Efimov Trimer Formation via Ultracold Four-Body Recombination

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We discuss the collisional formation of Efimov trimers via ultracold four-body recombination. In particular, we consider the reaction $A + A + A + B \to A_3 + B$ with A and B ultracold atoms. We obtain expressions for the *four*-body recombination rate up to an overall constant and show that it reflects the *three*-body Efimov physics either as a function of collision energy or as a function of the two-body s-wave scattering length between A atoms. In addition, we briefly discuss issues important for experimentally observing this interesting and unexplored process.

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The exquisite experimental control possible in ultracold atomic gases has enabled the observation of unique and bizarre quantum states. For instance, the many-body phenomena of Bose-Einstein condensation [1,2] and Fermi degeneracy [3,4] have both been observed and used for a wide range of studies [5–8]. Weakly bound diatomic Feshbach ‘‘halo’’ molecules have also been observed [9] and their dynamics probed [10]. Especially relevant to the present work, Efimov physics [11] was finally observed experimentally in three-body recombination of cesium atoms [12], and even more recently in $Cs + Cs_2$ collisions [13]. These experimental observations of Efimov physics were preceded by a considerable amount of theoretical work due to its general importance for ultracold three-body collisions (see, for instance, Refs. [14–17]), and we now have a remarkably complete characterization of these processes.

Our goal for this Letter is to examine ultracold four-body collisions. In particular, we want to explore the possibility of producing Efimov trimers via four-body recombination. Since the experimental evidence for the Efimov effect is from low-energy three-body collisions rather than from bound trimers themselves, producing bound trimers is a natural next step. A scheme for doing this in the tight confinement of an optical lattice has been proposed [18], but here we investigate the possibility for producing them in free space with four-body recombination somewhat like three-body recombination has been used experimentally to produce weakly-bound dimers [19]. Note that energy and momentum conservation require a four-body collision to produce a bound trimer.

Besides the intrinsic interest of Efimov states, it is also important to develop the theory of the fundamental process of four-body recombination quantum mechanically. Compared with three-body collisions, our knowledge of ultracold four-body collisions is still quite rudimentary. The reason is clear: solving the Schrödinger equation with three additional degrees of freedom is a much more difficult task. There have, of course, been many studies of four-body systems, but only recently have some relevant to ultracold gases begun to appear [20–23]—none of which has addressed four-body recombination (*see Note added*).

The system we consider in this Letter is an ultracold mixture of atoms A and B. We take A to be bosons distinguishable from B. Our goal is to produce Efimov trimers A_3 via the four-body recombination process

$$A + A + A + B \to A_3 + B. \tag{1}$$

To this end, we will assume that the two-body s-wave scattering length among A atoms a_{AA} is infinite to give the most favorable case for Efimov states. We will also assume that the interspecies scattering length a_{AB} is finite and that any dimer states, which are likely for real systems, lie much deeper than the Efimov trimer states. As we will show below, monitoring the loss of B atoms provides a convenient indicator for the formation of A_3 with many advantages over alternative schemes.

Our treatment of this process is asymmetrical in A and B, mirroring the differences in a_{AA} and a_{AB}. The two-body interactions for the A_3 subsystem are well-described by the zero-range model [11]. The advantage of this model is that the three-body solutions are especially simple in the $|a_{AA}| \to \infty$ limit [11]. Extending this model to four-body systems is not straightforward, however. Instead, we borrow an idea from Rydberg physics [24]—and from many-body theories of Bose-Einstein condensates [8]—to model the AB interaction. Since the wavelength of the A atoms, either when they are free or in an Efimov molecule, is much larger than the size of atom B, the AB interactions can be approximated by the Fermi contact potential [25] (atomic units are used throughout)

$$V_{AB}(r_{i4}) = \frac{2\pi a_{AB}}{\mu_{AB}} \delta(r_{i4}), \qquad i = 1, 2, 3, \tag{2}$$

where μ_{AB} is the two-body reduced mass and r_{i4} is one of the AB interparticle distances.

