Efimov physics in ultracold three-body collisions

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Abstract.
We discuss some of our recent work on the near-threshold behavior of ultracold three-body collisions and their relation to a recent experiment [T. Kraemer, et al., Nature 440, 315 (2006)]. In particular, we discuss the role of Efimov physics in this experiment and other ultracold collisions and how this role can be understood within the adiabatic hyperspherical representation.

1. Introduction
Three-body collisions are taking on increasingly visible roles in the field of ultracold atomic gases. One reason for this is the high degree of control possible in these systems. In particular, the two-body s-wave scattering length \( a \) can be controlled across a wide range of values — from essentially \(-\infty\) to \(+\infty\), in principle — using Feshbach resonances. This control, which has proven so useful in studying their microscopic behavior as many-body systems, also allows unprecedented studies of their behavior as few-body systems. In the process, the range of fields impacted by ultracold atomic physics has grown even larger.

The impact of other fields on ultracold atomic physics has, in turn, also grown larger. Just as two-body collision physics helped shape the development of Bose-Einstein condensate and degenerate Fermi gas experiments through the determination of scattering lengths and understanding of loss processes, three- and four-body collision physics is now helping to refine those experiments. The two-body problem is unquestionably more mature, but a great deal of progress has been made over the past few years on the few-body problem through the combined efforts of atomic, nuclear, and chemical physicists.

Of central importance in understanding the behavior of ultracold three-body processes is the effect discovered by Vitaly Efimov [1, 2, 3]. Specifically, Efimov predicted that three identical bosons that have no two-body bound states have an infinity of three-body bound states if \( |a| \to \infty \). Curiously, one consequence of this already-intriguing prediction is that the number of three-body bound states decreases as the interparticle attraction is increased (since \( a \) then decreases in magnitude).

Actually, it is more accurate to say that the conceptual framework developed by Efimov is central to our understanding of ultracold three-body collisions rather than the Efimov effect itself. This qualification is simply a reflection of the fact that an ultracold gas consists of free atoms, so that there are no three-body bound states present. What Efimov’s analysis truly revealed was that three-body systems behave universally for energies near the three-body breakup threshold — either below or above — and that this behavior is determined primarily
by the underlying two-body scattering length. It is the latter property that earns the label “universal” since any two-body interactions that give the same scattering length should then give the same three-body behavior near threshold.

The most important outcome of Efimov’s analysis in the context of our work described here is that there is an effective $-1/R^2$ three particle interaction for $r_0 \ll R \ll |a|$ where $R$ is the overall size of the system and $r_0$ is the characteristic length of the two-body interaction. The properties of such a potential are well known and include, among other things, the fact that there are an infinite number of bound states whose energies accumulate exponentially at the threshold when $|a| \rightarrow \infty$ — which is precisely the property that Efimov used to identify the effect that now bears his name. In fact, this exponential (or geometric) spacing is a telltale feature of what we have come to label “Efimov physics” [4]. That is, physics that derives from the framework that Efimov established for the large $|a|$ limit. Since we have found that such physics pervades all manners of ultracold three-body collisions, this catchall phrase probably has outlived its usefulness and a better term should be sought — as has been argued by others [5].

To be a little more concrete, the processes that we are interested in — and which are likely to manifest Efimov physics — are as follows:

\[
\begin{align*}
A + B + C & \rightarrow AB^* + B, BC^* + A, CA^* + B & \text{Three-body recombination} \quad (1) \\
& \rightarrow AB + C, BC + A, CA + B & \quad (2) \\
\end{align*}
\]

\[
\begin{align*}
AB^* + C & \rightarrow AB^* + C & \text{Elastic scattering} \quad (3) \\
& \rightarrow AB + C & \text{Vibrational relaxation} \quad (4) \\
& \rightarrow AC + B & \text{Reactive scattering} \quad (5)
\end{align*}
\]

