

Limits on Universality in Ultracold Three-Boson Recombination

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The recombination rate for three identical bosons has been calculated to test the limits of its universal behavior. It has been obtained for several different collision energies and scattering lengths a up to 10^5 a.u., giving rates that vary over 15 orders of magnitude. We find that universal behavior is limited to the threshold region characterized by $E \lesssim \hbar^2/2\mu_{12}a^2$, where E is the total energy and μ_{12} is the two-body reduced mass. The analytically predicted infinite series of resonance peaks and interference minima is truncated to no more than three of each for typical experimental parameters.

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The development of Bose-Einstein condensates (BECs) with tunable properties makes possible condensates with a wide range of interaction strengths. Several experiments [1–5] have investigated these properties by changing the atomic interactions with an external magnetic field near a diatomic Feshbach resonance. As is well known, these interactions are characterized at low temperatures by the two-body scattering length a , which covers the full continuum of positive and negative values near the Feshbach resonance. In fact, all of the essential properties of BECs are determined by the scattering length.

Because the two-body scattering length is the only relevant parameter, the precise shape of the two-body potential does not matter for the many-body physics. One of the remarkable results to emerge from recent work on ultracold collisions is that this property holds even for the low temperature *three-body* physics. This shape independence has allowed theorists to choose any convenient two-body potential that reproduces the desired scattering length. We again exploit this freedom in the present work to study three-body recombination. Three-body recombination is the process by which three free atoms collide to form a diatomic molecule and an unbound atom, setting free enough kinetic energy to make both atom and molecule escape from typical traps.

The universal behavior of the three-body recombination rate makes it possible to derive analytical expressions for $a > 0$ [6–8] and for $a < 0$ [9]. In the former case, theory predicts an infinite number of minima in the rate as $a \rightarrow +\infty$; and in the latter case, an infinite number of maxima as $a \rightarrow -\infty$. The physics behind both features is closely related to the Efimov effect [10]. In fact, it has been suggested that measuring the recombination rate while tuning through a Feshbach resonance might make possible some of the first direct experimental evidence of this intriguing effect.

Tuning through such Feshbach resonances can dramatically limit the density and lifetime of BECs, however, since the three-body recombination rate was predicted [6–9,11]—and recently verified experimentally [5]—to increase with the scattering length as a^4 .

More recently, three-body recombination has been used to create composite bosons by pairing fermions in ultracold gases [12,13]. The ultimate goal of this endeavor has recently been achieved with the observation of Bose-condensed pairs of fermion atoms [14]. Despite its importance and recent advances, much work remains for the theory of three-body recombination. In particular, the universal behavior of the recombination rate has not yet been tested by accurate calculations.

In this Letter, we show that the recombination rate for identical bosons is universal only for collision energies in the threshold regime. Generically, the threshold regime is characterized by $k|a| \lesssim 1$, or equivalently, when the collision energy is the smallest energy in the system. For $a > 0$, the energy scale is set by the two-body binding energy; for $a < 0$, by the height of a potential barrier or, in some cases, by a two-body shape resonance. Therefore, for a fixed total three-body energy E , the relation $E \lesssim E_{12}$ indicates when the system is in the threshold regime where universal behavior is expected. In this expression, $E_{12} = \hbar^2/2\mu_{12}a^2$ is the two-body binding energy and μ_{12} is the two-body reduced mass.

The experimental consequences of restricting the range of universal behavior are striking. At any nonzero temperature, rather than observing an *infinite* series of resonances or minima, only a finite number of either will be observable as the scattering length is scanned from $-\infty$ to $+\infty$ —and even those will be washed out. For instance, at 1 nK, only three resonances and three minima can be hoped to be seen.

We further show that the analytical formulas derived in Refs. [6–9] hold only at zero energy. At finite energies, when the scattering length is tuned out of the threshold regime ($E > E_{12}$), the analytical formulas break down because they do not take proper account of three important finite energy effects: unitarity, thermal averaging, and higher partial waves. Unitarity limits the rate to finite values at finite temperatures for large scattering lengths and leads to a saturation effect [5,15]. Thermal averaging takes account of the fact that experiments are performed at fixed temperature rather than fixed collision

energy, and higher partial waves must always be included, in principle. A generalized Wigner threshold law [16] guarantees that the $J^\pi = 0^+$ contribution dominates at threshold, where J is the total orbital angular momentum and π is the overall parity. The next leading contribution, 2^+ , grows with energy as E^2 and with scattering length as a^8 and can quickly become comparable to the 0^+ rate.

