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Origin of the Three-body Parameter Universality in Efimov Physics

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In recent years extensive theoretical and experimental studies of universal few-body physics have advanced our understanding of universal Efimov physics. Whereas theory had been the driving force behind our understanding of Efimov physics for decades, recent experiments have contributed an unexpected discovery. Specifically, measurements have found that the so-called *three-body parameter* determining several properties of the system is universal, even though fundamental assumptions in the theory of the Efimov effect suggest that it should be a variable property that depends on the precise details of the short-range two- and three-body interactions. The present Letter resolves this apparent contradiction by elucidating previously unanticipated implications of the two-body interactions. Our study shows that the three-body parameter universality emerges because a universal effective barrier in the three-body potentials prevents the three particles from simultaneously getting close together. Our results also show limitations on this universality, as it is more likely to occur for neutral atoms but less likely to extend to light nuclei.

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In the early 70's, Vitaly Efimov predicted a strikingly counterintuitive quantum phenomenon [1], today known as the Efimov effect: in three-body systems for which the two-body s-wave scattering length a is much larger than the characteristic range r_0 of the two-body interaction, an infinite number of three-body bound states can be formed even when the short-range two-body interactions are too weak to bind a two-body state (a < 0). The Efimov effect, once considered a mysterious and esoteric effect, is today a reality that many experiments in ultracold quantum gases have successfully observed and continue to explore [2–14].

One of the most fundamental assumptions underlying our theoretical understanding of this peculiar effect is that the weakly bound three-body energy spectrum, and other low-energy three-body scattering observables, should depend on a three-body parameter that encapsulates all details of the interactions at short distances [15]. So, while these details are critical in determining the deeply bound three-body spectrum often of interest to spectroscopists, they only enter ultracold properties through this single parameter [15]. Because of its connection to these short-range details, the three-body parameter has been viewed as nonuniversal since its value for any specific system was expected to depend on the precise details of the underlying two- and three-body interactions [16–18].

In nuclear physics, this picture seems to be consistent, i.e., properties of three-body weakly bound states are sensitive to the nature of the two- and three-body short-range interactions [17]. More recently, however, Berninger *et al.* [3] have experimentally explored this issue for alkali atoms whose scattering lengths are magnetically tuned near different Fano-Feshbach resonances [19]. Even though the short-range physics can be expected to vary from one resonance to another, Efimov resonances were found for values of the magnetic field at which $a=a_{3b}^{-}=-9.1(2)r_{vdW}$, where r_{vdW} is the van der Waals length [20, 21]. Therefore, in each of these cases, the three-body parameter was approximately the same, thus challenging a fundamental assumption of the universal theory. Even more striking has been the observation that the Efimov resonance positions obtained for ³⁹K [4], ⁷Li [5–7], ⁶Li [8–11], and ⁸⁵Rb [12] were also measured to be consistent with values of a_{3b}^-/r_{vdW} found for ¹³³Cs [3]. (Note that the work in Ref. [7] also provided early suggestive evidence of such universal behavior.) These observations provide strong evidence that the three-body parameter has universal character for spherically-symmetric neutral atoms, and therefore suggest that *something else* beyond the universal theory needs to be understood.

This Letter precisely identifies the physics beyond the universal theory that explains the universality of the three-body parameter, and presents theoretical evidence to support the recent experimental observations. Previous work has shown that the three-body parameter can be universal — that is, independent of the details of the interactions — in three-polar-molecule systems [22] and in three-atom systems near narrow Fano-Feshbach resonance [23, 24], although recent work has shown that the latter case likely requires even more finely-tuned conditions [25]. Our present numerical analysis, however, adds another, broader class of systems with a universal three-body parameter: systems with two-body interactions that efficiently suppress the probability to find any pair of particles separated by less than r_0 . This class of systems, therefore, is more closely related to systems near broad Fano-Feshbach resonances [19].

