Universal equation for Efimov states

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Efimov states are a sequence of shallow three-body bound states that arise when the two-body scattering length is large. Efimov showed that the binding energies of these states can be calculated in terms of the scattering length and a three-body parameter by solving a transcendental equation involving a universal function of one variable. We calculate this universal function using effective field theory and use it to describe the three-body system of ^{4}He atoms. We also extend Efimov's theory to include the effects of deep two-body bound states, which give widths to the Efimov states.

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The interactions of nonrelativistic particles (such as atoms) with short-range interactions at extremely low energies are determined primarily by their S-wave scattering length a. If $|a|$ is much larger than the characteristic range l of their interaction, low-energy atoms exhibit universal properties that are insensitive to the details of the interaction potential. In the two-body sector, the universal properties are simple and familiar. The differential cross section for two identical bosons with relative wave number $k \ll 1/l$ and mass m is $d\sigma/d\Omega = 4a^2/(1+k^2 a^2)$. If $a>0$, there is also a shallow two-body bound state (the dimer) with binding energy $B_2 = \hbar^2/ma^2$. In the three-body sector, there are also universal properties that were first deduced by Efimov [1]. The most remarkable is the existence of a sequence of three-body bound states with binding energies geometrically spaced in the interval between $\hbar^2/ma^2$ and $\hbar^2/ml^2$. The number of these "Efimov states" is roughly $\ln(|a|/l)/\pi$ if $|a|$ is large enough. In the limit $|a| \to \infty$, there is an accumulation of infinitely many three-body bound states at threshold (the "Efimov effect"). The knowledge of the Efimov binding energies is essential for understanding the energy dependence of low-energy three-body observables. For example, Efimov states can have dramatic effects on atom-dimer scattering if $a>0$ [1,2] and on three-body recombination if $a<0$ [3,4].

A large two-body scattering length can be obtained by fine-tuning a parameter in the interatomic potential to bring a real or virtual two-body bound state close to the two-atom threshold. The fine-tuning can be provided accidentally by nature. An example is the ^{4}He atom, whose scattering length $a = 104$ Å [5] is much larger than the effective range $l \approx 7$ Å. Another example is the two-nucleon system in the $^3S_1$ channel, for which the deuteron is the shallow bound state. This system provided the original motivation for Efimov's investigations [1]. In the case of atoms, the fine-tuning can also be obtained by tuning an external electric field [6] or by tuning an external magnetic field to the neighborhood of a Feshbach resonance [7]. Such resonances have, e.g., been observed for ^{23}Na and ^{85}Rb atoms [8] and are used to tune the interactions in Bose-Einstein condensates. An important difference from He is that the interatomic potentials for Na and Rb support many deep two-body bound states.

Efimov derived some powerful constraints on low-energy three-body observables for systems with large scattering length [1]. They follow from the approximate scale invariance at length scales R in the region $l \ll R \ll |a|$ and the conservation of probability. He introduced polar variables H and ξ in the plane whose axes are $1/a$ and the energy variable $\mathrm{sgn}(E)|mE|^{1/2}/\hbar$, and showed that low-energy three-body observables are determined by a few universal functions of the angle ξ. In particular, the binding energies of the Efimov states are solutions to a transcendental equation involving a single universal function of ξ [1]. In this paper, we calculate this universal function for the case of three identical bosons and apply Efimov's equation to the ^{4}He trimer. We also extend Efimov theory to atoms with deep two-body bound states.

The existence of Efimov states can easily be understood in terms of the equation for the radial wave function $f(R)$ in the adiabatic hyperspherical representation of the three-body problem [9,10]. The hyperspherical radius for three identical atoms with coordinates $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ is $R^2 = (r_{12}^2 + r_{13}^2 + r_{23}^2)/3$, where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. If $|a| \gg l$, the radial equation for three atoms with total angular momentum zero reduces in the region $l \ll R \ll |a|$ to

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial R^2} + \frac{s_0^2 + 1/4}{R^2}\right] f(R) = E f(R), \tag{1}$$

where $s_0 \approx 1.00624$. This looks like the Schrödinger equation for a particle in a one-dimensional, scale-invariant $1/R^2$ potential. If we impose a boundary condition on $f(R)$ at short distances of order l, the radial equation (1) has solutions at discrete negative values of the eigenvalue $E = -B_3$, with B_3 ranging from order $\hbar^2/ml^2$ to order $\hbar^2/ma^2$. The corresponding eigenstates are called Efimov states. As $|a| \to \infty$, their spectrum approaches the simple law $B_3^{(n)} \sim 515^n \hbar^2/ma^2$.