We obtain the recombination rates by solving the Schrödinger equation numerically using the adiabatic hyperspherical representation (see Refs. [7,16,17] for details of our implementation). The key to this approach is that the dynamics of the three-body system are reduced to the motion on a set of coupled effective potentials that depend only on the hyperradius R . The hyperradius is a collective coordinate that represents, in some sense, the overall size of the system. The effective potentials are determined by solving the adiabatic equation

$$H_{\text{ad}}\Phi_\nu(R; \Omega) = U_\nu(R)\Phi_\nu(R; \Omega),$$

where Ω denotes the five hyperangles representing all degrees of freedom besides R . The adiabatic Hamiltonian H_{ad} includes the kinetic energy for these hyperangles as well as all interactions. The effective potentials $U_\nu(R)$ are then used in the radial equations (atomic units will be used unless otherwise noted)

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

where F_ν is the hyperradial wave function, E is the total energy, and the three-body reduced mass μ is related to the atomic mass m by $\mu = m/\sqrt{3}$. The nonadiabatic coupling $W_{\nu\nu'}$ is responsible for inelastic transitions such as three-body recombination. The effective potentials give a very intuitive picture for these complicated systems. Moreover, the calculations can be made as accu-

rate as desired by including more channels in the equation above (all rates quoted here are accurate to at least three digits and were obtained with seven channels). The radial equations (1) are solved using the variational R -matrix method [18] in order to extract the S matrix.

The three-body recombination rate K_3 is defined in terms of the S matrix as [7,16,17]

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

where $k = \sqrt{2\mu E}$ is the hyperradial wave number, and i and f label the initial and final channels, respectively. The present results were obtained using the mass of helium atoms and the model dimer potential $v(r) = D\text{sech}^2(r/r_0)$ with D and r_0 adjusted to give a single two-body s -wave bound state.

In the adiabatic hyperspherical representation, recombination for $a > 0$ is driven primarily by the broadly peaked nonadiabatic coupling between the lowest three-body entrance channel and the highest molecular channel [7]. In this picture, there are two indistinguishable pathways for recombination, leading to the so-called “Stückelberg oscillations.” This interference phenomena modifies the a^4 dependence of the rate, suppressing it for certain values of a . At zero energy, the analytic results predict these minima to be equally spaced on a logarithmic scale and separated by a factor of approximately $e^{\pi/\alpha} \approx 22.7$, where $\alpha = 1.0064$.

For $a < 0$, the recombination rate is enhanced for particular values of a and, in the adiabatic hyperspherical representation, can be interpreted as three-body tunneling through a potential barrier in the entrance channel [7]. The nonadiabatic coupling is localized at small R behind this barrier so that recombination is suppressed for energies below the barrier maximum. That is, unless the collision energy matches the energy of a three-body

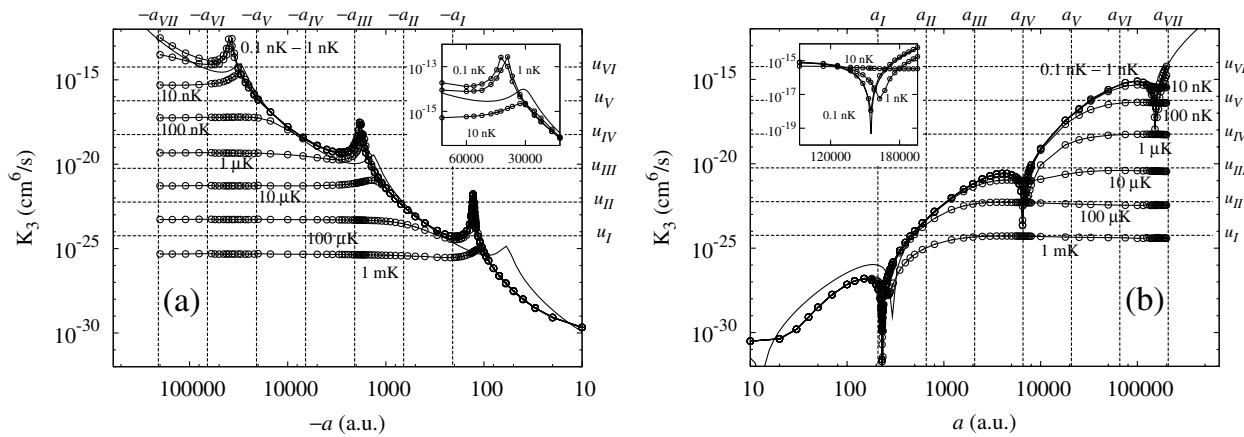


FIG. 1. Three-body recombination rate for (a) $a < 0$ and (b) $a > 0$. The horizontal lines represent the unitarity limit u_N for each energy (reported as a temperature using $E = k_B T$). The vertical lines represent the boundary of the threshold regime a_N . The solid curve represents the analytical formula Eq. (3). The insets show the third resonance peak (a) and third interference minima (b) from $a = 0$.

resonance trapped behind this barrier. Under these conditions, transmission through the barrier jumps and strong enhancement of the recombination rate can be observed. As with the interference minima, these resonances can be associated with Efimov physics [10], and are also predicted to be equally spaced on a logarithmic scale (separated by a factor of about 22.7). Figure 1 shows the $J^\pi = 0^+$ recombination rates calculated at energies in the range 0.1 nK to 1 mK. Figure 1(a) shows the first three resonance peaks for $a < 0$, and Fig. 1(b) shows the first three interference minima for $a > 0$. For small values of the scattering length, the rates for all energies lie along a common, *universal* curve. For any given energy, the rates depart from this universal curve at some point, with the highest energies departing soonest.

