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General Theoretical Description of N-Body Recombination

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Formulas for the cross section and event rate constant describing recombination of N particles are derived in terms of general S-matrix elements. Our result immediately yields the generalized Wigner threshold scaling for the recombination of N bosons. A semianalytical formula encapsulates the overall scaling with energy and scattering length, as well as resonant modifications by the presence of N-body states near the threshold collision energy in the entrance channel. We then apply our model to the case of four-boson recombination into an Efimov trimer and a free atom.

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Few-body processes have played an increasingly crucial role in the physics of strongly interacting quantum gases. Three-body recombination in particular [1] contributes strongly to atom loss and is primarily responsible for controlling the lifetime of Bose-Einstein condensates (BEC) because the kinetic energy released in the reaction is usually sufficient to eject the collision partners from the trapping potential [2]. At ultracold temperatures, the physics of three-body recombination is largely controlled by the effective long-range potential in the entrance (three-body) channel. Hence, a threshold analysis of these potentials immediately yields information about the scaling behavior of the event rate constant K_3 with respect to both the energy E and the (s-wave) scattering length a. For instance, a threshold analysis shows that K_3 scales as a^4 and E^0 for bosons [1], making three-body recombination an important process in the ultracold limit. In contrast, the long-lived nature of the ultracold polarized Fermi gas is explained by the E^2 scaling of K_3 near threshold [3]. Further, the presence of Efimov states [4] near the threshold collision energy resonantly enhances recombination [1]. This resonant feature was exploited to confirm the existence of Efimov states in experiments with ultracold cesium [5]. The increasing number of experiments observing Efimov physics [6] highlights the importance of few-body physics in our understanding of strongly interacting quantum gases.

The natural extension of three-body recombination is to four bodies. Considerable progress has in fact been made towards the calculation of four-body processes, notably collision cross sections involving two-body fragmentation channels [7] and bound-state energies [8]. Scattering processes involving four or more free atoms are far more complex and require a deep analysis of the multiparticle continua [9,10]. Nevertheless, recent studies have proposed four-body recombination as an efficient process for the production of Efimov trimers [9,10]. Four-boson borromean states (four-body bound states with no bound subsystems) with universal properties tied to Efimov physics were recently predicted [11], further explored [10], and measured by the Innsbruck group [12] in atom loss due to recombination. The present analysis is concerned with the recombination of N particles into a channel with $N-1$ particles bound together and one free.

We use hyperspherical coordinates (see [13,14] for useful reviews), in which Jacobi vectors $\vec{\rho}_i$ are transformed to a set of angular coordinates collectively denoted Ω, plus a radial coordinate called the hyperradius R defined by $\mu_N R^2 = \sum_{i=1}^{N-1} \mu_i \rho_i^2$, where $\mu_N = [(\prod_i m_i)/M]^{1/(N-1)}$ is the N-body reduced mass, $M = \sum_i m_i$ is the total mass of the system and μ_i is the reduced mass associated with the ith Jacobi vector. At large R, the solutions to the angular portion of the Schrödinger equation yield the fragmentation channels of the N-body system, and the quantum numbers labeling those solutions index the S matrix.

Derivation of the generalized cross section.—This formulation begins by considering scattering by a purely hyperradial potential in d dimensions, and then obtains the generalized cross section "by inspection." For clarity, we adopt a notation that resembles the usual derivation in three dimensions.

In d dimensions, the wave function at large R behaves as

$$\Psi^I \to e^{i\vec{k}\cdot\vec{R}} + f(\hat{k},\hat{k}')\frac{e^{ikR}}{R^{(d-1)/2}}. \quad (1)$$

Equivalently, an expansion in hyperspherical harmonics is written in terms of unknown coefficients $A_{\lambda\mu}$:

$$\Psi^{II} = \sum_{\lambda,\mu} A_{\lambda\mu} Y_{\lambda\mu}(\hat{R})[j_\lambda^d(kR)\cos\delta_\lambda - n_\lambda^d(kR)\sin\delta_\lambda]. \quad (2)$$

Here, $Y_{\lambda\mu}$ are hyperspherical harmonics (solutions to the free-space angular equation $[\Lambda^2 - \lambda(\lambda + d - 2)]Y_{\lambda\mu} = 0$, where Λ^2 is the grand angular momentum operator [14]) and j_λ^d (n_λ^d) are hyperspherical Bessel (Neumann) functions [14].