Efimov's constraints can be derived by constructing a solution to Eq. (1) that is valid in the region $l \ll R \ll |a|$. In the case of a bound state with energy $E = -B_3$, the radial variable is $H^2 = mB_3/\hbar^2 + 1/a^2$ and the angular variable ξ is

$$\xi = -\arctan(a\sqrt{mB_3}/\hbar) - \pi\theta(-a), \tag{2}$$

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where $\theta(x)$ is the unit step function. Since we are interested in low energies $|E| \sim \hbar^2/ma^2$, the energy eigenvalue in Eq. (1) can be neglected. The most general solution therefore has the form [1]

$$f(R) = \sqrt{HR}[Ae^{is_0 \ln(HR)} + Be^{-is_0 \ln(HR)}], \qquad (3)$$

which is the sum of outgoing and incoming hyperspherical waves. The dimensionless coefficients A and B can depend on ξ. At shorter distances $R \sim l$ and longer distances $R \sim |a|$, the wave function becomes very complicated. Fortunately, we can avoid solving for it by using simple considerations based on unitarity [1].

We first consider the short-distance region. Efimov assumed implicitly that there are no deep two-body bound states with binding energies $B \gg \hbar^2/ma^2$. Thus the two-body potential supports no bound states at all if $a<0$ and only the dimer with binding energy $B_2 = \hbar^2/ma^2$ if $a>0$. We will address the complication of deep two-body bound states later. The probability in the incoming wave must then be totally reflected by the potential at short distances, so we can set $B = Ae^{i\theta}$. The phase θ can be specified by giving the logarithmic derivative $R_0 f'(R_0)/f(R_0)$ at any point $l \ll R_0 \ll |a|$. The resulting expression for θ has a simple dependence on H:

$$\theta/2 = s_0 \ln(H/c\Lambda_*). \qquad (4)$$

The denominator $c\Lambda_*$ is a complicated function of R_0 and $R_0 f'(R_0)/f(R_0)$. It differs by an unknown constant c from the three-body parameter Λ_* introduced in Ref. [2].

We next consider large distances $R \sim |a|$. In general, an outgoing hyperspherical wave incident on the $R \sim |a|$ region can either be reflected or else transmitted to $R \to \infty$ as a three-atom or atom-dimer scattering state. The reflection and transmission amplitudes are described by a dimensionless unitary 3×3 matrix that is a function of ξ only. For $-\pi<\xi<-\pi/4$, scattering states with $R\to\infty$ are kinematically not allowed. The probability is therefore totally reflected, so we must have $B = Ae^{i\Delta(\xi)}$, where the phase Δ depends on the angle ξ. Compatibility with the constraint from short distances requires $\theta = \Delta(\xi) \bmod 2\pi$. Using Eq. (4) for θ and inserting the expression for H, we obtain Efimov's equation [1]

$$B_3 + \frac{\hbar^2}{ma^2} = \frac{\hbar^2\Lambda_*^2}{m}\; e^{2\pi n/s_0} \exp[\Delta(\xi)/s_0], \qquad (5)$$

where ξ is given by Eq. (2) and the constant c was absorbed into $\Delta(\xi)$. Note that we measure B_3 from the three-atom threshold and Λ_* is only defined up to factors of $\exp[\pi/s_0]$. Once the universal function $\Delta(\xi)$ is known, the Efimov binding energies B_3 can be calculated by solving Eq. (5) for different integers n. This equation has an exact discrete scaling symmetry: if there is an Efimov state with binding energy B_3 for the parameters a and Λ_*, then there is also an Efimov state with binding energy $\lambda^2 B_3$ for the parameters $\lambda^{-1}a$ and Λ_* if $\lambda = \exp[n'\pi/s_0]$ with n' an integer.

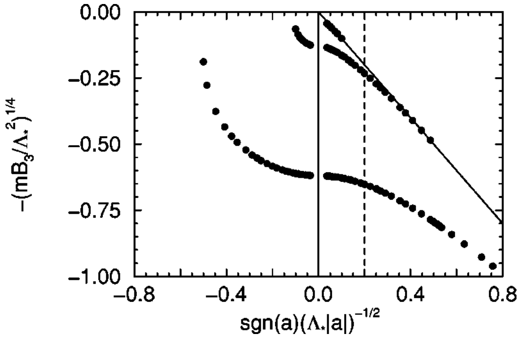

FIG. 1. The energy variable $-(mB_3/\hbar^2\Lambda_*^2)^{1/4}$ for three shallow Efimov states as a function of $\mathrm{sgn}(a)(\Lambda_*|a|)^{-1/2}$.