Given the success of the adiabatic hyperspherical representation in describing the three-body continuum [14,15], we will use it here to treat the four-body continuum as well. Since we want to use the known solutions for the A_3 subsystem, we build the four-body hyperspherical coordinates from the three-body ones. The four-body hyperradius R_4 and hyperangle α_4 are thus defined as

$$\mu_4 R_4^2 = \mu_{3,4}\rho_3^2 + \mu_3 R_3^2 \quad \text{and} \quad \tan\alpha_4 = \sqrt{\frac{\mu_3}{\mu_{3,4}}}\frac{R_3}{\rho_3}. \tag{3}$$

Here, $\mu_3 = m_A/\sqrt{3}$, $\mu_{3,4} = 3m_A m_B/(3m_A + m_B)$, and $\mu_4 = \sqrt{\mu_3\mu_{3,4}}$. Finally, ρ_3 denotes the distance from the A_3 center of mass to B; R_3, the three-body hyperradius; and α_3, the three-body Delves' hyperangle [26].

The representation we use, however, is not fully adiabatic since we will not include V_{AB} in the adiabatic Hamiltonian $H_{\rm ad}$. Rather, we will include them later as coupling between the channels in a mixed adiabatic-diabatic representation. This choice, together with our definition of coordinates, permits separation of variables in the adiabatic equation, utilizing the known solutions for the A_3 subsystem. Mathematically, this procedure begins with the four-body Schrödinger equation

$$[T_{R_4} + V_{AB}(r_{14}) + V_{AB}(r_{24}) + V_{AB}(r_{34}) + H_{\rm ad}]\Psi = E\Psi,$$

where T_{R_4} is the hyperradial kinetic energy and

$$H_{\rm ad} = T_{\Omega_4} + T_{\Omega_3} + V_{123}, \tag{4}$$

which includes the hyperangular kinetic energies T_{Ω_i} and all of the interactions among A atoms in V_{123}. The notation Ω_3 denotes collectively all of the three-body hyperangles; and Ω_4, all remaining hyperangles. In the ultracold limit, only the zero total orbital angular momentum solution is relevant by the generalized Wigner threshold law [27]. And, since Efimov states only exist for zero orbital angular momentum of A_3, the angular momentum of B relative to A_3 must also be zero. The channels for the four-body problem are thus defined from

$$H_{\rm ad}\Phi_\nu^{(4)} = U_\nu(R_4)\Phi_\nu^{(4)}. \tag{5}$$

Separation of variables allows ($\nu \equiv \{\beta, n\}$)

$$\Phi_\nu^{(4)}(R_4;\Omega_4,\Omega_3) = u_{\beta n}(R_4;\Omega_4)\Phi_\beta^{(3)}(\Omega_3). \tag{6}$$

For four-body recombination, we will need to find not only the $A_3 + B$ bound channels, but also the four-body continuum channels $A + A + A + B$.

For the $A_3 + B$ channels ($\beta = 0$), we use [11]

$$\Phi_0^{(3)}(\Omega_3) = \sum_{l=1}^{3}\frac{2\sinh(s_0\alpha_3^{(l)})}{\sin(2\alpha_3^{(l)})} \tag{7}$$

$$(T_{\Omega_3} + V_{123})\Phi_0^{(3)} = -\frac{s_0^2 + \frac{1}{4}}{2\mu_3 R_3^2}\Phi_0^{(3)} \tag{8}$$

where the summation is over the three possible three-body Jacobi sets, each with its own Delves' hyperangle $\alpha_3^{(l)}$; $s_0 \approx 1.0062$ is a universal constant. Substituting Eq. (7) into Eq. (6), and the result into Eq. (5), gives the equation for the bound trimer channels:

$$\left(-\frac{\partial^2}{\partial\alpha_4^2} - \frac{s_0^2 + \frac{1}{4}}{\sin^2\alpha_4}\right)u_{0n} = \lambda_{0n}^2 u_{0n}, \quad U_{0n} = \frac{\lambda_{0n}^2 - \frac{1}{4}}{2\mu_4 R_4^2}. \tag{9}$$

