Mass dependence of ultracold three-body collision rates

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We show that many aspects of ultracold three-body collisions can be controlled by choosing the mass ratio between the collision partners. In the ultracold regime, the scattering length dependence of the three-body rates can be substantially modified from the equal mass results. We demonstrate that the only nontrivial mass dependence is due solely to Efimov physics. We have determined the mass dependence of the three-body collision rates for all heteronuclear combinations relevant for two-component atomic gases with resonant *s*-wave interspecies interactions, i.e., three-body systems with two identical bosons or two identical fermions.

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The achievement of quantum degeneracy in ultracold gases with different atomic species $[1]$ has driven experimental studies of several novel phenomena. The observation of interspecies Feshbach resonances in boson-fermion mixtures [2] allows considerable flexibility for exploring new regimes by controlling the interspecies interactions. Boson-mediated Cooper pairing [3], for instance, can substantially increase the critical temperature for a phase transition to the Bardeen-Cooper-Schrieffer (BCS) regime. The collapse of the fermionic component as well as the phase separation of both components can be studied [4] along with the creation of ultracold polar molecules $[5]$. It is worth noting that heteronuclear boson-fermion molecules are composite fermions which allows a new type of crossover between an atomic Bose-Einstein condensate and a molecular Fermi-type superfluidity [6]. Heteronuclear boson-boson and fermion-fermion mixtures have also been studied $[7]$, but no Feshbach resonances have yet been reported.

The magnetic field sensitivity of the hyperfine states is the key to controlling the interatomic interactions in ultracold gases. By applying an external magnetic field near a diatomic Feshbach resonance, the *s*-wave scattering length *a*, which characterizes the low-energy interatomic interactions, can take any value from the weakly $(a \rightarrow 0)$ to the strongly $(|a| \rightarrow \infty)$ interacting limits. Even though two-body loss processes can usually be minimized by using resonances in the lowest hyperfine states, three-body loss processes can still be substantial. Fortunately, near the resonance, when $|a| \ge r_0$ (with r_0 being the characteristic range of the interatomic interactions) processes such as vibrational relaxation, $X + X_2^*$ \rightarrow *X*+*X*₂, three-body recombination, *X*+*X*+*X* \rightarrow *X*+*X*₂², and collision-induced dissociation, $X + X_2^* \rightarrow X + X + X$, no longer depend on the details of the interactions and universal predictions can be made.

Recent experiments have underscored the importance of knowing the *a* dependence of three-body rates in order to determine the atomic and molecular lifetimes. In fact, threebody losses have been used to locate Feshbach resonances [2] and to create ultracold molecules [8]. While general results for threshold [9] and scattering length scaling laws of three-body equal mass systems $[10]$ have been obtained, however, there are no similarly general scaling laws for heteronuclear systems. The specific case of recombination in a two-component Fermi gas has been investigated, though, and found to scale as a^6 for $a>0$, and minima were predicted as

a function of the mass ratio between the collision partners [11].

In this paper, we demonstrate that the mass ratio has a large impact on ultracold threebody collisional losses, allowing a certain degree of control. Using the simple physical picture developed in Ref. [10], extended to include heteronuclear systems, we have determined that the scattering length scaling laws can differ substantially from the equal mass results $[10]$. For instance, in a system with two identical fermions that are much heavier than the third atom, relaxation of weakly bound heteronuclear molecules scales approximately as *a*−7—an even stronger suppression than the $a^{-3.33}$ scaling found when all three atoms have equal mass [10,12]. This scaling was derived in Ref. [12] to explain the long molecular lifetimes observed experimentally for molecules formed of fermions in different spin states. It was their long lifetimes that made further experiments with these molecules feasible $[8,13]$. The stronger suppression found here might open other experimental avenues.

In our picture, the mass dependence enters via the threebody effective potentials and is associated with Efimov physics $[14]$. In fact, we demonstrate here that the only nontrivial mass dependence is due solely to Efimov physics. We determine the mass dependence of the collision rates for threebody systems relevant to all two-component atomic gases with resonant interspecies *s*-wave interactions, which amounts to systems with two identical bosons or two identical fermions. In this work, we analyze the cases where the intraspecies interactions are not resonant so that only the interspecies scattering length is important. We have also assumed that the atoms are spin polarized. These cases, though, are those most likely to be relevant for current experiments.