Such a suppression could derive from the usual classical suppression of the probability for two particles to exist between r and r + dr in regions of high *local* velocity $\hbar k_L(r)$, which is proportional to $[mdr/\hbar k_L(r)]$ (m being the particle mass), the time spent classically in that interval dr (see Ref. [26]). It is possible that there could be an additional suppression as well, through quantum reflec-

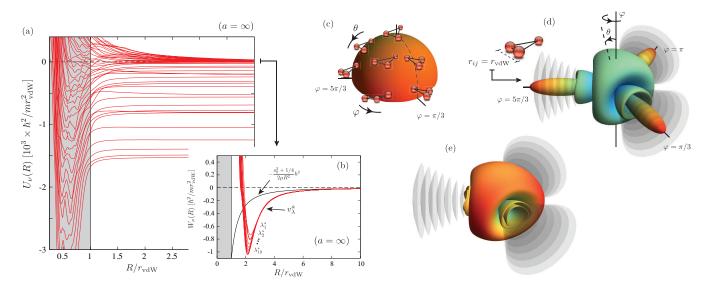


FIG. 1: (a) The full energy landscape for the three-body potentials at $a = \infty$ for our v_{λ}^{a} model potential. (b) effective diabatic potentials W_{ν} relevant for Efimov physics for v_{λ}^{a} with an increasingly large number of bound states (λ_{n}^{*} is the value of λ that produces $a = \infty$ and n s-wave bound states). W_{ν} converge to a universal potential displaying the repulsive barrier at $R \approx 2r_{\rm vdW}$ that prevents particles access to short distances. (c)-(e) demonstrate the suppression of the wave function inside the potential well through the channel functions $\Phi_{\nu}(R; \theta, \varphi)$ for R fixed near the minima of the Efimov potentials in (b). (c) shows the mapping of the geometrical configurations onto the hyperangles θ and φ . (d) and (e) show the channel functions, where the "distance" from the origin determines $|\Phi_{\nu}|^{1/2}$, for two distinct cases: in (d) when there is a substantial probability to find two particles inside the potential well (defined by the region containing the gray disks) and in (e) with a reduced probability — see also our discussion in Fig. 2. In (d) and (e), we used the potentials $v_{\rm sch}$ and v_{λ}^{a} , respectively, both with n = 3.

tion from a potential *cliff* [27]. Systems supporting many bound states, such as the neutral atoms used in ultracold experiments with their strong van der Waals attraction, clearly exhibit this suppression. In general, a finite-range two-body potential that supports many bound states decreases steeply with decreasing interparticle distance r, starting when $r/r_{\rm vdW} \lesssim 1$, at which point the potential cliff plays a role analogous to a repulsive potential for low-energy scattering. We demonstrate this fact by showing that the three-body parameter in the presence of many two-body bound states roughly coincides with that for a 100% reflective two-body model potential, where the two-body short-range potential well is replaced by a hard-sphere.

The starting point for our investigation of the universality of the three-body parameter is the adiabatic hyperspherical representation [18, 28]. This representation offers a simple and conceptually clear description by reducing the problem to the solution of the "hyperradial" Schrödinger equation :

$$\begin{bmatrix} -\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + W_{\nu}(R) \end{bmatrix} F_{\nu}(R) + \sum_{\nu' \neq \nu} W_{\nu\nu'}(R) F_{\nu'}(R) = EF_{\nu}(R). \quad (1)$$

