows a fit of the quantity $E_3^{\mathrm{ZR}}/|E_2^{\mathrm{ZR}}|$ to a fourth-order polynomial. Our fit predicts that the trimer becomes unbound with respect to the dimer for $\kappa_{c,3} \approx 8.20$, which compares favorably with the $\kappa_{c,3}$ value of 8.173 determined for zero-range interactions [20]. This good agreement demonstrates that the stochastic variational approach employed in this work is capable of accurately describing universal few-body bound states. Non-universal trimer states can, at least in principle, exist for $\kappa \gtrsim 8.6$, corresponding to a scaled hyperangular eigenvalue $s_{0,\mathrm{unit}} < 1$ [17, 27, 38, 39]. Whether or not non-universal states exist depends on the details of the underlying two-body potential. For the Gaussian model potential considered here, it was shown [40, 41] that non-universal three-body physics comes into play for mass ratios larger than those considered here.

We now discuss the energetics of the four-body system. For zero-range interactions with $1/a_s = 0$, the $s_{0,\mathrm{unit}}$ value is greater than 1 for $\kappa < 10$ [40–42], suggesting that four-body bound states are, provided they exist, universal. Circles and triangles in Fig. 2 show the quantity $E_4/|E_2^{\mathrm{ZR}}|$ for, respectively, the energetically lowest-lying and second lowest-lying states with $L^{\Pi} = 1^+$ symmetry for (a) $\kappa = 9.5$, (b) $\kappa = 9.75$ and (c) $\kappa = 10$ as a function of r_0/a_s. The four-body energies are obtained by the stochastic variational approach. For comparison, the dashed lines in Fig. 2 show the quantity $E_2/|E_2^{\mathrm{ZR}}|$, and the crosses and solid lines show the quantity $E_3/|E_2^{\mathrm{ZR}}|$. The four-body ground state energy lies below the three-body energy for small r_0/a_s. For $\kappa = 9.5$, 9.75 and 10, the four-body ground state energy "dives down" around $r_0/a_s \approx 0.015$, 0.011 and 0.008, respectively. In this regime, the four-body state acquires non-universal characteristics. For slightly larger r_0/a_s, the energy of the first excited state drops below the energy of the trimer and then "traces" the three-body energy [43]. We refer to the feature where the four-body system acquires a new bound state as resonance-like feature. The existence and characteristics of the resonance-like feature depend on the details of the two-body interaction model employed. Away from the resonance-like feature, the four-body energy shows a very similar range dependence as the three-body energy, suggesting that the four-body energy is roughly a constant multiple of the three-body energy. Moreover, it is clear from Fig. 2 that E_3/E_4 increases with increasing mass ratio [44]. A precise extrapolation of the four-body energies to the zero-range limit is challenging since numerical issues limit our calculations to $r_0/a_s \gtrsim 0.004$ and the resonance-like feature prevents us to perform unambiguous fits. We estimate that the

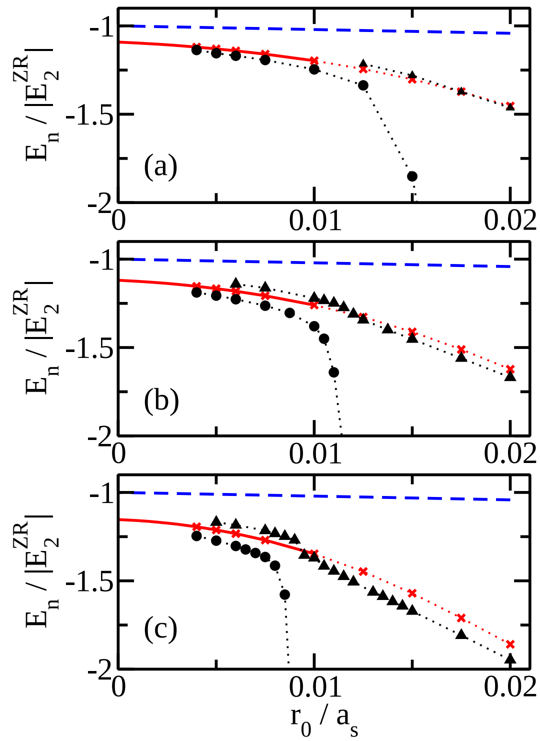

FIG. 2: (Color online) Scaled energies as a function of r_0/a_s for (a) $\kappa = 9.5$, (b) $\kappa = 9.75$, and (c) $\kappa = 10$. The dashed lines show $E_2/|E_2^{\mathrm{ZR}}|$ while the crosses (stochastic variational energies) and solid lines (fit) show $E_3/|E_2^{\mathrm{ZR}}|$ (these energies are also shown in Fig. 1). Circles and triangles show $E_4/|E_2^{\mathrm{ZR}}|$ for the energetically lowest-lying and second lowest-lying four-body states, respectively. Dotted lines serve as a guide to the eye.