The universal function $\Delta(\xi)$ could be determined by solving the three-body equation for the Efimov binding energies in various potentials whose scattering lengths are so large that effective range corrections are negligible. It can be calculated more easily by using the effective field theory (EFT) of Ref. [2] in which the effective range can be set to zero. In Ref. [2], the dependence of the binding energy on a and Λ_* was calculated for the shallowest Efimov state and $a>0$. In order to extract the universal function $\Delta(\xi)$, we have calculated the binding energies of the three lowest Efimov states for both signs of a. In Fig. 1, we plot $-(mB_3/\hbar^2\Lambda_*^2)^{1/4}$ as a function of $\mathrm{sgn}(a)(\Lambda_*|a|)^{-1/2}$ for these three branches of Efimov states. The binding energies for deeper Efimov states and for shallower states near $(\Lambda_*|a|)^{-1/2}=0$ can be obtained from the discrete scaling symmetry. A given two-body potential is characterized by values of a and Λ_* and corresponds to a vertical line in Fig. 1, such as the dashed line shown. The intersections of this line with the binding energy curves correspond to the infinitely many Efimov states. Those states with $B_3 \gtrsim \hbar^2/ml^2$ are unphysical. For $B_3\to\infty$, the angle ξ goes to $-\pi/2$. The ratio of the binding energies of successive Efimov states therefore approaches $\exp[2\pi/s_0]\approx 515$. However, for the shallowest Efimov states, this ratio exhibits significant deviations from the asymptotic value. If $a>0$, there is an Efimov state at the atom-dimer threshold $B_3 = \hbar^2/ma^2$ when $s_0 \ln(a\Lambda_*) = 1.444 \bmod \pi$. The sequence of binding energies B_3 in units of $\hbar^2/ma^2$ is 1, 6.8, 1.4×10^3, ... Consequently, the ratio of B_3 for the two shallowest Efimov states can range from 6.8 to 210. If $a<0$, there is an Efimov state at the three-atom threshold $B_3=0$ when $s_0 \ln(a\Lambda_*) = 1.378 \bmod \pi$. The sequence of binding energies B_3 in units of $\hbar^2/ma^2$ is 0, 1.1×10^3, 6.0×10^5, ... Thus, the ratio of B_3 for the two shallowest Efimov states can range from ∞ to 550.

Using Eq. (5) with $n=0$, we have extracted the universal function $\Delta(\xi)$ from the data for the middle branch in Fig. 1. The extracted values of $\Delta(\xi)$ are given in Table I. An analytic expression for $\Delta(\xi)$ is not known, but we can obtain parametrizations in various regions of ξ by fitting the data:

$$\xi \in \left[-\frac{3\pi}{8}, -\frac{\pi}{4}\right]: \Delta = 3.10x^2 - 9.63x - 2.18, \qquad (6)$$

TABLE I. The values of the universal function $\Delta(\xi)$.

ξ	$\Delta(\xi)$	ξ	$\Delta(\xi)$	ξ	$\Delta(\xi)$
−0.785	−2.214	−0.965	−5.712	−1.482	−8.009
−0.787	−2.539	−1.019	−6.123	−1.502	−8.059
−0.791	−2.897	−1.065	−6.415	−1.651	−8.373
−0.797	−3.194	−1.104	−6.634	−1.681	−8.427
−0.804	−3.448	−1.166	−6.943	−1.745	−8.534
−0.820	−3.864	−1.214	−7.151	−1.817	−8.641
−0.836	−4.196	−1.296	−7.461	−1.988	−8.843
−0.852	−4.469	−1.347	−7.632	−2.197	−9.009
−0.868	−4.701	−1.408	−7.814	−2.395	−9.095
−0.899	−5.076	−1.443	−7.910	−2.751	−9.110
−0.933	−5.434				

$$\xi \in \left[-\frac{5\pi}{8}, -\frac{3\pi}{8}\right]: \Delta = 1.17y^3 + 1.97y^2 + 2.12y - 8.22, \tag{7}$$

$$\xi \in \left[-\pi, -\frac{5\pi}{8}\right]: \Delta = 0.25z^2 + 0.28z - 9.11, \tag{8}$$

where $x=(-\pi/4-\xi)^{1/2}$, $y=\pi/2+\xi$, and $z=(\pi+\xi)^2 \exp[-1/(\pi+\xi)^2]$. These parametrizations deviate from the numerical results in Table I by less than 0.013. The discontinuity at $\xi=-3\pi/8$ and $\xi=-5\pi/8$ is less than 0.016. This accuracy is sufficient for most practical calculations using Eq. (5).