Identification of the incoming wave parts of Ψ^{I} and Ψ^{II} yields the coefficients $A_{\lambda\mu}$, whose insertion into Eq. (2) gives

$$f(\hat{k},\hat{k}') = \left(\frac{2\pi}{k}\right)^{(d-1/2)} \sum_{\lambda\mu} i^{\lambda} e^{-i(d/2-1+\lambda)\pi/2 - i\pi/4} Y^{*}_{\lambda\mu}(\hat{k}) \times Y_{\lambda\mu}(\hat{k}')(e^{2i\delta_{\lambda}} - 1). \tag{3}$$

The immediate generalization of this elastic scattering amplitude to an anisotropic short-range potential is

$$f(\hat{k},\hat{k}') = \left(\frac{2\pi}{k}\right)^{(d-1/2)} \sum_{\lambda\mu\lambda'\mu'} i^{\lambda} e^{-i\eta_{\lambda}} Y^{*}_{\lambda\mu}(\hat{k}) Y_{\lambda'\mu'}(\hat{k}') \times (S_{\lambda\mu,\lambda'\mu'} - \delta_{\lambda\lambda'}\delta_{\mu\mu'}), \tag{4}$$

where $\eta_{\lambda} = (d/2 - 1 + \lambda)\pi/2 + \pi/4$. Upon integrating $|f(\hat{k},\hat{k}')|^2$ over all final hyperangles $\hat{k}$, and *averaging* over all initial hyperangles $\hat{k}'$ as would be appropriate to a gas phase experiment, we obtain the average integrated elastic scattering cross section by a short-range potential:

$$\sigma^{\rm dist} = \left(\frac{2\pi}{k}\right)^{d-1} \frac{1}{\Omega(d)} \sum_{\lambda\mu\lambda'\mu'} |S_{\lambda\mu,\lambda'\mu'} - \delta_{\lambda\lambda'}\delta_{\mu\mu'}|^2, \tag{5}$$

where $\Omega(d) = 2\pi^{d/2}/\Gamma(d/2)$ is the total solid angle in d dimensions [14]. This last expression is immediately interpreted as the generalized average cross section resulting from a scattering event that takes an initial channel into a final channel, $i \equiv \lambda'\mu' \rightarrow \lambda\mu \equiv f$. Since this S matrix is manifestly unitary in this representation, it immediately applies to inelastic collisions as well, including N-body recombination. It is worth noting that the sum in Eq. (5) should include degeneracies, and that the cross section should be appropriately averaged over initial spin substates and collision energies.

In this form, we can *interpret* the generalized cross section derived above in terms of the unitary S-matrix computed by solving the exact coupled-channels reformulation of the few-body problem within the adiabatic hyperspherical representation [15]. In principle this can describe collisions of an arbitrary number of particles. Identical particle symmetry is handled by summing over all indistinguishable amplitudes before taking the square, averaging over incident directions and momenta for a given energy, followed by integrating over distinguishable final states to obtain the total cross section: $\sigma^{\rm indist} = N_p \sigma^{\rm dist}$. Here N_p is the number of terms in the permutation symmetry projection operator (e.g., for N identical particles, $N_p = N!$).

The cross section for total angular momentum J and parity Π includes an explicit $2J + 1$ degeneracy. Hence, the total generalized cross section (with dimensions of length^{d-1}) for N particles in all incoming channels i to scatter into the final state f, properly normalized for identical particle symmetry, is given in terms of general S-matrix elements as

$$\sigma^{\rm indist}_{fi}(J^{\Pi}) = N_p \left(\frac{2\pi}{k_i}\right)^{d-1} \frac{1}{\Omega(d)} \sum_i (2J+1)|S^{J^{\Pi}}_{fi} - \delta_{fi}|^2. \tag{6}$$

