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

D. Blume$^{1,2}$

$^1$Department of Physics and Astronomy, Washington State University, Pullman, Washington 99164-2814, USA
$^2$ITAMP, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, Massachusetts 02138, USA

(Dated: May 2, 2014)

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.

PACS numbers:

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

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 $0.5 \times 10^6$ 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 $E_z \approx -\hbar^2/(2\mu a_s^2)$ in both cases: here, $\mu$ is the reduced mass of the constituents (the two atoms and two mesons, respectively).

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 [2], 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 [3–5]. In either case, the description of the Efimov scenario requires two parameters, the $s$-wave scattering length and a three-body parameter $\kappa$ [5]. The latter may be determined by the characteristic length of the underlying two-body potential [23] (a scenario more likely to apply to nuclear systems).

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. Another crucial distinction is that the states considered here have continuous scale invariance while Efimov states exhibit discrete scale invariance. 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 $\kappa$ 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 $\kappa > 5$ [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, 24, 25]), 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]. 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 [20, 29] that can be realized with cold atoms [30, 32], electrons [34] 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 $m$,

$$H = \sum_{j=1}^{n-1} -\frac{\hbar^2}{2M} \nabla^2_{r_j} + \frac{\hbar^2}{2m} \nabla^2_{r_n} + \sum_{j=1}^{n-1} V_{tb}(r_{jn}),$$

(1)
where
\[ V_{tb}(r_{jn}) = -V_0 \exp \left[-r_{jn}^2/(2r_0^2)\right]. \] (2)

Here, \( \vec{r}_j \) denotes the position vector of the \( j \)th 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 Gaussian potential \( V_{tb} \) with depth \( V_0 \) and range \( r_0 \). In the following, we are interested in the regime where the two-body free-space \( s \)-wave scattering length \( a_s \) of \( V_{tb} \) is positive and \( r_0 \ll a_s \). Throughout, we express lengths in units of \( a_s \) and energies in units of \( |E_{2R}^R| \), where \( E_{2R}^R \) denotes the relative \( s \)-wave energy of the two-body system with zero-range interactions (realized when \( r_0 \rightarrow 0 \)). \( E_{2R}^R = -\hbar^2/(2\mu a_s^2) \) 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 separate off the center-of-mass degrees of freedom and expand the relative wave function in terms of explicitly correlated Gaussians \[35\]. To construct basis functions with good total relative angular momentum \( L \), projection quantum number \( M_L \), and parity \( \Pi \), we employ the global vector approach \[36, 37\], which has been used extensively to describe nuclear systems. Throughout, we limit ourselves to states with \( M_L = 0 \). The anti-symmetry of the basis functions with respect to the exchange of pairs of identical fermions is ensured through the application of an anti-symmetrizer. The parameters of the explicitly correlated Gaussian basis functions are optimized semi-stochastically. According to the generalized Ritz variational principle \[32\], the approach yields variational upper bounds for the eigenenergies of the ground and excited states. Our stochastic variational calculations for \( n = 3 \) and 4 reported below employ up to 1000 and 3500 basis functions, respectively.

We first consider the \( n = 3 \) system with \( L^I = 1^- \) 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 normalized by \( |E_{2R}^R| \), as a function of \( r_0/a_s \) for various mass ratios (\( \kappa = 8.25 - 10.5 \), where \( \kappa = M/m \)). As expected, the trimer energy becomes more negative with increasing \( \kappa \) 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 \( \kappa \). For comparison, the dashed line shows the quantity \( E_2/|E_{2R}^R| \) as a function of \( r_0/a_s \); 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 \( r_0/a_s \leq 0.01 \) \[38\]. The symbols in the inset of Fig. 1 show the extrapolated zero-range energies \( E_3^{ZR} \) of the trimer, scaled by \( |E_{2R}^R| \), as a function of the mass ratio \( \kappa \). The solid line shows a four-parameter fit.