Here, the hyperradius R describes the overall size of the system; ν is the channel index; $\mu = m/\sqrt{3}$ is the three-body reduced mass for particle masses m; E is the total energy; and F_{ν} is the hyperradial wave function. The nonadiabatic couplings $W_{\nu\nu'}$ drive inelastic transitions, and the effective hyperradial potentials W_{ν} support bound and resonant states. To treat problems with deep two-body interactions — necessary to see strong insidethe-well suppression — requires us to solve Eq. (1) for two-body model interactions that support many bound states, a challenge for most theoretical approaches. Using our recently developed methodology [29], however, we have treated systems with up to 100 two-body rovibrational bound states and have solved Eq. (1) beyond the adiabatic approximation. Here, the universality of the three-body parameter is analyzed for a number of model potentials, one of then being the usual Lennard-Jones potential:

$$v_{\lambda}^{a}(r) = -\frac{C_{6}}{r^{6}} \left(1 - \lambda^{6}/r^{6}\right),$$
 (2)

where λ is adjusted to give the desired value of a and number of bound states. The other short-ranged potential models used here, namely, $v_{\rm sch}$, v_{λ}^{b} and $v_{\rm vdW}^{\rm hs}$, can be found in Ref. [26].

Figure 1 (a) shows the adiabatic potentials U_{ν} at $|a| = \infty$ obtained using the potential v_{λ}^{a} above supporting 25 dimer bound states. At first glance, it is difficult to identify any universal properties of these potentials. Efimov physics, however, occurs at a very small energy scale near the three-body breakup threshold. Indeed, a closer analysis of the energy range $|E| < \hbar^2/mr_{\rm vdW}^2$ [Fig. 1 (b)]

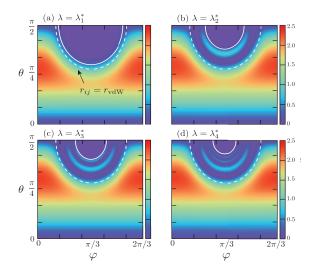


FIG. 2: Density plot of the three-body probability density $|\Phi_{\nu}(R;\theta,\varphi)|^2 \sin 2\theta$ which determines the three particle configuration [see Fig. 1 (c)] in the θ - φ hyperangular plane for a fixed R (sin 2θ is the volume element). (a)–(d) show the results for an R near the minima of the Efimov potentials in Fig. 1 (b) for the first four scattering length poles of the v_{λ}^{a} model as indicated. (a) shows that there is a negligible probability to find the particles at distances smaller than $r_{\rm vdW}$ (outer dashed circle) and, of course, inside the $1/r^{12}$ repulsive barrier (inner solid circle). For higher poles, i.e., as the strength of the hard-core part of v_{λ}^{a} potential decreases, the potential becomes deeper and penetration into the region $r < r_{\rm vdW}$ is now classically allowed. Nevertheless, (b)–(e) show that inside-the-well suppression still efficiently suppresses the probability to find particle pairs at distances $r < r_{\rm vdW}$, found to be in the range 2%-4%.

reveals the universal properties of the key potential curve controlling Efimov physics.

Figure 1 (b) shows one of our most important pieces of theoretical evidence for the three-body parameter universality: the effective adiabatic potentials W_{ν} obtained us- $\log v_{\lambda}^{a}$ for more and more two-body bound states converge to a single universal curve. [In some cases in Fig. 1 (b) we have manually diabatized W_{ν} near sharp avoided crossings in order to improve the visualization.] As one would expect, the usual Efimov behavior for the effective potentials, $W_{\nu} = -\hbar^2 (s_0^2 + 1/4)/2\mu R^2$ with $s_0 \approx 1.00624$, is recovered for $R > 10r_{\rm vdW}$. It is remarkable, however, that the W_{ν} also converge to a universal potential curve for $R < 10r_{\rm vdW}$ and, more importantly, these effective potentials display a repulsive wall or barrier at $R \approx 2r_{\rm vdW}$. This barrier prevents the close collisions that would probe the small R nonuniversal three-body physics, including three-body forces known to be important in chemistry, thus producing the three-body parameter universality as we confirm below. This is in fact our most striking result: a sharp cliff or attraction in the twobody interactions produces a strongly repulsive universal barrier in the effective three-body interaction potential.