In these reactions, $A$, $B$, and $C$ represent arbitrary atoms. They can be indistinguishable bosons, indistinguishable fermions, or any combination thereof. They can also have the same or different masses. Our only assumption, that the interparticle interactions are short-ranged (i.e., fall off faster than $1/r^2$), is certainly satisfied for ground state atoms. For the purposes of this paper, we will also assume that at least two of the scattering lengths are resonant ($|a| \gg r_0$). In the above processes, the superscripted asterisk indicates a vibrationally excited state of the molecule. Note that at ultracold temperatures only those reactions that are exothermic (or superelastic) will proceed. In fact, they will have a finite, non-zero rate constant at zero temperature. Since the energy released in the reaction appears as relative kinetic energy of the fragments, these are generally loss processes as the molecular binding energies are typically much higher than the trapping potential confining the ultracold gas. If the gas temperature is higher than the binding energy in a given case, then the time-reverse of that process is possible. For instance, if the temperature is larger than the $AB^*$ binding energy, then the time-reversed version of Eqs. (1) and (2), collision-induced dissociation, will occur. Similarly, for sufficiently high temperatures, the time-reversed processes to vibrational relaxation Eq. (4) and reactive scattering (5) are also possible.

These exothermic processes are especially important near a Feshbach resonance since the scattering length $a$ has a pole there and the rates for these processes scale with $a$. For example, it has been known for many years that the three-boson recombination rate is proportional to $a^4$ [6, 7, 8]. Moreover, in this regime where $|a| \gg r_0$, Efimov physics begins to play a dominant role. In particular, it determines the primary dependence of all three-body rates on the scattering length and on the masses [9, 10]. Only the energy dependence is not a consequence of Efimov’s predictions, being determined instead at distances large compared to $|a|$ [11].

In this paper, we will discuss how we have built on the foundation laid by Efimov to derive the scattering length scaling laws for essentially all of the processes listed above. We obtain the mass and energy dependence for each reaction as well. A significant part of our effort goes into direct numerical solution of the Schrödinger equation to verify that our derived results are
correct and to put limits on their range of validity. All together, this information allows us to identify the dominant process and symmetry at threshold, which, in turn, helps experimentalists design better experiments as well as interpret them. This knowledge has also led us to identify physical systems that are more favorable to the observation of the geometric scaling of features so characteristic of the Efimov effect.

2. Theoretical Background

We solve the three-body Schrödinger equation using the adiabatic hyperspherical representation [12, 13, 14]. For particles interacting via short-range potentials, this representation rigorously discretizes the three-body continuum which is the most difficult aspect of this problem. Moreover, this representation treats all breakup channels — two- and three-body — on an equal basis. The dynamics of the three-body system is reduced to motion on a set of coupled, one-dimensional effective potentials that depend only on the hyperradius $R$. The hyperradius is a collective coordinate that gives, in some sense, the overall size of the system according to

$$
\mu R^2 = \mu_{12} \rho_{12}^2 + \mu_{12,3} \rho_{12,3}^2.
$$

(6)

In this expression, $\rho_{12}$ and $\rho_{12,3}$ are the Jacobi vectors, $\mu_{12}$ and $\mu_{12,3}$ are their associated reduced masses, and $\mu = \sqrt{\mu_{12} \mu_{12,3}}$ is a three-body reduced mass. The remainder of the system’s coordinates are the angles in the six-dimensional space of center-of-mass coordinates ($\rho_{12}, \rho_{12,3}$).

These hyperangles can be chosen in many different ways, but we use a modified Smith-Whitten coordinate system to simplify the symmetrization of the wave function [13].

The effective potentials are determined by solving the adiabatic equation

$$
H_{\text{ad}} \Phi_\nu(R; \Omega) = U_\nu(R) \Phi_\nu(R; \Omega), \quad \text{with} \quad H_{\text{ad}} = \frac{\Lambda^2}{2\mu R^2} + V(R, \Omega).
$$

(7)

In these expressions, $\Omega$ denotes the five hyperangles, and the adiabatic Hamiltonian $H_{\text{ad}}$ includes the kinetic energy for these hyperangles (in the first term) as well as all interactions in $V$. The effective potentials $W_{\nu\nu}(R)$ — composed of $U_\nu(R)$ plus a diagonal non-adiabatic correction — are then used in the hyperradial equations (atomic units will be used unless otherwise noted),

$$
\left( -\frac{1}{2\mu} \frac{d^2}{dR^2} + W_{\nu\nu} \right) F_\nu + \sum_{\nu' \neq \nu} W_{\nu\nu'} F_{\nu'} = EF_\nu,
$$

(8)

where $F_\nu$ is the hyperradial wave function and $E$ is the total energy. The nonadiabatic coupling $W_{\nu\nu'}$ includes first and second derivative coupling terms (for details, see Ref. [13]) and is responsible for inelastic transitions.