The physically acceptable solution of Eq. (9) is

$$u_{0n}(R_4;\alpha_4) = N_4\cos\alpha_4 \sin^{(1/2)+is_0}(\alpha_4)\,{}_2F_1\left(\frac{3}{4} + \frac{is_0}{2} - \frac{\lambda_{0n}}{2}, \frac{3}{4} + \frac{is_0}{2} + \frac{\lambda_{0n}}{2}; \frac{3}{2}; \cos^2\alpha_4\right) \tag{10}$$

with N_4 the normalization constant. To avoid the Thomas collapse [28], we simply require that the three-body hyperradial wave functions vanish for $R_3 \le R_0$ where R_0 roughly represents the size of the ground Efimov state. This regularization leads to a transcendental equation for λ_{0n}, and it can be shown explicitly that the Efimov trimer energies are recovered from U_{0n} in the limit $R_4 \to \infty$. We include the diagonal coupling $Q_{\nu\nu} = \langle\langle\frac{d\Phi_\nu}{dR_4}|\frac{d\Phi_\nu}{dR_4}\rangle\rangle$ to get the most physical potentials $W_\nu(R_4) = U_\nu(R_4) - \frac{1}{2\mu_4}Q_{\nu\nu}(R_4)$.

We follow the same logic for the $A + A + A + B$ channels. The only difference is that $\Phi_\beta^{(3)}$ is now a three-body continuum function, but still for $|a_{AA}| \to \infty$. That is, we replace s_0 in Eqs. (7)–(10) by is_β ($\beta > 0$), where s_β are real numbers determined by

$$\sqrt{3}s_\beta\cos\left(\frac{\pi}{2}s_\beta\right) = 8\sin\left(\frac{\pi}{6}s_\beta\right). \tag{11}$$

The resulting $u_{\beta m}$ satisfy the same boundary condition at R_0 as the bound channels. Asymptotically, $\lambda_{\beta m} \to s_\beta + 2m + \frac{3}{2}$ with $m = 0, 1, 2, \ldots$ labeling the four-body continuum states possible for each β. The four-body continuum potentials thus behave as $1/R_4^2$ for $R_4 \gg R_0$.

If we expand the total four-body wave function as

$$\Psi(R_4,\Omega_4,\Omega_3) = \sum_\nu F_\nu(R_4)\Phi_\nu^{(4)}(R_4;\Omega_4,\Omega_3), \tag{12}$$

then the nonadiabatic couplings between four-body continuum and atom-trimer channels vanish since $\Phi_\beta^{(3)}$ are independent of R_4 and form an orthonormal set. Recombination is thus driven only by the diabatic couplings

$$V_{\nu'\nu} = \langle\nu'|V_{AB}(r_{14}) + V_{AB}(r_{24}) + V_{AB}(r_{34})|\nu\rangle \tag{13}$$

and occurs predominantly at the crossings in Fig. 1 which shows the lowest atom-trimer and four-body continuum potentials, multiplied by R_4^2 for clarity. In the vicinity of the crossings, the coupling $V_{\nu'\nu}$ behaves to a good approximation as $\zeta a_{AB}/(\mu_{\rm AB}R_4^3)$. The unitless constant ζ originates from the numerical evaluation of $V_{\nu'\nu}$, has a weak dependence on the channel numbers, and is on the order of 10^{-3}. While the two sets of potentials in Fig. 1 cross in several places, the lowest two $A_3 + B$ potentials do not cross a continuum channel. In our model, then, the lowest two Efimov trimers can only be populated by weak nonadiabatic transitions between atom-trimer channels. This conclusion is independent of R_0, but for more realistic, finite range two-body potentials, all the channels will likely be coupled at small R_4. Note that because all of the states of interest here display strongly repulsive potentials at small R_4 in Fig. 1, no four-body parameter [22,23] is required in

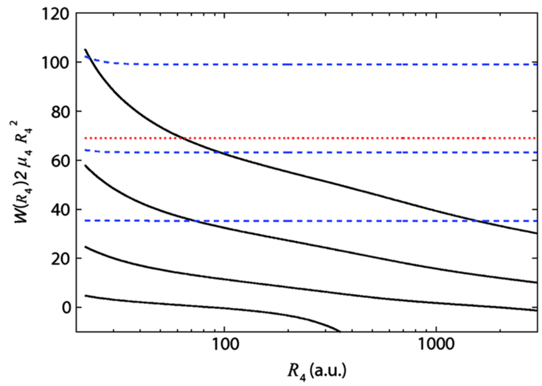

FIG. 1 (color online). The lowest four-body adiabatic hyperspherical potentials W_ν multiplied by $2\mu_4 R_4^2$ to better show their behavior. Black solid lines denote atom-trimer potentials for $\beta = 0$ and $n = 1, 2, 3, 4$; blue dashed lines, four-body continuum potentials for $\beta = 1$ ($s_1 = 4.465$) and $m = 0, 1, 2$; and the red dotted line, the four-body continuum potential with $\beta = 2$ ($s_2 = 6.818$) and $m = 0$. We take $R_0 = 10$ a.u. for all curves.