Qualitatively, this universality derives from the re-

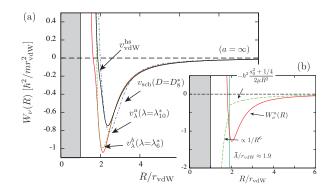


FIG. 3: (a) The Efimov potential obtained from the different two-body potential models used here. The reasonably good agreement between the results obtained using models supporting many bound states $(v_{\rm sch}, v_{\lambda}^{a} \text{ and } v_{\lambda}^{b})$ and $v_{\rm vdW}^{\rm hs}$ [obtained by replacing the deep potential well with a hard wall but having only one (zero-energy) bound state] supports our conclusion that the inside-the-well suppression of the wave function is the main physical mechanism behind the universality of the three-body effective potentials. The differences between these potentials are seen to cause differences of a few percent in the three-body parameter. (b) Comparison between the effective potential proposed by Ref. [39] (green dashed curve) and the one (red solid curve) constructed to describe our findinings: $2\mu r_{\rm vdW}^2 W_{\nu}^{(u)}(R)/\hbar^2 \approx -(s_0^2 + 1/4)/X^2 - b_3/X^3 - b_4/X^4 - b_5/X^5 + b_{16}/X^{16}$, where $X = R/r_{\rm vdW}$ and $b_3 = 2.334, b_4 = 1.348, b_5 = 44.52, b_6 = 4.0 \times 10^4$.

duced probability to find particles inside the attractive two-body potential well. This effect is clear from the channel functions Φ_{ν} [18, 28], in Figs. 1 (c)-(e) and the hyperangular probability densities in Fig. 2. In the adiabatic hyperspherical representation, the space forbidden to the particles fills an increasingly larger portion of the hyperangular volume as R decreases. This evolution can be visualized as the dashed lines in Fig. 2 (a)–(d) expanding outward. In the process, the channel function Φ_{ν} is squeezed into an increasingly small volume, driving its kinetic energy higher and producing the repulsive barrier in the universal Efimov potential. Moreover, this suppression implies that the details of the interaction should be largely unimportant. Consequently, different two-body model potentials should give similar three-body potentials. Figure 3 (a) demonstrates this universality by comparing W_{ν} obtained from different potential models supporting many bound states. Perhaps more importantly, it compares them with the results obtained from the twobody model $v_{\text{vdW}}^{\text{hs}}$ that replaces the deep well by a hard wall, essentially eliminating the probability of observing any pair of atoms at short distances. Quantitatively, however, the fact that the barrier occurs only at $R \approx 2r_{\rm vdW}$ indicates that universality might not be as robust as in the cases discussed in Refs. [22–25]. It is thus important to quantify the value of the three-body parameter to assess the size of nonuniversal effects.

In principle, the three-body parameter could be defined in terms of *any* observable related to the Efimov

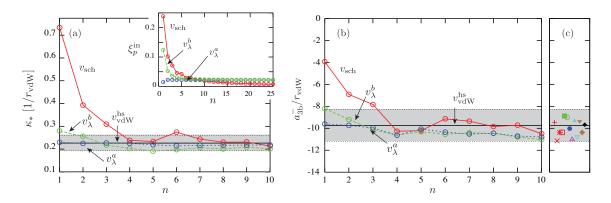


FIG. 4: Values for the three-body parameter (a) κ_* and (b) a_{3b}^- as functions of the number *n* of two-body *s*-wave bound states for each of the potential model studied here. (c) Experimental values for a_{3b}^- for 133 Cs [3] (red: $\times, +, \square$, and *), 39 K [4] (magenta: \triangle), 7 Li [5] (blue: •) and [6, 7] (green: \blacksquare and °), 6 Li [8, 9] (cyan: \blacktriangle and ∇) and [10, 11] (brown: \checkmark and \diamond), and 85 Rb [12] (black: \blacklozenge). The gray region specifies a band where there is a $\pm 15\%$ deviation from the v_{vdW}^{hs} results. The inset of (a) shows the suppression parameter ξ_p^{in} [Eq. (S.5) in Ref. [26]] which can be roughly understood as the degree of sensitivity to nonuniversal corrections. Since ξ_p^{in} is always finite — even in the large *n* limit — nonuniversal effects associated with the details of the short-range interactions can still play an important role. One example is the large deviation in κ_* found for the v_{sch} (n = 6) model, caused by a weakly bound *g*-wave state. For n > 10 we expect κ_* and a_{3b}^- to lie within the range of $\pm 15\%$ established for $n \leq 10$.

