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DOI: [10.1103/PhysRevLett.108.073201](https://doi.org/10.1103/PhysRevLett.108.073201)
Efimov physics in heteronuclear four-body systems

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We study three- and four-body Efimov physics in a heteronuclear atomic system with three identical heavy bosonic atoms and one light atom. We show that exchange of the light atom between the heavy atoms leads to both three- and four-body features in the low-energy inelastic rate constants that trace to the Efimov effect. Further, the effective interaction generated by this exchange can provide an additional mechanism for control in ultracold experiments. Finally, we find that there is no true four-body Efimov effect — that is, no infinite number of four-body states in the absence of two- and three-body bound states — resolving a decades-long controversy.

PACS numbers:

Few-body physics has benefitted greatly from ultracold experiments on quantum gases in recent years. Many long-standing predictions have been verified and new phenomena identified due to the extraordinary ability to control and measure these systems. One of the more spectacular results for few-body physics was the observation of Efimov physics in Cs [1], experimentally validating Efimov’s surprising, 35-year old prediction [2] by confirming its predicted influence on three-body recombination [3]. Several measurements of Efimov physics have now been made [1, 4–13] and even include features traceable via theory [14] to four-body processes [10, 15].

One natural question to ask is whether there is an Efimov effect for $N>3$ bodies. The Efimov effect in this case is defined as the existence of an infinite number of $N$-body bound states when no subsystems are bound [16, 19]. Part of the answer was provided in Ref. [16]: there is no Efimov effect for $N>3$ equal mass particles. While generally interpreted to imply no Efimov effect is possible for $N>3$ (see, for example, [17]), this result does not preclude the possibility of an Efimov effect for systems with unequal masses. In fact, Ref. [18] recently reported that three identical fermions interacting resonantly with a fourth particle do have an Efimov effect for a small range of mass ratios. The question of an Efimov effect for $N=4$ with three identical bosons, however, remains open despite prior study: $H_3L$ systems ($H$ and $L$ are heavy and light particles, respectively) were analyzed in Ref. [19] with the conclusion that no Efimov effect occurs. When this system was revisited in Ref. [20], however, the opposite conclusion was reached.

In this Letter, we settle this controversy: there is no true four-body Efimov effect for $H_3L$ with bosonic $H$s. Although our conclusion is in agreement with Ref. [19], our reasoning is very different. We have, however, identified one universal four-body state [14, 24–26] attached to each three-body Efimov state. We also show that the low-energy scattering observables simultaneously display distinct three- and four-body features characteristic of the three-body Efimov effect. Moreover, we find that, in the context of ultracold collisions, the $s$-wave two-body scattering length $a_{HL}$ between $H$ and $L$ atoms can be used to tune the effective heavy-heavy scattering length $a_{HH}^*$ when $a_{HL}>0$, opening up new avenues for control in few-body systems.

Since an exact solution of the four-body problem remains a substantial challenge, we apply the Born-Oppenheimer (BO) approximation as described in Refs. [19, 20], assuming that the mass $m$ of $L$ is much less than the mass $M$ of $H$. Besides the practical benefit of reducing the four-body problem to a three-body problem, the BO approximation provides a useful conceptual framework and allows us to directly comment on the analysis in Refs. [19, 20]. Although we will focus on bosonic $H$s, our analysis can be generalized straightforwardly.

We first recall that the three-body Efimov effect occurs when at least two scattering lengths are much larger than a characteristic two-body interaction range $r_0$ [2] even in the heteronuclear case [37, 38]. Thus, for $H_2L$, Efimov physics will occur for $|a_{HL}|>|r_0$. Applying the BO approximation with $\rho$ the $H+H$ distance yields a BO potential with the universal long-range behavior $-\chi_0^2\hbar^2/2m\rho^2$, $\chi_0=0.567143$, in the region $r_0<\rho<|a_{HL}|$ [17, 21]. The three-body problem has thus been reduced to an effective two-body problem with scattering length $a_{HH}^*$. In the limit $|a_{HL}|\to\infty$, the Efimov region of this potential extends to infinity and supports an infinite number of Efimov states with the characteristic geometric relation between bound state energies [2]

$$E_{n+1}/E_n = e^{-2\pi/s_0}, \quad n = 0, 1, 2, ...$$  \hspace{1cm} (1)

where $s_0^2=\chi_0^2M/2m - 1/4$.