Universality can be exploited to greatly reduce the calculational effort required to predict three-body observables for atoms with large a. The observables can be calculated once and for all as functions of a and Λ_* either by using the EFT or by solving the Schrödinger or Faddeev equation with various methods. The binding energies obtained by solving Efimov's equation (5) are shown in Fig. 2. Simple expressions can be given for other observables, such as the S-wave atom-dimer scattering length:

$$a_{12} = a\{1.46 - 2.15 \tan[s_0 \ln(a\Lambda_*) + 0.09]\}, \tag{9}$$

as well as the phase shifts and the rate constant for three-body recombination at threshold [11]. Given a and a measured or calculated value of B_3 for one Efimov state as input, one can read off Λ_* from Fig. 2. Predictions for other three-body observables, such as the atom-dimer scattering length in Eq. (9), are then immediate.

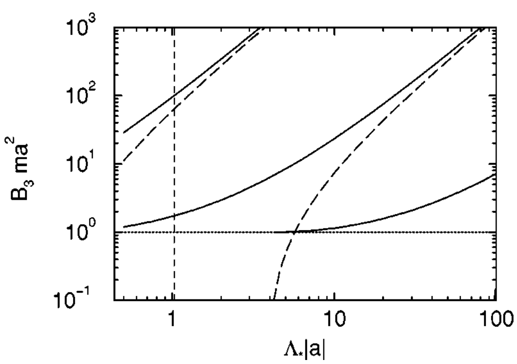

FIG. 2. The Efimov binding energies $B_3 m a^2/\hbar^2$ as a function of $|a|\Lambda_*$ for $a>0$ (solid lines) and $a<0$ (dashed lines). Vertical dashed line gives $|a|\Lambda_*$ for LM2M2/TTY potentials (cf. Ref. [15]). The horizontal dotted line is the atom-dimer threshold ($a>0$).

TABLE II. The values of B_2, $B_3^{(0)}$, $B_3^{(1)}$, and a_{12} for four model potentials from Ref. [15], the value of $a_B\Lambda_*$ determined from $B_3^{(1)}$, and the predictions for $B_3^{(0)}$ from Eq. (5) and a_{12} from Eq. (9). All energies (lengths) are given in mK (Å). ($\hbar^2/m = 12.12$ K Å^2 for ^{4}He.)

Potential	B_2	$B_3^{(0)}$	$B_3^{(1)}$	a_{12}	$a_B\Lambda_*$	$B_3^{(0)}$	a_{12}
HFDHE2	0.830	116.7	1.67		1.258	118.5	87.9
HFD-B	1.685	132.5	2.74	135(5)	0.922	137.5	120.2
LM2M2	1.303	125.9	2.28	131(5)	1.033	130.3	113.1
TTY	1.310	125.8	2.28	131(5)	1.025	129.1	114.5

One of the most promising systems for observing Efimov states is ^{4}He atoms. The ^{4}He trimer has been observed [12], but no quantitative experimental information about its binding energy is available to date. The binding energy has been calculated accurately for various model potentials. They indicate that there are two trimers, a ground state with binding energy $B_3^{(0)}$ and an excited state with binding energy $B_3^{(1)}$. The most accurate calculations have been obtained by solving the Faddeev equations in the hyperspherical representation [13], in configuration space [14], and with hard-core boundary conditions [15]. These methods all give consistent results. The results of Ref. [15] for B_2, $B_3^{(0)}$, and $B_3^{(1)}$ and the atom-dimer scattering length a_{12} for four different model potentials are given in Table II. The discrepancies between B_2 and the large-a prediction $\hbar^2/ma^2$ are about 6–8 % [15]. They can be attributed to effective range corrections and provide estimates of the error associated with the large-a approximation.

We proceed to illustrate the power of universality by applying it to the ^{4}He trimer. For the scattering length a, we take the value $a_B \equiv \hbar/\sqrt{mB_2}$ obtained from the calculated dimer binding energy. We determine Λ_* by demanding that $B_3^{(1)}$ satisfy Eq. (5) with $n=1$. Solving Eq. (5) with $n=2$, we obtain the predictions for $B_3^{(0)}$ in the second-to-last column of Table II. The predictions are only 1–4 % higher than the calculated values, which is within the expected error for the large-a approximation. This demonstrates that the ground state of the ^{4}He trimer can be described by Efimov's equation (5). If we use the calculated values of a as input instead of B_2, the predicted values of $B_3^{(0)}$ are larger than the calculated values by 11–21 %.

We can use the value of $a_B\Lambda_*$ determined from the excited state of the trimer to predict the atom-dimer scattering length a_{12} and compare with the calculated values in the fourth column of Table II. The predictions for the four model potentials are given in the last column of Table II. They are smaller than the calculated values by about 13%. If the calculated value of a is used as input they are smaller by about 28%. It should be possible to account for these differences quantitatively by taking into account higher order corrections [11].