The event rate constant [recombination probability per second for each distinguishable N group within a (unit volume)$^{(N-1)}$] is the generalized cross section Eq. (6) multiplied by a factor of the N-body hyperradial "velocity" (including factors of $\hbar$ to explicitly show the units of K_N):

$$K^{J^{\Pi}}_{N} = \frac{\hbar k_i}{\mu_N} \sigma^{\rm indist}_{fi}(J^{\Pi}). \tag{7}$$

Treatment of N bosons.—The structure of a relevant S-matrix element from an adiabatic hyperspherical viewpoint is seen to be $S^{J^{\Pi}}_{fi} = \langle \Phi^{J^{\Pi}}_{f}(R;\Omega)F_f(R)|\hat{S}| \times \Phi^{J^{\Pi}}_{i}(R;\Omega)F_i(R)\rangle$, where $\Phi^{J^{\Pi}}_{i}$ and $\Phi^{J^{\Pi}}_{f}$ are the channel functions (i.e., solutions to the hyperangular part of the Schrödinger equation in the limit $R \rightarrow \infty$) for the entrance and final channel, respectively. For all N-body entrance channels we have $i \rightarrow \lambda$, where λ is the hyperangular momentum quantum number associated with eigenfunction $Y_{\lambda\mu}$. The functions F_i and F_f are the large R solutions to the coupled hyperradial equations obtained in the adiabatic hyperspherical representation [15] (in units where $\hbar = 1$):

$$\left[\frac{-1}{2\mu_N}\frac{\partial^2}{\partial R^2} + W_i(R) - E\right]F_i + \sum_{f\neq i} V_{if}(R)F_f = 0. \tag{8}$$

Asymptotically (as $R \rightarrow \infty$) the couplings $V_{if}(R)$ vanish and the effective potentials in the N-body continuum channels are expressed in terms of an *effective* angular momentum quantum number l_e:

$$W_{\lambda}(R) \rightarrow \frac{l_e(l_e+1)}{2\mu_N R^2} \quad \text{with} \quad l_e = (2\lambda + d - 3)/2. \tag{9}$$

Near threshold, the recombination cross section is controlled by the *lowest* N-body entrance channel $i = \lambda \rightarrow \lambda_{\rm min} = 0$. For N identical bosons in a thermal (non-quantum-degenerate) gas cloud, the dominant contribution to Eq. (6) is from $J^{\Pi} = 0^{+}$. Further, unitarity of the S matrix allows us to write the *total* rate constant summed over all final channels (using $d = 3N - 3$) as

$$K^{0^+}_{N} = \frac{2\pi\hbar N!}{\mu_N} \frac{(2\pi/k)^{(3N-5)}}{\Omega(3N-3)} (1 - |S^{0^+}_{00}|^2). \tag{10}$$

Based on prior hyperspherical treatments for three [16] and four [10] bosons, in cases where one or more $(N-1)$-body state is bound with no bound states of fewer particles, we expect the hyperradial potentials to schematically look like those sketched in Fig. 1. Monte Carlo calculations [17] of N-boson systems provide evidence of superborromean states which could produce the topology shown in Fig. 1. For four bosons, potentials with the topology shown occur at negative scattering lengths ($a < 0$).

The semiclassical (WKBJ) treatment of Berry [18] can be generalized, giving a *complex* phase shift δ_{l_e} for collisions of N identical bosons. The phase shift is acquired in terms of the phase ϕ accumulated in the classically allowed region ($R_3 < R < R_2$), and the tunneling integral γ in the classically forbidden regions:

$$\phi = \int_{R_3}^{R_2} q(R)dR; \quad \text{and} \quad \gamma = \text{Im}\int_{R^*}^{(3N-5)/2k} q(R)dR, \tag{11}$$

where $q(R) = \sqrt{2\mu_N[E - W'(R)]}$ (W' is the effective potential including the Langer correction [19]), and R^* is the hyperradius at which the inelastic coupling to the exit channel peaks [typically at hyperradii much greater than the range of the two-body interaction r_0; i.e., $r_0 \ll R^* \lesssim R_3$ for recombination into a universal $(N-1)$-body state].