Similarly, all of the universal results [17] for low-energy three-body scattering apply to $H_2L$. For instance, when $a_{HL}>0$, there is a weakly bound $HL$ molecule, and $a_{HH}^*$ is the atom-diatom $H+HL$ scattering length [17],

$$a_{HH}^* \propto \cot[s_0\ln(a_{HL}/r_0) + \Phi]|a_{HL}|.$$  \hspace{1cm} (2)

The poles in $a_{HH}^*$ occur at those values of $a_{HL}$ when an Efimov state becomes bound, so their positions are characteristically log-periodic in $a_{HL}$. Their overall position,
however, is determined by the short-range three-body phase \( \Phi \) [3, 22, 39]. Equation (2) thus shows that \( a_{HL} \) provides a control over \( a_{HH}^* \) that could prove advantageous when \( a_{HH}^* \) cannot be easily be controlled directly via, for example, a Feshbach resonance [23].

In general, the \( H \)'s also interact directly. However, so long as the direct \( H + H \) interaction is short-ranged — even if it is repulsive — the large-potential surface that must behave as

\[
\Phi \equiv \frac{\rho}{L} + \kappa \rho^2 + \lambda \rho^4
\]

result for three bosons, we expect an Efimov effect for \( H_3L \) as long as the direct \( H + H \) interaction changes only \( E_0 \) (or, equivalently, \( \Phi \)) and not the characteristic log-periodic behavior. Consequently, manipulating the direct \( H + H \) interaction allows control of \( \Phi \) and thus the position of the family of log-periodic Efimov features.

Applying the BO approximation to \( H_3L \) reduces it to an effective three-body problem for \( H_3 \). We thus expect that our knowledge of Efimov physics and universality for three identical bosons should apply and provide at least a basic understanding of the system [19, 20]. For simplicity, we assume that the \( H \) atoms do not interact directly. Per the argument above, this assumption will not materially affect our conclusions. The \( H + H \) interaction then comes solely from mediation by the \( L \) and is characterized by the effective \( H + H \) scattering length \( a_{HH}^* \). Based on the result for three bosons, we expect an Efimov effect for \( H_3 \) when \( |a_{HH}^*| \to \infty \) [20].

To determine whether the \( |a_{HH}^*| \to \infty \) limit actually produces an Efimov effect for \( H_3L \), we adopt the following definition [16, 19]: a true four-body Efimov effect exists if the four-body system possesses an infinity of stable bound states when there is a zero-energy three-body bound state and no other two- or three-body bound states. Under these conditions, the four-body Efimov effect is completely independent of any three-body Efimov effect, making the resulting states fundamentally different from the universal four-body states discussed in Refs. [14, 24–26].

If it exists, a true four-body \( H_3L \) Efimov effect will occur for \( |a_{HH}^*| \to \infty \) and \( a_{HL} < 0 \). This case gives a zero-energy \( H_2L \) bound state but no \( HL \) bound state and is precisely the case identified in Ref. [19]. They concluded that no Efimov effect is possible because the BO potential surface has no long-range component. Naus and Tjon [20] correctly pointed out that it is not the BO potential surface that must behave as \(-R^{-2}\), but rather the adiabatic hyperspherical potential where the hyperradius \( R \) measures the overall size of the system (see, for example, Refs. [27, 28] for a discussion of hyperspherical coordinates in this context). They concluded that because \( |a_{HH}^*| \to \infty \), the conditions of the Efimov effect for \( H_3 \) are fulfilled and there is thus a four-body Efimov effect. Unfortunately, neither analysis provides a definitive answer.