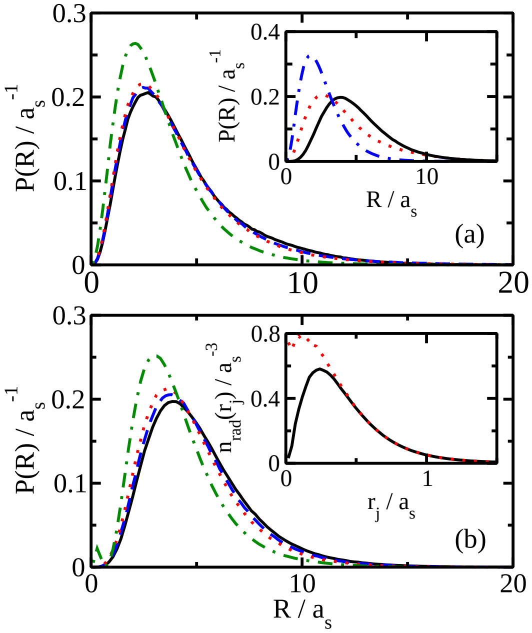

FIG. 3: (Color online) (a) Solid, dashed, dotted and dash-dotted lines show $P(R)$ of the energetically lowest-lying state for $n = 3$, $\kappa = 8.5$ and $r_0/a_s = 0.004$, 0.005, 0.006 and 0.015, respectively. Inset: Dotted, dash-dotted and solid lines show $P(R)$ for $n = 3$ ($\kappa = 8.5$ and $r_0/a_s = 0.004$), $n = 3$ ($\kappa = 9.75$ and $r_0/a_s = 0.004$), and $n = 4$ ($\kappa = 9.75$ and $r_0/a_s = 0.004$), respectively. (b) Solid, dashed, dotted and dash-dotted lines show $P(R)$ for $n = 4$, $\kappa = 9.75$ and $r_0/a_s = 0.004$, 0.005, 0.006 and 0.015, respectively. For $r_0/a_s = 0.004, 0.005$ and 0.006, the energetically lowest-lying state is considered. For $a_s/r_0 = 0.015$, the energetically second-lowest lying state is considered. Inset: Solid and dotted lines show $n_{\mathrm{rad}}(r_j)$ for the heavy and light particles, respectively, for $n = 4$, $\kappa = 9.75$, $r_0/a_s = 0.004$ and 1^+ symmetry.

four-body system becomes bound around $\kappa_{c,4} = 9.5$.

To provide further evidence that the four-body states are—away from the resonance-like feature—universal, we analyze the hyperradial density $P(R)$, where $\mu R^2 = \sum_{j=1}^{n-1} M(\vec{r}_j - \vec{R}_{\mathrm{cm}})^2 + m(\vec{r}_n - \vec{R}_{\mathrm{cm}})^2$ and $\vec{R}_{\mathrm{cm}}$ denotes the center-of-mass vector of the n-body system. A small hyperradius R implies that all n particles are close together while a large hyperradius implies that two or more particles are far away from each other [48]. The hyperradial density $P(R)$, normalized such that $\int_0^\infty P(R)dR = 1$, indicates the likelihood of finding the n-particle system with a given R. We calculate the hyperradial densities as well as other structural properties by sampling the n-particle density obtained by the stochastic variational approach via a Metropolis walk [49].

Figures 3(a) and 3(b) show the hyperradial densities $P(R)$ for $n = 3$ ($\kappa = 8.5$ and $L^\Pi = 1^-$) and $n = 4$ ($\kappa = 9.75$ and $L^\Pi = 1^+$) for various r_0/a_s [45]. For these mass ratios, the three- and four-body systems support very weakly-bound states. To allow for a direct comparison, dotted and solid lines in the inset of Fig. 3(a) show the hyperradial densities for $n = 3$ ($\kappa = 8.5$) and $n = 4$ ($\kappa = 9.75$) for $r_0/a_s = 0.004$. The hyperradial densities for $n = 3$ with $\kappa = 8.5$ and $n = 4$ with $\kappa = 9.75$ agree qualitatively. They have a small amplitude for $R/a_s \ll 1$, peak around $R/a_s = 2$ and fall off exponentially for $R \gg a_s$ for all r_0/a_s considered. For fixed κ, the hyperradial densities move smoothly "outward" with decreasing r_0/a_s. Importantly, the hyperradial density has vanishingly small amplitude not only when $R \approx r_0$ but also for notably larger R values [46]. For $n = 3$, this is consistent with the hyperradial density obtained within the zero-range framework [20, 47], confirming that the three-body states considered are fully universal, i.e., fully determined by a_s. The qualitatively similar behavior of the $n = 3$ and 4 hyperradial densities for similarly weakly-bound states provides, combined with the energetics, strong evidence that the four-body states are also universal.