The effective potentials give a very intuitive picture for these complicated systems [6, 9, 11]. Moreover, the calculations can be made as accurate as desired by including more channels in Eq. (8) since they are exact in the limit that the expansion extends to infinity. The radial equations (8) are solved using the variational $R$-matrix method [15] in order to extract the $S$-matrix.

With the $S$-matrix in hand, the cross sections and rates for all possible processes can be calculated. For instance, the three-body recombination rate $K_3$ for identical bosons is [13]

$$
K_3 = \sum_{J,\pi} \sum_{i,f} \frac{192(2J + 1)\pi^2}{\mu k^4} |S_{f,i}^{J,\pi}|^2,
$$

(9)

where $k = \sqrt{2\mu E}$ is the hyperradial wave number, and $i$ and $f$ label the initial and final channels, respectively.
To derive the scattering length scaling laws, however, we are interested in approximate solutions of Eq. (8) rather than exact ones. So, we first approximate the effective potentials \( W_{\nu \nu}(R) \) using Efimov’s analysis [1, 2, 3]. That is, assuming that \( |a| \gg r_0 \) and \( E < 1/2 \mu a^2 \), the real two-body potentials can be replaced by a zero range potential that reproduces the correct scattering length. Under these conditions, the lowest energy effective potentials \( W_{\nu \nu}(R) \) take one of two forms (assuming no deeply bound two-body states),

\[
W_{\nu \nu}(R) = -\frac{s_0^2 + \frac{1}{4}}{2\mu R^2} \quad \text{or} \quad W_{\nu \nu}(R) = +\frac{p_0^2 - \frac{1}{4}}{2\mu R^2},
\]

representing attractive and repulsive Efimov potentials, respectively. These potentials are universal and hold in the range \( r_0 \ll R \ll |a| \) [16]; all higher-lying channels have repulsive \( 1/R^2 \) potentials for both cases. The coefficients \( s_0 \) and \( p_0 \) (and those of the higher-lying channels) can be determined to any desired precision as the zeroes of transcendental equations already derived by Efimov [1, 2, 3]. At \( R \gg |a| \), the potentials are those for free particles, given by the hyperspherical harmonic potentials or simply by two-body-like atom-molecule potentials, namely

\[
W_{\nu \nu}(R) = \frac{\lambda(\lambda + 4) + \frac{15}{4}}{2\mu R^2} \quad \text{and} \quad W_{\nu \nu}(R) = -E_{AB^*} + \frac{\ell(\ell + 1)}{2\mu R^2},
\]

where \( \lambda \) is a positive integer, \( E_{AB^*} \) is the binding energy of \( AB^* \), and \( \ell \) is the relative angular momentum between the atom and molecule. At \( R \) smaller than \( r_0 \), the potentials depend strongly on the details of the two-body potentials and are not universal.

Armed with these approximate potentials and the knowledge that the non-adiabatic coupling in Eq. (8) generally peaks at a distance comparable to the size of the more strongly bound state, the \( S \)-matrix elements in Eq. (9) can be approximated in the ultracold regime using a combination of one-dimensional scattering for the classically allowed regions [1, 2, 3, 17] and WKB for tunneling. Explicitly, the WKB tunneling integral is (including the Langer correction)

\[
|S_{fi}|^2 \approx \exp \left[ -2\int \sqrt{2\mu \left( W_{\nu \nu}(R) + \frac{1/4}{2\mu R^2} - E \right)} \, dR \right].
\]

We have checked several cases numerically to verify that this expression is sufficient to obtain the near-threshold behavior of the various rates. More details of this analysis are given in Refs. [9, 10].

3. Results and Discussion

As already discussed, Efimov physics — in the loosest sense of this term — manifests itself in the \( 1/R^2 \) behavior of the effective adiabatic potentials. The fact that both attractive and repulsive potentials are possible leads to a natural classification of all three-body systems interacting via short-ranged potentials into those that have purely repulsive potentials in the \( |a| \to \infty \) limit and those that have at least one attractive potential in this limit [9]. These results, combined with the techniques described above, allow us to obtain analytic expressions for the dependence of essentially all possible ultracold collision rates on the scattering length, mass, and energy [9, 10] — the length and mass scaling from Efimov physics and the energy scaling from a generalized Wigner analysis [11].