Although otherwise sound, the argument of Ref. [20] is limited by its reliance on the BO approximation — a problem they identified but did not address. The issue with the BO approximation is that for \( a_{HL} < 0 \), \( L \) becomes unbound when \( \rho \geq |a_{HL}| \) [19], and its spectrum becomes continuous. Since a zero-energy \( L \) is no longer fast compared to the \( H \)'s, the BO approximation breaks down. Naus and Tjon dealt with this issue by following Ref. [19] and simply set the BO potential to zero for \( \rho \geq |a_{HL}| \). Under this questionable approximation, \( a_{HH}^* \) can be defined and adjusted to infinity, so that they conclude there is an infinite series of bound \( H_3L \) states, i.e. the four-body Efimov effect.

Where the BO approximation fails, however, the adiabatic hyperspherical approximation is perfectly valid, retaining a discrete spectrum for all \( R \). In particular, the lowest \( H_2L \) adiabatic hyperspherical potential coincides with the BO potential for \( R \leq |a_{HL}| \) and crosses zero energy at \( R \sim |a_{HL}| \) much like the BO potential [30]. For larger \( R \), the potential increases to a barrier [29] then falls to zero as \( l_{\text{eff}}(l_{\text{eff}}+1)\hbar^2/2M + l_{\text{eff}} = 3/2 \) [30, 31].

Having taken care to define the \( H_2L \) hyperradius \( R \) such that it reduces to the \( H + H \) distance \( \rho \) in the \( M/m \to \infty \) limit, we can regard this adiabatic hyperspherical potential as an effective \( H + H \) interaction. The \( l_{\text{eff}}=3/2 \) non-s-wave character of this potential, however, prevents the scattering length \( a_{HH}^* \) from even being defined. Consequently, in a dramatic breakdown of the BO approximation, there is no Efimov effect. This conclusion has been confirmed by direct calculation of the four-body adiabatic hyperspherical potentials for \( H_3L \) with \( M/m = 30 \) [32] using the correlated Gaussian approach [33].

Even though our finding no true four-body Efimov effect agrees with the conclusions of Ref. [19] and contradicts the conclusions of Ref. [20], we believe the former were right for the wrong reason and the latter underestimated the consequences of the breakdown of the BO approximation. In the end, it is this breakdown that excludes the possibility of a true four-body Efimov effect in this system.

**FIG. 1**: Schematic energy spectrum for \( H_3L \). Solid lines denote bound states and dashed lines denote resonances.
The possibility of true four-body Efimov states is not the only phenomenon of interest in $H_3 L$. Continuing to $a_{HL}>0$ such that $a_{HL} \gg r_0$, including $a_{HL} \to \infty$, the BO approximation displays no pathologies since $L$ is bound for all $H$ configurations, and we can safely think about the three-body $H_3$ motion on the lowest BO potential surface, which we take from Ref. [19]. Based on the known three-body results [17, 27, 34], we expect an adiabatic hyperspherical potential of the form

$$W_0 = -\frac{g_0^2}{2\mu R^2} + \frac{1}{2} \frac{\mu R}{\hbar^2}, \quad a_{HL} \ll R \ll |a_{HH}^*|,$$  

with $g_0=1.00624$ and $\mu=M/\sqrt{\pi}$ that approaches the three-body break-up threshold. In this case, that threshold corresponds physically to $HL+H+H$. The lower limit of $R$ in Eq. (3) is modified from the usual three-body problem [34] due to the fact that the characteristic range of the effective two-body $H+H$ potential is no longer $r_0$, but rather $a_{HL}$ as defined by the size of the $HL$ bound state.