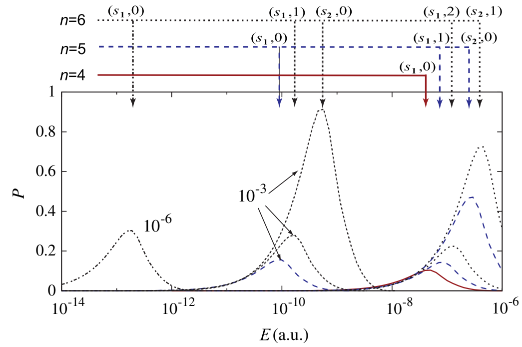

FIG. 2 (color online). The recombination probability for several transitions (s_β, m) labels the initial continuum channel and n labels the final state of the Efimov trimer. The probabilities must be multiplied by the factors indicated. We have taken $R_0 = 10$ a.u. and $a_{AB} = 100$ a.u..

the description of four-body recombination to Efimov trimers.

The four-body recombination rate K_4 is related to the recombination probability $|T_{fi}|^2$ by $K_4 \propto |T_{fi}|^2/k^7$ where $k = \sqrt{2\mu_4 E}$ is the incident four-body wave vector and the unknown proportionality constant is a number that depends on the number of identical particles. Because the couplings $V_{\nu'\nu}$ are quite small, the peaks of $|T_{fi}|^2$ occur at $E \approx W_\nu(R_c)$,

$$W_\nu(R_c) \approx \frac{(s_\beta + 2m + \frac{3}{2})^2}{2\mu_{3,4}R_0^2} e^{-(\pi/s_0)(2n - s_\beta - 2m + ((2\gamma - s_0)/\pi) - 1)}, \tag{14}$$

where R_c is the value of R_4 at the crossing and $\gamma = 0.30103$. This expression shows that for a given initial channel (s_β, m), there is a geometrically spaced sequence of peaks in energy for recombination to Efimov trimers n. This characteristic feature of the three-body Efimov physics is thus evident in the four-body physics as well. Moreover, the spacing of the features is $\exp(-2\pi/s_0)$ just as one would predict from the three-body physics.

To illustrate this point, we show in Fig. 2 $P = |T_{fi}|^2$ for several transitions. We calculated $|T_{fi}|^2$ for recombination from the lowest continuum channel (s_1, 0) into the $n = 4$ and 5 states including only these three channels in the Schrödinger equation. These otherwise exact solutions show that the recombination probability does indeed peak at the crossings, thus showing the expected log-periodic spacing of peaks. Since this calculation confirmed our predictions and a full calculation is prohibitively expensive, we estimate the other peaks in Fig. 2 by shifting the peaks from the three-channel calculation based on the crossing energy (14) and scaling them taking into account the difference in their heights.

Up to this point, our analysis has assumed $|a_{AA}| = \infty$. If we let it be finite instead, then the above analysis applies in the regime $|a_{AA}| \gg |a_{AB}|$. We further require $a_{AA} < 0$ so that there are no weakly bound dimers and thus no three-body recombination of A atoms to compete with four-body recombination. Under these conditions, the four-body adiabatic potentials behave as described above for $|a_{AB}| \ll R_4 \ll |a_{AA}|$. For $R_4 \gg |a_{AA}|$, the $A + A + A + B$ potentials approach the four-body hyperspherical harmonic potentials $W_\nu \approx \frac{\lambda(\lambda+7)+12}{2\mu_4 R_4^2}$ with λ a non-negative integer, and the $A_3 + B$ potentials approach the trimer bound energies. It follows that at energies $a_{AA}^{-1} \ll k \ll a_{AB}^{-1}$, K_4 keeps the structure described above.