Efimov implicitly assumed in his derivation of Eq. (5) that there were no deep two-body bound states [1]. If such states are present, the Efimov states become resonances that can decay into a deep two-body bound state and a recoiling atom. Thus their energies are given by complex numbers $E=-B_3-i\Gamma_3/2$. If a potential supports many two-body bound states, the direct calculation of the widths Γ_3 by solving the Schrödinger equation is very difficult [16]. However, one can show that the cumulative effect of all deep two-body bound states on low-energy three-body observables can be taken into account by including one additional low-energy parameter η. Three-body recombination into a deep two-body bound state with binding energy $B\sim\hbar^2/ml^2$ can only take place if $R\sim l$. It is obvious that the atoms that form the bound state must approach to within a distance of order l, since the size of the bound state is of order l. However, the third atom must also approach the pair to within a distance of order l, because it must recoil with momentum $\sqrt{4mB/3}\sim\hbar/l$, and the necessary momentum kick can be delivered only if $R\sim l$. The atoms can approach such short distances only by following the lowest continuum adiabatic hyperspherical potential, because it is attractive in the region $l\ll R\ll|a|$, while all other potentials are repulsive. Thus all pathways to final states including a deep two-body bound state must flow through this lowest continuum adiabatic potential. Note the lowest continuum state can be either a three-atom state or an atom-dimer state. See, e.g., Fig. 5 in Ref. [10] for an explicit calculation of these potentials. The cumulative effects of three-body recombination into deep two-body bound states can therefore be described by the reflection probability $e^{-\eta}$ for hyperspherical waves entering the region $R\sim l$ of this potential. Up to corrections suppressed by $l/|a|$, the low-energy three-body observables are all determined by a, Λ_*, and η.

We proceed to generalize Efimov's equation (5) to the case in which there are deep two-body bound states. Again, we combine the analytic solution (3) to the radial equation in the region $l\ll R\ll|a|$ with simple probability considerations at $R\sim|a|$ and $R\sim l$. Since the existence of deep two-body bound states plays no role in the unitarity constraint at $R\sim|a|$, we still have $B=Ae^{i\Delta(\xi)}$ with the same universal function $\Delta(\xi)$ given in Eqs. (6)–(8). In the unitarity constraint at $R\sim l$, we need to take into account that only a fraction of the probability that flows to short distances is reflected back to long distances through the lowest adiabatic hyperspherical potential associated with the three-atom or atom-dimer continuum. Denoting the reflection probability by $e^{-\eta}$, the coefficient B in Eq. (3) can be written $B=Ae^{i\theta+\eta/2}$. The compatibility condition $\theta-i\eta/2=\Delta(\xi)\bmod 2\pi$ then becomes

$$B_3+\frac{i}{2}\Gamma_3+\frac{\hbar^2}{ma^2}=\frac{\hbar^2\Lambda_*^2}{m}\;e^{2\pi n/s_0}e^{(\Delta(\xi)+i\eta/2)/s_0},\quad(10)$$

where ξ is defined by Eq. (2) with $B_3\to B_3+i\Gamma_3/2$. To solve this equation, we need the analytic continuation of $\Delta(\xi)$ to complex values of ξ. The parametrization (6)–(8) for $\Delta(\xi)$ should be accurate for complex ξ with sufficiently small imaginary parts, except perhaps near $\xi=-\pi$ where it has an essential singularity. If B_3 and Γ_3 for one Efimov state are known, they can be used to determine Λ_* and η. The remaining spectrum of Efimov states and their widths can then be calculated by solving Eq. (10). For infinitesimal η, the widths approach $\Gamma_3\to(\eta/s_0)(B_3+\hbar^2/ma^2)$. The widths of the deeper Efimov states increase geometrically just like the binding energies, as has been observed in numerical calculations [16]. If η is so large that $B_3\sim\Gamma_3$, the Efimov states cease to exist in any meaningful sense.

We have calculated the universal function $\Delta(\xi)$ that appears in Efimov's equation (5) for the binding energies B_3 of Efimov states. This equation can be used as an operational definition of the three-body parameter Λ_* introduced in Ref. [2]. If B_3 for one Efimov state is known, it can be used to determine Λ_*, and then universality predicts all low-energy three-body observables as functions of a and Λ_*. In Eq. (10), we have generalized Efimov's equation to permit deep two-body bound states. The generalization involves an additional inelasticity parameter η, but the spectrum is determined by the same universal function $\Delta(\xi)$.

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