In the adiabatic hyperspherical representation, the analytic recombination expression is derived under the assumption that the collision energy is in the threshold regime. It is natural, then, to conclude that the analytic expression—and thus the universal behavior—is valid only in the threshold regime. The collision energy is in the threshold regime when it is smaller than other characteristic energies of the system. One obvious energy scale is the two-body binding energy E_{12} .

In Fig. 1, the vertical dashed lines mark the scattering lengths determined from the relation $E \approx E_{12}$ for each energy. It is clear that the two-body binding energy provides a reasonable estimate for the domain of universal behavior; i.e., for each energy, the rate curve for a less than this limit follows the common curve. For $a < 0$, a more restrictive limit can be determined from the adiabatic potential since the threshold regime in this case requires energies less than the potential barrier maximum, $U_{\max} = 0.079/\mu a^2$ [11], which reduces the limiting a by about a factor of 3. For example, in a ^{23}Na condensate at a temperature of 100 nK, the recombination rate is expected to be universal only for $-3200 < a < 8650$ a.u.; for ^{87}Rb , for $-1650 < a < 4450$ a.u. All of these values are well within the range that is already experimentally accessed near Feshbach resonances.

We also show in Fig. 1 the analytical results [6–9]:

$$K_3 = \begin{cases} \frac{4590(a^4/m) \sinh(2\eta_*)}{\sin^2[\alpha \ln(3|a|/2r_0) + \Phi + 1.63] + \sinh^2 \eta_*} & a < 0, \\ 360(a^4/m) \sin^2[\alpha \ln(3a/2r_0) + \Phi] & a > 0, \end{cases} \quad (3)$$

where Φ and η_* are unknown parameters. Φ represents an unknown small- R phase [6,7] (related to Λ_* in Refs. [8,9]) and is chosen to give the best fit to the third interference minimum at 0.1 nK. The additional 1.63 rad of the $a < 0$ phase is predicted in [9]. The value $\eta_* = 0.1$ was found to give the best fit for $a < 0$. There is generally very good agreement with the numerical results for large, positive a/r_0 , and Eq. (3) appears to be essentially exact for zero energy recombination. It relies on the effective range expansion, however, and gets increasingly worse as $|a|$ decreases due to order r_0/a errors (here, $r_0 = 15$ a.u.). The agreement is more qualitative for $a < 0$ due to the

small shift of the resonance peak positions. We found, though, that a 15% change in the extra $a < 0$ phase gives good agreement with the 0.1 nK curve. It is worth pointing out that both Eq. (3) and the present results do not include the full physics of the Feshbach resonance, only the change in the scattering length.

One factor left out of Eq. (3) is unitarity (although a “unitarized” version has been proposed [15] to help explain the experimental results in Ref. [5]). As the collision energy grows large compared to E_{12} for a fixed scattering length, the probability of recombination approaches unity for the 0^+ partial wave. More relevant for experiments, unit recombination probability is also reached as the scattering length is increased at fixed collision energy E . The horizontal dashed lines in Fig. 1 denote the unitarity limit— $u_N = 192\pi^2/\mu k_N^4$, obtained from Eq. (2) by setting $|S|^2 = 1$ —for each energy shown. From the figure, it is clear that the recombination rate reaches the unitarity limit for positive a outside the threshold regime. For negative a , however, while the rate does saturate, it does so at a value about a factor of 10 below unitarity.

A second factor neglected in Eq. (3) is the thermal average. Experiments are performed at fixed temperatures rather than fixed energies, so the thermal average becomes crucial for proper comparison with experiment. In the threshold regime, the recombination rate is constant as a function of energy, so the thermal average has no effect. Since we consider exactly the situation when the system is no longer in the threshold regime, thermal averaging can have significant effects. The thermally averaged recombination rate is

$$\langle K_3 \rangle(T) = \frac{1}{2(k_B T)^3} \int K_3(E) E^2 e^{-E/k_B T} dE, \quad (4)$$

where k_B is Boltzmann’s constant. Figure 2 illustrates the effects of thermal averaging at 0.1 and 1 μK near the second resonance peak and second interference minima. For energies solidly within the threshold regime, thermal averaging has little effect. For energies on the border of