When $a_{HL}$ is tuned to give $a_{HH}^* \to \infty$, the Efimov potential (3) extends to infinity, producing an infinite series of four-body bound states below the $HL+H+H$ threshold with binding energies $E_{n+1}/E_n=e^{-2\pi/g_0}$. These states are not true four-body Efimov states since there is an $HL$ bound state, but they can be regarded as three-body Efimov states of $HL+H+H$ much like the homonuclear equivalents discussed in Ref. [14, 17, 33]. They are indicated with the notation $(HL)H_2$ in Fig. 1 where the $H_2L+H$ and $HL+H+H$ thresholds intersect since $a_{HH}^* \to \infty$ at these points.

Figure 1 sketches the energy trajectories for $H_3 L$ as a function of $a_{HL}$. In addition to the $(HL)H_2$ Efimov states, there are the $H_2L$ Efimov states, and associated with each of the universal (highly excited) $H_2L$ states we find — for both $M/m=50$ and $M/m=30$ — one $H_2L$ state that appears to be the analog of the universal four-boson states in Refs. [14, 15, 24-26]. We find that its binding energy within our BO treatment is universally related to the binding energy of the associated $H_2L$ Efimov state by $E_{H_2L}/E_{H_2L} \approx 0.4$ for both of the mass ratios we have calculated. Note that the binding energies are defined relative to the next lowest breakup threshold ($HL+H+H$ for $H_2L$ states and $H_2L+H$ for $H_3 L$ states).

Figure 2 shows our numerically calculated three-body recombination rates $K_3$ for $HL+H+H \to H_2L+H$ with $M/m=30$ (see Ref. [28] for details of our numerical methods). Although there may be several final $H_2L$ Efimov states available, our calculation shows that recombination into the most weakly bound Efimov state dominates. In fact, the main peaks in Fig. 2(c) occur where an $H_2L$ Efimov state just becomes bound. The separation between the main peaks is thus determined by $s_0$ from the $H_2L$ Efimov effect: for $M/m=30$, $a_{HL}^{(2)}/a_{HL}^{(1)}=e^{\pi/s_0}=4.34$. Note that the adiabatic hyperspherical approach gives $e^{\pi/s_0}=3.96$ [34, 35], giving an indication of the BO approximation error for this mass ratio. For consistency, we will quote only BO results in the rest of this Letter. The factor of 5.5 between these two main peaks in Fig. 2 does not match this prediction because the criterion $a_{HL} \gg r_0$ is not well satisfied.

Since each main peak corresponds to a pole of $a_{HH}^*$, $K_3$ shows Efimov features characteristic of the $H_3$ motion where $a_{HH}^* /a_{HL} \gg a_{HL}$. When this condition is satisfied, the rates are given by the usual universal three-body expressions [17, 36] with the short-range length scale set to $a_{HL}$.

$$K_3^{(a_{HH}^*<0)} = \frac{C'}{\mu} \sin^2(\varphi_0) \left| a_{HH}^* \right|^4,$$

$$K_3^{(a_{HH}^*>0)} = \frac{C}{\mu} \sin^2(\varphi_0) \ln\left(\frac{a_{HH}^*/a_{HL}}{\Phi} + \sin^2(\varphi)\right) + \sin^2(\varphi_0)^2 \left( a_{HH}^* \right)^4.$$  

In these expressions, $C$ and $C'$ are universal constants. But, because the final $H_2L$ state is an Efimov state, $\Phi$, $\Phi'$ and $\eta$ depend not on short-range four-body physics, but rather on the short-range physics of the $H_2L$ states — no additional four-body parameter is needed [14, 24, 25]. The $a_{HH}^*/K_3$ projection in Fig. 3 supports this conclusion, showing that the Efimov features related to the $H_3$ motion described by Eq. (4) are approaching universal values of $a_{HH}^*/a_{HL}$ in the limit $a_{HL} \gg r_0$.