We now discuss the energetics of the four-body system. Circles and triangles in Fig. 2 show the quantity \( E_4/|E_{2R}^R| \) for, respectively, the energetically lowest-lying and second lowest-lying states of the four-body system with \( L^I = 1^+ \) 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. Dotted lines are shown as a guide to the eye. For comparison, the dashed lines in Fig. 2 show the quantity \( E_{2s}/|E_{2R}^R| \), and the crosses and solid lines show the quantity \( E_3/|E_{2R}^R| \) (the symbols show the stochastic variational energies and the solid line shows the fit; see also Fig. 1). The ground state energy of the four-body system lies below that of the three-body system for small \( r_0/a_s \). For \( \kappa = 9.5, 9.75 \) and 10, the ground state energy of the four-body system “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 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 the ratio between the four- and three-body energy increases with increasing mass ratio \( \frac{r_0}{a_s} \). A precise extrapolation of the four-body energies to the zero-range limit is challenging for two reasons: (i) Numerical issues limit our calculations to \( \frac{r_0}{a_s} \gtrsim 0.004 \). (ii) The existence of the resonance-like feature prevents us to perform unambiguous fits. We estimate that the 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 \( P(R) \). The hyperradius provides a measure of the system size \(^{17}\). A small hyperradius implies that all \( n \) particles are close together while a large hyperradius implies that two or more particles are far away from each other. In Eq. (3), \( \vec{R}_{\text{em}} \) denotes the center-of-mass vector of the \( n \)-body system. 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 \(^{18}\).

Figures 3(a) and 3(b) show the hyperradial densities \( P(R) \) for \( n = 3 \) (\( \kappa = 8.5 \) and \( L^1 = 1 \)) and \( n = 4 \) (\( \kappa = 9.75 \) and \( L^1 = 1 \)) for various \( r_0/a_s \). 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 \( \kappa \), 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 \(^{15}\). For the three-body system, this is consistent with the hyperradial density obtained within the zero-range framework \(^{20,16}\), 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 of the three-body system for \( \kappa = 9.75 \) and \( r_0/a_s = 0.004 \). The three-body system is more tightly bound than the four-body system with the same \( \kappa \) 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 \( \sqrt{3} \) \( \mu \) baryons \(^{9,10}\). 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 of a given \( \kappa \) loosely resemble those of the trimer with smaller \( \kappa \) but comparable binding energy. Solid and dotted lines in the inset of Fig. 3(b) show the radial density \( n_{\text{rad}}(r_j) \), normalized such that \( 4\pi \int_0^\infty n_{\text{rad}}(r_j) r_j^2 \,dr_j = 1 \), for the heavy
and light particles of the $n = 4$ system; the position vector $\vec{r}_j$, $j = 1, \ldots, n$, is measured with respect to $\vec{R}_{\text{cm}}$ 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 $r_j$, $r_{\text{rad}}$ 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 consisting of three heavy particles and one light particle 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 $\text{H}_2^+$ or $\text{H}_2$ glue together the protons by way of the exchange interaction $^{49}$. 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 $13.384 < k < 13.607^{22}$.

Acknowledgments: DB thanks Javier von Stecher for suggesting to look at heavy-light mixtures with positive scattering length and Seth Rittenhouse for fruitful discussions. Support by the NSF through grants PHY-0855332 and PHY-1205443 is gratefully acknowledged. This work was additionally supported by the National Science Foundation through a grant for the Institute for Theoretical Atomic, Molecular and Optical Physics at Harvard University and Smithsonian Astrophysical Observatory.