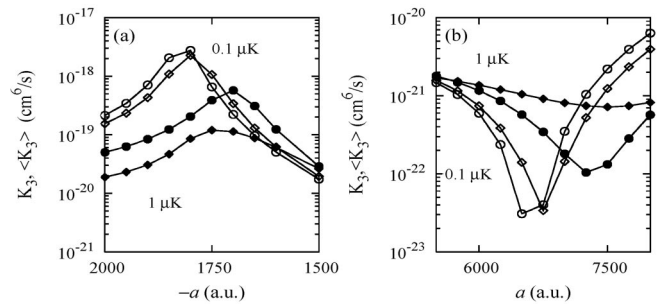


FIG. 2. Thermally averaged recombination rate (a) near the second resonance peak and (b) near the second interference minimum. Circles and diamonds represent K_3 and $\langle K_3 \rangle$, respectively, at 0.1 μK (empty symbols) and 1 μK (filled symbols).

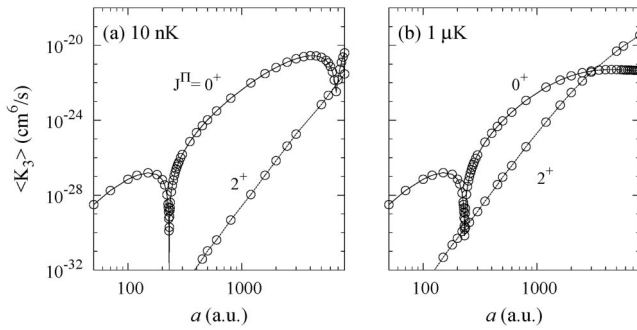


FIG. 3. Comparison of the 0^+ and 2^+ recombination rate for $a > 0$ and temperatures of (a) 10 nK and (b) $1 \mu\text{K}$.

the threshold regime, however, averaging reduces the intensity of both the peaks and minima, making their observation much more difficult.

A third factor not included in Eq. (3) is the contribution from higher partial waves. The $J^\pi = 2^+$ rate was calculated for $-3000 < a < 8000$ a.u. and energies from 0.1 nK up to 1 mK. The 2^+ threshold law is $K_3 \propto E^2 a^8$ [16], so for a finite energy, there will be a scattering length for which the 2^+ contribution is comparable to 0^+ . Figure 3 shows the thermally averaged 2^+ rate at 10 nK and $1 \mu\text{K}$ along with 0^+ for $a > 0$. (For $a < 0$, the 2^+ recombination rate is many orders of magnitude smaller than for 0^+ , making it completely negligible for the present range of scattering lengths and energies.) It is clear from Fig. 3 that the 2^+ rate dominates 0^+ at the second interference minimum for $1 \mu\text{K}$ so that the total rate will show just one minimum. At 10 nK, the 2^+ rate is merely comparable to 0^+ at the second minimum, cutting its depth in the total rate. For energies below 10 nK, the 2^+ recombination rate is negligible in this range of scattering length; for larger scattering lengths, however, the 2^+ recombination rate can contribute substantially.

Taken together, the unitarity limit, thermal averaging, and higher partial waves restrict the analytic results for ultracold three-body recombination to the threshold regime, i.e., when $E \lesssim E_{12}$.

Assuming that the only effect of a Feshbach resonance is to change the scattering length, the experimental consequences of these limitations could be rather dramatic. Near a Feshbach resonance, a changes, for instance, from its background value to $+\infty$, then to $-\infty$, then back to its background value—all while the system is at essentially the same temperature. The analytic expressions predict that the three-body recombination rate grows like a^4 as the resonance is approached, goes through an infinite number of minima as $a \rightarrow +\infty$, then has an infinite number of resonances as a returns from $-\infty$. Each series of features reflects Efimov physics, so measuring them might reveal evidence for this effect. The present calculations show, however, that the infinite series are truncated to a small number [$\approx \alpha/\pi \ln(3a_c/2r_0)$, where

$a_c = \hbar/\sqrt{2\mu_{12}E}$] for typical collision energies E and that the contrast of the surviving features may be considerably reduced. The recombination rate is thus not a good candidate for observing physics related to the Efimov effect except at extremely low temperatures.

Even though we have shown that the universal behavior described by existing analytic expressions is limited to the threshold regime, scattering lengths up to a few thousand atomic units are included. Moreover, a new sort of universal behavior dictated by the unitarity limit may take over and modifications to the analytic expressions along these lines have already been proposed [15]. Since we have used only one model potential, we are not in a position to discuss any universal behavior outside of the threshold regime. We expect, however, that recombination for $a > 0$ will be much as we have shown in Fig. 1 since it takes place at large distances where differences in the two-body potential will have little effect. For $a < 0$, the situation is just the opposite since recombination is a small distance process. The resonance positions as well as the $a \rightarrow -\infty$ limiting rate will likely then depend on the two-body potential.

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