The other approach that we have taken, solving the three-body Schrödinger equation directly (see, for example, Refs. [6, 4, 13]), allows us to calculate essentially exact solutions [18] as a check on the analytical results — both ours and others [17, 19, 20]. In most cases we have verified the analytic results. In addition, we have been able to put bounds on the range of applicability of
the analytic expressions [4]. In only a couple of cases have we found that an analytic result is not fully supported numerically. We have discussed one such case in Ref. [10].

In fact, it was our early numerical calculations [6] — rather than analytic results — that provided the prediction recently verified experimentally by Rudi Grimm’s group [21]. Specifically, we predicted that the three-body recombination rate for identical bosons should show strong resonant enhancement for negative scattering lengths and that these resonances would be equally spaced on a log $|a|$ scale (to compensate the geometric scaling) due to their origins in Efimov physics. The former prediction was obtained numerically while the latter was obtained through a physical argument. Braaten and Hammer later provided a general analytic expression that contained both properties we had predicted [22]. Our more recent calculations [4] also reproduced both of these properties and showed, for the first time, what the recombination rate $K_3$ should look like as a function of $a$ at finite temperatures (see Fig. 1).

![Figure 1](image)

**Figure 1.** (Colour online) Our calculated recombination length, $\varrho \propto K_3^{1/4}$ [6], for the Cs measurement of Ref. [21] (red lines and symbols). These are adapted from the calculations in Ref. [4] by scaling those results with the mass and adjusting $r_0$, which is a free parameter in our two-body model, to fit the experimental peak position. The best fit value of $r_0 \sim 100$ a.u. turned out to be quite close to the van der Waal’s length for Cs, i.e. the natural length scale for the Cs-Cs interaction. The curves for all temperatures and $a$ were then produced with this same $r_0$. The agreement with the experimental data (black symbols) is quite good for all temperatures. (Experimental data courtesy of H.C. N"{a}gerl.)

The Grimm-group experiment [21] found exactly the resonant enhancement we had predicted in [6] as well as the temperature dependence we had predicted in [4], thus providing the first solid experimental evidence of Efimov physics. Unfortunately, they were not able to see more than one resonance, so could not verify the most characteristic feature of Efimov physics: the geometric
spacing of the features. One benefit of our ability to describe the mass, scattering length, and energy dependence of ultracold three-body collisions is that we can direct the experimentalists to systems that should allow them to see this behavior. For instance, in Ref. [23] we point out that a system that is a mixture of Cs and Li should show exactly the same resonant behavior observed in Cs alone, except that the spacing between the resonances should require only about a factor of 5 change in $a$ rather than a factor of almost 23. This reduction greatly improves the chances of being able to observe multiple peaks — of course, the cost is an increase in experimental complexity with the introduction of a second species.

To get a better understanding of the connection of the recombination resonance shown in Fig. 1 to the Efimov effect, it is useful to examine the approximate adiabatic hyperspherical potentials sketched in Fig. 2. These potentials were constructed following the description given previously. In particular, for the region $r_0 \ll R \ll |a|$, the lowest three-body breakup channel (labeled $\alpha$ in the figure) has the attractive $1/R^2$ character predicted by Efimov. The key observation is that for $a < 0$, there is a barrier in the initial free atom channel. Just as with any barrier, it is possible to have a resonance. In this case, it is a three-body shape resonance. In a normal collision, the potentials are fixed, and the collision energy is varied to reveal the resonant behavior. Since the collision energy is fixed by the temperature in an ultracold gas, however, we must scan the scattering length to see the resonance. As the scattering length is changed, the position of the barrier grows proportional to $|a|$; and its height, to $1/a^2$. The resonance energy thus decreases as $|a|$ increases and at some particular $a$ will coincide with the collision energy, giving the observed resonance. The recombination rate is enhanced when this happens because the amplitude of the scattering wave function behind the barrier — where the coupling to the atom-dimer channel peaks — grows much larger on resonance.