It is in the zero energy limit that the effects of finite a_{AA} reveal themselves. When $E \to 0$, recombination into the most weakly bound Efimov trimer dominates. Since the size of this trimer is on the order of $|a_{AA}|$, we expect recombination to occur at $R_4 \approx |a_{AA}|$. So, employing a WKB analysis similar to that described in Ref. [16], we find that the recombination probability is

$$P = C(a_{AB})(k|a_{AA}|)^7 \sin^2(k_n|a_{AA}| + \Phi), \tag{15}$$

where C is a proportionality constant, Φ is a short-range phase independent of a_{AA}, and $k_n = \frac{2}{R_0}\frac{\mu_4}{\mu_3}\exp[-(n\pi + \gamma)/s_0]$ is the wave number for the final trimer state n at $E = 0$. When $|a_{AA}|$ increases by a factor of 22.7, a new atom-trimer channel appears and k_n changes to k_{n+1} which, in turn, changes the period of the a_{AA}-dependent oscillations. It turns out that recombination into a particular atom-trimer state will show about seven full oscillations in K_4 as a function of a_{AA}. From the relation $K_4 \propto P/k^7$, Eq. (15) also shows that K_4 will be constant in the threshold regime, $ka_{AA} \lesssim 1$, and proportional to $|a_{AA}|^7$. This scaling will apply to K_4 for any system without identical fermions.

If the trimers cannot be experimentally observed directly, then their production can be measured through the loss of either A or B atoms. In an ultracold mixture of the two, it is much better to observe the B atoms, however, as other few-body processes will lead to loss of A atoms and thus mask the effects we predict. The best choice is to make the B atoms spin-polarized fermions. In this case, $A + A + A + B$ recombination is unaffected, but the competing loss processes involving two or more B atoms can be avoided as they will be suppressed near threshold [27]. There remains the possibility for loss of B atoms in $A + A + B$ collisions, but for $|a_{AA}| = \infty$ or a_{AA} finite but negative, the three-body potentials are all repulsive [29], and only deeply bound dimer channels are available. The various loss rates for this system are thus small [29]. Measuring the loss of B atoms should then provide a signature of Efimov trimer formation.

The primary processes competing with $A + A + A + B$ recombination for $|a_{AA}| \to \infty$ are three- and four-body recombination of A atoms since they will deplete the A atoms. If, as we have assumed, there are no A_2 bound states, then there is no $A + A + A$ recombination. For realistic systems with A_2 states, however, we can consider the effect of $A + A + A$ recombination via the rate equations, which suggest that $A + A + A + B$ recombination can be made dominant by increasing the density n_B of B atoms. To estimate the required n_B, we require that the rate of depletion of A atoms is dominated by four-body recombination, or $K_4 n_B > K_3$. Observing the three sets of peaks shown in Fig. 2 thus requires n_B to be on the order of 10^{15}, 10^{15}, and 10^{17} atoms/cm^3 in order of increasing energy of the peaks, using $|T_{fi}|^2 = 10^{-7}$, 10^{-4}, and 10^{-1} for the three sets of peaks, respectively, and assuming that the overall constants in K_3 and K_4 are of similar magnitude. For the three-body recombination probability, we use 10^{-3} [15]. These probabilities, however, are not expected to be universal as they depend on short-range physics. Consequently, our density estimates can change—assuming equal three- and four-body probabilities, for instance, gives n_B of 10^{11}, 10^{14}, and 10^{19} atoms/cm^3. So, with this level of uncertainty, there is hope that the first two peaks might be within experimental reach. Unfortunately, the competing $A + A + A + A$ recombination process has not yet been treated theoretically [24], so its dependence on a_{AA} beyond the overall $|a_{AA}|^7$ scaling is not known. By making $n_B \gg n_A$, though, this process might be made less important than $A + A + A + B$ recombination. These two processes can also be separated by the dependence of the latter on a_{AB} [30].

To summarize, we have taken the first steps in understanding ultracold four-body recombination into Efimov trimers. By carefully setting up the problem, we were able to obtain largely analytical results. In the process, we showed that the four-body recombination should show prominent, geometrically spaced peaks that reflect the three-body Efimov physics. In fact, these peaks are separated by precisely the factor one expects from the three-body physics. Further, we proposed a potentially useful scheme using the spectator B atoms to detect these trimer-forming events. Observing the four-body recombination loss is only the first step—studying the trimers produced is the real goal.

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Note added.—Recently, a treatment of $A + A + A + A$ recombination appeared in Ref. [31].

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