The inelastic amplitude is incorporated into the phase by letting $\phi \to \phi + i\eta$ [20]. Applying the connection formulas for each of the classical turning points R_1, R_2, and R_3 shown in Fig. 1 gives the phase shift:

$$\delta_{l_e} = \delta_{l_e}^{(0)} - \arctan[\tfrac{1}{4}e^{-2\gamma}\cot(\phi + i\eta - \pi/2)]. \tag{12}$$

Here, $\delta_{le}^{(0)}$ is the real semiclassical phase shift derived by ignoring the interior region, which does not contribute to the inelastic probability. The S-matrix element describing scattering from one N-boson state to another is then simply $S_{00} = e^{2i\delta_{l_e}}$, and the total probability to recombine into all available final channels is

$$1 - |S_{00}|^2 = \frac{e^{-2\gamma}}{2}\frac{\sinh(2\eta)}{\cos^2\phi + \sinh^2\eta}A(\eta, \gamma, \phi), \tag{13}$$

where the function $A(\eta, \gamma, \phi)$:

$$A(\eta, \gamma, \phi) = \left|1 + \frac{e^{-2\gamma}}{4}\tanh(\eta + i\phi)\right|^{-2} \tag{14}$$

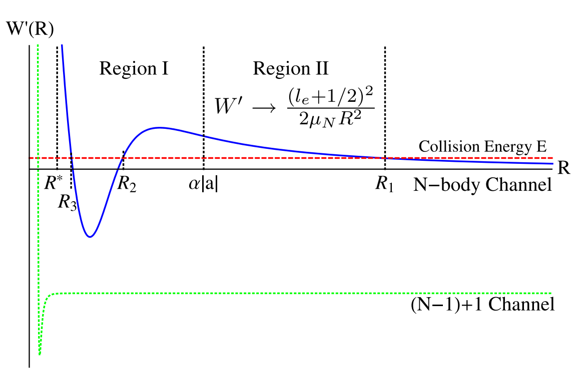

FIG. 1 (color online). A schematic representation of the N-boson hyperradial potential curves is shown. When a metastable N-boson state crosses the collision energy threshold at $E = 0$, N-body recombination into a lower channel with $N - 1$ atoms bound plus one free atom is resonantly enhanced.

is equal to unity in the threshold limit *unless* both $\eta \to 0$ and $\phi \to \pi/2$.

The threshold energy dependence of $K_N^{0^+}$ is found by breaking γ into two pieces corresponding to the regions shown in Fig. 1:

$$\gamma_{II} = \int_{\alpha|a|}^{(3N-5)/2k} |q(R)|dR; \quad \gamma_I = \text{Im}\int_{R^*}^{\alpha|a|} q(R)dR. \tag{15}$$

For recombination into a *universal* $(N-1)$-body bound state, we expect $R^* \gg r_0$, in which case γ, ϕ, and η are also universal. A simple calculation shows $e^{-2\gamma_{II}} = [2k\alpha|a|/(3N-5)]^{3N-5}$. It is convenient to introduce an α-independent function $C(a) = C_N\alpha^{(3N-5)}e^{-2\gamma_I}$. The constant C_N must be adjusted to give the correct overall scale of $K_N^{0^+}$. The full N-boson recombination rate constant in the ultracold limit is then

$$K_N^{0^+} = \frac{\pi\hbar N!}{\mu_N\Omega(3N-3)}\left(\frac{4\pi|a|}{3N-5}\right)^{3N-5}\frac{C(a)\sinh(2\eta)}{\cos^2\phi + \sinh^2\eta}. \tag{16}$$

Note that this is a quantitative result valid in the threshold regime. It is a *constant* (independent of k), and scales roughly as $|a|^{3N-5}$ (in agreement with [21]). Hence, N-body processes could contribute to the total atom loss at higher particle density n through terms of the form $-K_N n^N$: $\frac{dn}{dt} = \sum_{N=2}^{N_{\max}} -L_N n^N$, where the atom-loss rate L_N is related to the event rate by $L_N = K_N/(N-1)!$ provided each recombination event ejects N atoms from the trapped gas. (Recall also that for a quantum-degenerate Bose gas, the above expressions for K_N must be divided by $N!$ [22].) For $N = 3$, Eq. (16) is consistent with the expression found by Braaten and Hammer [20] and the