The dash-dotted line in the inset of Fig. 3(a) shows the hyperradial density for $n = 3$, $\kappa = 9.75$ and $r_0/a_s = 0.004$. The three-body system is more tightly bound than the four-body system with the same κ and r_0/a_s (solid line). In a naive picture, one may imagine that the four-body system is comprised of a trimer with a fourth atom loosely attached to the trimer. Structures like this have been observed for the excited tetramer state attached to the Efimov trimer state comprised of three identical bosons [9, 10]. Our analysis of the pair distribution functions and radial densities indicates that the situation for the tetramers considered here is different. The structural properties of the tetramer for a given κ loosely resemble those of the trimer with smaller κ but comparable binding energy. Solid and dotted lines in the inset of Fig. 3(b) show the radial density $n_{\mathrm{rad}}(r_j)$, normalized such that $4\pi \int_0^\infty n_{\mathrm{rad}}(r_j) r_j^2 dr_j = 1$, for the heavy and light particles of the $n = 4$ system; the position vector $\vec{r}_j$, $j = 1, \cdots, n$, is measured with respect to $\vec{R}_{\mathrm{cm}}$ and $r_j = |\vec{r}_j|$. For large r_j, the radial densities of the heavy particles and the light particle are nearly indistinguishable. For small r_j, n_{rad} goes to zero for the heavy particles but has an appreciable amplitude for the light particle, suggesting that the light particle is "shared" among the heavy particles.

In summary, we analyzed heavy-light mixtures in three spatial dimensions, where the heavy-light pairs interact through short-range potentials with positive s-wave scattering lengths. Despite the Pauli exclusion principle, which acts as an effective repulsion between the identical heavy fermions, the four-body system supports a universal bound state if the mass ratio between the heavy and light particles is larger than about 9.5. The light particle acts as a mediator that "glues" the four-body system together, just as electrons in H_2^+ or H_2 glue together the protons by way of the exchange interaction [50]. Although the three-body energy shows a fairly strong dependence on r_0, we found that the ratio E_4/E_3 is, away from the resonance-like feature, roughly constant for a fairly wide range of r_0/a_s values, suggesting that the universal four-body states can be observed in cold atom experiments with current technologies. The existence of universal tetramer states opens the possibility to search for novel tetramer phases in many-body systems, promising a rich phase diagram of heavy-light mixtures on the positive scattering length side. In the future, it will be interesting to investigate how the universal four-body states discussed here are affected by non-universal three- and four-body states and how these states are connected to Efimov tetramers that have been predicted to exist for $13.384 < \kappa < 13.607$ [22].

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[43] For $\kappa = 9.5$, the energy of the four-body state with 1^+ symmetry lies slightly below the energy of the three-body state with 1^- symmetry for $r_0/a_s = 0.02$ but not for $r_0/a_s = 0.0175$ and 0.015.

[44] We also performed calculations for $\kappa = 10.25$ and 10.5. For these mass ratios, the finite-range effects of the three-body system are already fairly large (see Fig. 1). For the r_0/a_s considered, we also observe that the four-body energy is, away from the resonance-like feature (which moves to smaller r_0/a_s with increasing κ), roughly a constant multiple of the three-body energy.

[45] For $n = 4$ and $r_0/a_s = 0.015$, the hyperradial density of the energetically second lowest-lying state with 1^+ symmetry is shown [this is the state whose energy is shown by a triangle in Fig. 2(b)]; for all other cases, the hyperradial density of the energetically lowest-lying state is shown. The wave function of the energetically second lowest-lying state has a node in the hyperradial coordinate, which leads to the vanishing of the hyperradial density around $r_0/a_s \approx 0.5$.

[46] For $n = 3$ and $R = 10r_0$ ($r_0/a_s = 0.004$ and $\kappa = 8.5$), the amplitude of the hyperradial density is more than 1000 times smaller than the corresponding hyperradial peak density. For $n = 4$ and $R = 50r_0$ ($r_0/a_s = 0.004$ and $\kappa = 9.75$), the amplitude of the hyperradial density is more than 1000 times smaller than the corresponding hyperradial peak density.

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