Interestingly, for larger mass ratios, $H_2L$ Efimov states with non-zero orbital angular momentum $j$ are possible [34, 35]. In this case, the universal constant $s_0$ in Eq. (1) is determined from $s_0^2=\chi_0^2 M/(2m-j(j+1))-1/4$, and there will be an Efimov effect for $H_2L$ so long as $s_0^2>0$. Higher angular momentum Efimov states have not yet been observed because experiments have focused mostly on identical particles which have no such states.
and because \( j > 0 \) Efimov states produce extremely narrow recombination peaks as seen in Fig. 3. The mass ratio in Fig. 3, \( M/m = 50 \), supports \( j = 2 \) Efimov states, but is not sufficient for higher \( j \) states. Because \( e_H = j \neq 0 \) for the \( H_2L \) system, there is no \((HL)H_2\) Efimov effect associated with these states. Their narrow \( K_3 \) peaks thus show no substrate of the sort seen on the main peaks.

The periods for each of the three different families of Efimov peaks are indicated in Fig. 3. Because none of the respective scattering lengths are strongly in the universal limit, however, the calculated periods do not match the predicted ones. The main \( j = 0 \) \( H_2L \) Efimov peaks highlighted by the \( a_{HL} - K_3 \) projection should have a period of \( e^{\pi/\eta_0} \approx 3.08 \). The calculated spacings are larger than this, but appear to be approaching the expected value as \( a_{HL} \) increases. Similarly, for \( j = 2 \), the expected period is 10.46 while the calculated one is 17.5, and the predicted period of the \((HL)H_2\) Efimov substructure on the main peaks highlighted in the \( a_{HH}^* - K_3 \) projection is \( e^{\pi/\eta_0} \approx 50 \). The magnitude of the deviations from the predictions likely reflects what can be observed since it is difficult to penetrate deeply into the universal regime experimentally.

So far, we have not taken advantage of all of the freedom that this heteronuclear system affords to manipulate the Efimov features. In particular, since \( a_{HH}^* \) depends only on the total \( H + H \) interaction, i.e. effective plus direct interactions, it can be tuned by either interaction — or both. Intriguingly, this freedom also allows experimental control of both \( a_{HL}^* \) and \( \Phi \) (or \( \Phi^* \)). Controlling the former via either \( a_{HL} \) or a direct interaction with scattering length \( a_{HH}^* \) allows the various Efimov features seen, for instance, in Figs. 2 and 3 to be mapped out. Controlling the latter makes it possible to shift all of these features — something not possible so far in three-body systems. Moreover, in the neighborhood of a pole in \( a_{HH}^* \), it should be possible to exert both types of control largely independently.

To illustrate the effect of tuning the direct interaction, we show in Fig. 4 the numerically calculated rates for the relaxation process \( H_2L(n)+H \rightarrow H_2L(n-1)+H \) as a function of \( a_{HH}^* \) where \( n \) labels the most weakly bound \( H_2L \) state. This tuning was accomplished by including a short-range, direct \( H + H \) interaction in addition to an effective \( H + H \) interaction. The behavior of \( V_{rel} \) in Fig. 4 is also found in the three-boson system. In fact, when \( a_{HH}^* \gg a_{HL} > 0 \), \( V_{rel} \) has the same form as in three-boson systems \[ 17 \]

\[
V_{rel}^{(a_{HH}^* > 0)} = \frac{A \sinh 2\eta}{\sin^2 \left[ \ln(a_{HH}^*/a_{HL}) + \Phi \right] + \sinh^2 \eta a_{HH}^*},
\]

where \( A \) is a universal constant, but \( \eta \) and \( \Phi \) depend on the short-range details of the relaxed \( H_2L \) bound state — although not on a separate four-body parameter.

To conclude, we have studied Efimov physics in the four-body heteronuclear system \( H_3L \) with bosonic \( H \) atoms, showing that there is no true four-body Efimov effect. We have, however, identified a universal four-body heteronuclear system — although not on a separate four-body parameter. We have, however, identified a universal four-body heteronuclear system — although not on a separate four-body parameter.
We thank C.H. Greene for critical and stimulating discussions of the four-body Efimov effect. This work was supported in part by the National Science Foundation and in part by the Air Force Office of Scientific Research. Y. W. also acknowledges support from the National Science Foundation under Grant No. PHY0970114.
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