Another way to see the evolution of the resonance with scattering length is shown in Fig. 3. The recombination rate for several different scattering lengths is shown as a function of the collision energy. This figure illustrates the discussion above, showing that the resonant behavior also appears as a function of energy and that the peak position moves closer to threshold as $|a|$
is increased [24]. The figure clearly shows how $K_3$ increases when sitting at a fixed energy while the scattering length approaches the resonance. At some point, this three-body shape resonance passes through threshold (one such curve is shown in the figure) to become instead a Feshbach resonance in the atom-dimer channel [25]. If it happens that there is no dimer bound state, then the shape resonance becomes a three-body bound state. In either case, because the wave function lies largely in the range of $R$ governed by the attractive $1/R^2$ potential, the resonance has the character of an Efimov state. In fact, if the scattering length is increased by another factor of 23 (for identical bosons), then the progression depicted in Fig. 3 repeats. Any further increase in $|a|$ by a multiple of 23 will also result in a similar progression.

![Figure 3](image)

**Figure 3.** (Colour online) The three-body recombination rate as a function of collision energy for several different negative scattering lengths near the resonance. Each curve is labeled save for the very last one whose peak has moved below threshold at $E = 0$. Its scattering length is $-867$ a.u.

### 4. Summary
The control that is possible in ultracold atomic experiments is making the rich physics of few-body systems accessible in ways that have not been possible previously. It was this control, for instance, that allowed Rudi Grimm’s group to obtain the first experimental evidence of Efimov physics 35 years after its prediction. We expect that the impact of few-body physics on ultracold experiments and the insights the latter provides for the former will only grow over the next few years.

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### References
[1] V. Efimov, Sov. J. Nucl. Phys. 12, 589 (1971).
[2] V. Efimov, Nucl. Phys. A210, 157 (1973).
[3] V. Efimov, Sov. J. Nucl. Phys. 29, 546 (1979).
[4] J.P. D’Incao, H. Suno, and B.D. Esry, Phys. Rev. Lett. 93, 123201 (2004).
[5] E. Braaten, (private communication).
[6] B.D. Esry, C.H. Greene, and J.P. Burke, Jr., Phys. Rev. Lett. 83, 1751 (1999).
[7] E. Nielsen and J. H. Macek, Phys. Rev. Lett. 83, 1566 (1999).
[8] P. O. Fedichev, M. W. Reynolds, and G. V. Shlyapnikov, Phys. Rev. Lett. 77, 2921 (1996).
[9] J.P. D’Incao and B.D. Esry, Phys. Rev. Lett. 94, 213201 (2005).
[10] J.P. D’Incao and B.D. Esry, Phys. Rev. A 73, 030702(R) (2006).
[11] B.D. Esry, C.H. Greene, and H. Suno, Phys. Rev. A 65, R010705 (2002).
[12] J. Macek, J. Phys. B 1, 831 (1968).
[13] H. Suno, B.D. Esry, C.H. Greene, and J.P. Burke, Jr., Phys. Rev. A 65, 042725 (2002).
[14] E. Nielsen, D. V. Fedorov, A. S. Jensen, and E. Garrido, Phys. Rep. 347, 373 (2001).
[15] M. Aymar, C.H. Greene, and E. Luc-Koenig, Rev. Mod. Phys. 68, 1015 (1996).
[16] J.P. D’Incao and B.D. Esry, Phys. Rev. A 72, 032710 (2005).
[17] E. Braaten and H.-W. Hammer, Phys. Rep. 428, 259 (2006).
[18] For all of the results we present, which are based on solutions of model systems, the rates are converged to at least three digits.
[19] D. S. Petrov, C. Salomon, and G. V. Shlyapnikov, Phys. Rev. Lett. 93, 090404 (2004).
[20] D. S. Petrov, Phys. Rev. A 67, 010703(R) (2003).
[21] T. Kraemer, M. Mark, P. Waldfurger, J.G. Danzl, C. Chin, B. Engeser, A.D. Lange, K. Pilch, A. Jaakkola, H.-C. Nägerl, and R. Grimm, Nature 440, 315 (2006).
[22] E. Braaten and H.-W. Hammer, Phys. Rev. Lett. 87, 160407 (2006).
[23] J.P. D’Incao and B.D. Esry, Phys. Rev. A 73, 030703(R) (2006).
[24] F. Bringas, M.T. Yamashita, and T. Frederico, Phys. Rev. A 69, 040702(R) (2004).
[25] E. Nielsen, H. Suno, and B.D. Esry, Phys. Rev. A 66, 012705 (2002).