physics [15]. Two of its possible definitions are [15]: the value of $1/a = 1/a_{3b}^- < 0$ at which the first Efimov resonance appears in three-body recombination (see for instance Ref. [30]) and $\kappa_* = (m|E_{3b}^0|/\hbar^2)^{1/2}$, where E_{3b}^0 is the energy of the lowest Efimov state at $|a| \to \infty$. Our numerical results for κ_* and a_{3b}^- are shown in Figs. 4(a) and (b), respectively, demonstrating their universality in the limit of many bound states. In fact, the values for κ_* and a_{3b}^- in this limit differ by no more than 15% from the $v_{\rm vdW}^{\rm hs}$ results — $\kappa_* = 0.226(2)/r_{\rm vdW}$ and $a_{3\rm b}^- = -9.73(3)r_{\rm vdW}$ [solid black line in Fig. 4(a) and (b)] — indicating, once again, that the universality of the three-body parameter is dependent upon the suppression of the probability density within the two-body potential wells. Given this picture, we attribute the non-monotonic behavior of κ_* and a_{3b}^- in Fig. 4 to the small but finite probability to reach short distances, which brings in nonuniversal effects related to the details of two- and three-body forces, including occasional interactions with an isolated perturbing channel. Nevertheless, our results for a_{3b}^- are consistent with the experimentally measured value for 133 Cs [2, 3], 39 K [4], ⁷Li [5–7], ⁶Li [8–11, 31], and 85 Rb [12], all of which lie within about 15% of the $v_{\rm vdW}^{\rm hs}$ result. The average of the experimental values differs from the present $v_{\rm vdW}^{\rm hs}$ result by less than 3%.

Previous treatments have failed to predict the universality of the three-body parameter for various reasons. In treatments using zero-range interactions, for instance, the three-body parameter enters as a free parameter to cure the Thomas collapse [32], preventing any statement about its universality. Finite range models devoid of a van der Waals tail, like those used in some of our own treatments [18] [corresponding to the results for $v_{\rm sch}$ with n = 2 and 3 in Figs. 4 (a) and (b)], have failed for lack of substantial suppression of the probability density in the two-body wells. Such models, however, are more appropriated to describe light nuclei having few bound states and shallow attraction. In contrast to Ref. [18], other models [24, 33–38] have found better agreement with experiments. Our analysis of these treatments, however, indicates that the two-body models used have many of the characteristics of our $v_{\rm vdW}^{\rm hs}$, therefore satisfying the prerequisite for a universal three-body parameter. A recent attempt [39] to explain this universality using an *ad hoc* hyperradial potential that bore little resemblance to ours [see Fig. 3 (b)]. This *ad hoc* three-body potential displayed strong attraction at short distances in contrast to our key finding, which to reiterate, is that a cliff of attraction for two bodies produces a universal *repulsive* barrier in the three-body system.

In summary, our theoretical examination shows that the three-body parameter controlling much of universal Efimov physics can also be a universal parameter under certain circumstances which should be realized in most ultracold neutral atom experiments. Provided the underlying two-body short-range interaction supports a large number of bound states, or it has some other property leading to the suppression of the wave function at short distances, three-body properties associated with Efimov physics can be expected to be universal. This surprising new scenario could not have been, and was not, anticipated from the simple model calculations to date. Ironically, increasing the complexity of the model simplified the outcome by effectively eliminating the impact of the deeply bound two- and three-body states on the low-energy bound and scattering three-body observables. That is, the three-body parameter becomes largely universal.

Acknowledgments

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