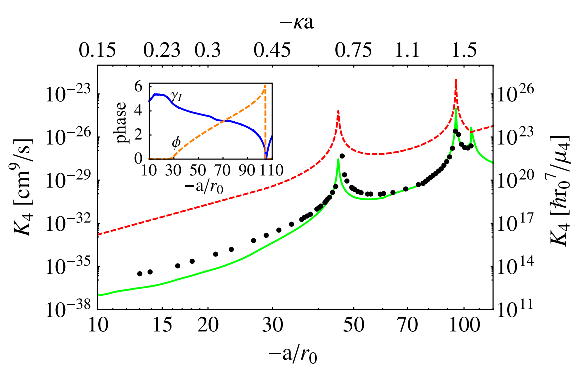

FIG. 2 (color online). The four-boson recombination rate constant $K_4^{0^+}$ is shown over approximately one range of the discrete scaling factor e^{π/s_0} [10]. The dots are obtained by numerically solving the coupled hyperradial equations, while the solid green curve is obtained from Eq. (16) with $N = 4$, $\eta = 0.01$, and $C_4 = 55$. The dashed red curve is a calculation using Eq. (16), but ignoring the additional suppression due to γ_I. The inset shows the universal phases ϕ and γ_I used in Eq. (16). While γ_I is shown here for $\alpha = 10$, results for $K_4^{0^+}$ are independent of α (see text).

phase ϕ acquires the universal log-periodicity characteristic of Efimov physics [4].

Recombination of four bosons with $a < 0$.—Now we specialize our results to the case of four identical bosons ($d = 9$, $J = 0$, $N_p = 4!$, and no degeneracy). Using numerical hyperradial potential curves for four bosons interacting via a short-range model potential [10], we obtain $K_4^{0^+}$ both by solving the coupled channels numerically and by using Eq. (16) specialized to $N = 4$. In Fig. 2, we show $K_4^{0^+}$ on an absolute scale [cm^9/s] (where we use parameters appropriate for ^{133}Cs: $m = 244\,188$ a.u. and $r_0 = 100$ a.u.), and in model units of $[\hbar r_0^7/\mu_4]$. The horizontal axis is shown in units of r_0 and in units of the universal "three-body parameter" $\kappa = \sqrt{m|E_{3B}^{(2)}|}/\hbar$, where $E_{3B}^{(2)}$ is the bound-state energy of the second Efimov trimer at unitarity. The overall magnitude of $K_4^{0^+}$ is governed by $-a/r_0$, while the position of the peaks is fixed with respect to $-\kappa a$. However, because κ and r_0 are related by a nonuniversal factor, the relationship between the two horizontal axes in Fig. 2 is model dependent. These results show good agreement between the two calculations demonstrating the validity of the WKBJ approximation. The results show the overall $|a|^7$ scaling modified by resonant peaks at

$$\kappa|a| \approx 0.65 \quad \text{and} \quad \kappa|a| \approx 1.36. \tag{17}$$

A cusp in K_4 appears at $\kappa|a| \approx 1.51$ [23] when a new atom-trimer channel appears (i.e., a new Efimov state becomes bound), whereas peaks appear when a four-boson state sits at the threshold of the entrance channel.

As was recently noted [10], *two* four-boson states are bound at slightly *less negative* values of a than the values of a at which an Efimov trimer becomes bound. In the potentials of Fig. 1 for $N = 4$, the entrance channel is capable of supporting four-boson bound states, but the second trimer-atom channel is not yet available. Because inelastic transitions occur at hyperradii of order the size of the lowest Efimov trimer, C, ϕ, and η are universal functions of a. We assume η is independent of a, and use $\eta = 0.01$ and $C_4 = 55$ in Fig. 2. For larger values of $|a|$, the universal structure of Fig. 2 repeats with the three-boson scale factor $e^{\pi/s_0} \approx 22.7$ [10]. The Innsbruck group has recently observed this universal connection between Efimov states and four-boson states and confirmed the spacing implied by Eq. (17), and the observed atom-loss rates are consistent with the absolute scale in Fig. 2 [12].

In conclusion, we have derived a general formula for the event rate constant for N-body recombination. The generalized Wigner threshold scaling laws immediately follow, and the overall scaling is resonantly modified by the presence of metastable N-body states near threshold. We then specialize to four bosons with $a < 0$.

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