[1] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga. Rev. Mod. Phys. 82, 1225 (2010).
[2] E. Braaten and M. Kusunoki. Phys. Rev. D 69, 074005 (2004).
[3] C. H. Greene. Physics Today 63, 40 (2010).
[4] F. Ferlaino and R. Grimm. Physics 3, 9 (2010).
[5] E. Braaten and H.-W. Hammer. Phys. Rep. 428, 259 (2006).
[6] L. Platter, H.-W. Hammer and U. Meißner. Phys. Rev. A 70, 52101 (2004).
[7] G. J. Hanna and D. Blume. Phys. Rev. A 74, 063604 (2006).
[8] H.-W. Hammer and L. Platter. Eur. Phys. J. A 32, 113 (2007).
[9] J. von Stecher, J. P. D’Incao and C. H. Greene. Nat. Phys. 5, 417 (2009).
[10] J. von Stecher. J. Phys. B 43, 101002 (2010).
[11] A. Deltuva. [arXiv:1202.0167] (to appear in Few-Body Systems).
[12] T. Kraemer, M. Mark, P. Waldburger, J. G. Danzl, C. Chin, B. Engeser, A. D. Lange, K. Pilch, A. Jaakkola, H.-C. Nägerl, and R. Grimm. Nature 440, 315 (2006).
[13] F. Ferlaino, S. Knoop, M. Berninger, W. Harm, J. P. D’Incao, H.-C. Nägerl, and R. Grimm. Phys. Rev. Lett. 102, 140401 (2009).
[14] S. E. Pollack, D. Dries, and R. G. Hulet. Science 326,
A. Zenesini, B. Huang, M. Berninger, S. Besler, H.-C. Nägerl, F. Ferlaino, R. Grimm, C. H. Greene, and J. von Stecher. [arXiv:1205.1921]

D. S. Petrov. Phys. Rev. A 67, 030703(R) (2003).

J. P. D’Incao and B. D. Esry. Phys. Rev. A 73, 030703(R) (2006).

J. P. D’Incao and B. D. Esry. Phys. Rev. A 73, 030702(R) (2006).

O. I. Kartavtsev and A. V. Malykh. J. Phys. B 40, 1429 (2007).

J. Levinsen and M. M. Parish. [arXiv:1207.0459]

J. Wang, J. P. D’Incao, B. D. Esry, and C. H. Greene. Phys. Rev. Lett. 105, 223201 (2010).

D. Blume and K. M. Daily. Phys. Rev. Lett. 105, 170403 (2010).

D. Blume and K. M. Daily. Phys. Rev. A 82, 063612 (2010).

J. P. D’Incao and B. D. Esry. Phys. Rev. A 73, 030702(R) (2006).

Y. Suzuki and K. Varga. Stochastic Variational Approach to Quantum Mechanical Few-Body Problems. Springer Verlag, Berlin (1998).

Y. Suzuki, W. Horiuchi, M. Orabi, and K. Arai. Few-Body Syst. 42, 33 (2008).

D. Rakshit, K. M. Daily, and D. Blume. Phys. Rev. A 85, 033634 (2012).

We fit a polynomial containing a constant, a linear and a quadratic term to the quantity $E_d/E_2$, where $E_2$ denotes the range-dependent two-body energy.

Y. Castin, C. Mora, and L. Pricoupenko. Phys. Rev. Lett. 97, 160404 (2006).

S. Endo, P. Naidon and M. Ueda. [arXiv:1203.4050] (2012).

E. Wille, F. M. Spiegelhalder, G. Kerner, D. Naik, A. Trenkwalder, G. Hendl, F. Schreck, R. Grimm, T. G. Tiecke, J. T. M. Walraven, S. J. J. M. F. Kokkelmans, E. Tiesinga, and P. S. Julienne. Phys. Rev. Lett. 100, 090405 (2008).

C. J. M. Mathy, M. M. Parish, and D. A. Huse. Phys. Rev. Lett. 106, 166404 (2011).

M. Iskin and C. A. R. Sá de Melo. Phys. Rev. Lett. 97, 100404 (2006).

M. Iskin and C. A. R. Sá de Melo. Phys. Rev. A 76, 013601 (2007).

Y. Nishida, D. T. Son, and S. Tan. Phys. Rev. Lett. 100, 090405 (2008).

M. Taglieber, A.-C. Voigt, T. Aoki, T. W. Hänsch, and K. Dieckmann. Phys. Rev. Lett. 100, 010401 (2008).

E. Wille, F. M. Spiegelhalder, G. Kerner, D. Naik, A. Trenkwalder, G. Hendl, F. Schreck, R. Grimm, T. G. Tiecke, J. T. M. Walraven, S. J. J. M. F. Kokkelmans, E. Tiesinga, and P. S. Julienne. Phys. Rev. Lett. 100, 090405 (2008).

B. H. Bransden and C. J. Joachain. Physics of Atoms and Molecules (2nd edition, Prentice Hall, 2003).