For short-range two-body interactions, the ultracold behavior of three-body systems can be derived from three-body effective potentials and couplings $[10]$ which, in the adiabatic hyperspherical representation, are determined from the adiabatic equation $[15]$,

$$
H_{\text{ad}}(R,\Omega)\Phi_{\nu}(R;\Omega) = U_{\nu}(R)\Phi_{\nu}(R;\Omega). \tag{1}
$$

This equation is obtained from the full Schrödinger equation by fixing the hyperradius *R*, leaving only dynamics in the hyperangles Ω through H_{ad} . By expanding the total wave function on the adiabatic basis Φ_{ν} , the Schrödinger equation (in atomic units) is reduced to:

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

where *E* is the total energy, F_v is the hyperradial wave function, and ν is a collective index that represents all quantum numbers necessary to label each channel. In the present case, the three-body reduced mass is $\mu = m/\sqrt{\delta(\delta + 2)}$ where *m* is the mass of the distinguishable particle and δ is the ratio of the different atom mass to the identical atom mass. This equation describes the collective radial motion under the influence of the effective potential W_v as well as any inelastic transitions controlled by the nonadiabatic couplings $V_{\nu\nu}$.

In the limit $|a| \ge r_0$, the effective potentials W_{ν} depend crucially on Efimov physics $[10,14]$. In Ref. $[10]$, we described a scheme that uses this fact to classify all equal-mass three-body systems with resonant *s*-wave pairwise interactions. In this scheme, each system falls into one of two categories: those with an attractive dipole (R^{-2}) potential in the range $r_0 \ll R \ll |a|$ and those only with repulsive dipole potentials. Which category a particular system falls into depends on its symmetry J^{π} (total angular momentum *J* and parity π) and the identical particle permutational symmetry, i.e., whether they are bosons or fermions. For heteronuclear systems, this basic classification scheme still holds, and the extension of the analysis of the three-body rates requires only slight modifications which, in turn, come almost entirely from the δ dependence of the dipole potential strengths.

For each category, there are three distinct regions in *R* that characterize the effective potentials (for a schematic picture, see Fig. 1 in Ref. [10]): $R \le r_0$, $r_0 \le R \le |a_{\delta}|$, and $R \ge |a_{\delta}|$ where $a_{\delta} = [\sqrt{\delta(\delta+2)/(\delta+1)}]^{1/2}a$. Replacing *a* by a_{δ} in these definitions is the first mass-dependent modification of our previous analysis. In the asymptotic region, $R \geq a_{\delta}$, the potentials can be derived analytically $[16]$. They are associated with molecular channels, which represent atom-molecule scattering, and with three-body continuum channels, which represent collisions of three free atoms, and are given respectively by

$$
W_{\nu} = E_{\nu l'} + \frac{l(l+1)}{2\mu R^2} \quad \text{and } W_{\nu} = \frac{\lambda(\lambda + 4) + 15/4}{2\mu R^2}.
$$
 (3)

The molecular bound state energy E_{vl} is labeled by the rovibrational quantum numbers v and l' ; l is the atom-molecule relative angular momentum; and λ labels the eigenstates of the hyperangular kinetic energy.

For $r_0 \ll R \ll |a_{\delta}|$, the potentials for the molecular and continuum channels $[Eq. (3)]$ are modified due to Efimov physics, establishing our classification scheme. In the first category, an attractive dipole potential occurs in the highest vibrationally excited *s*-wave molecular channel for $a > 0$ and in the lowest continuum channel for $a < 0$. The potentials for all higher-lying channels are repulsive. These potentials are conveniently parameterized by the coefficients s_0 and s_{ν} :

$$
W_{\nu}(R) = -\frac{s_0^2 + \frac{1}{4}}{2\mu R^2} \quad \text{and} \ W_{\nu}(R) = \frac{s_{\nu}^2 - \frac{1}{4}}{2\mu R^2}.
$$
 (4)

In the second category, the potentials for the weakly bound molecular channel and the continuum channels are repulsive and parametrized by coefficients p_0 and p_{ν} :

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$$
W_{\nu}(R) = \frac{p_0^2 - \frac{1}{4}}{2\mu R^2} \quad \text{and} \ W_{\nu}(R) = \frac{p_{\nu}^2 - \frac{1}{4}}{2\mu R^2}.
$$
 (5)

In both categories, however, deeply bound molecular channels are essentially independent of *a*. In the above equations, the coefficients s_0 , s_{ν} , p_0 , and p_{ν} depend on the number of resonant pairs, the number of identical particles, and the mass ratio δ between collision partners [14]. For $R \le r_0$, the potentials depend on the details of the interatomic interactions and can lead to resonance effects due to three-body shape or Feshbach resonances.

In the adiabatic hyperspherical representation, inelastic transitions at ultracold temperatures proceed via tunneling in the initial collision channel to where the coupling $V_{\nu\nu'}$ peaks—the coupling, of course, drives the transition. We have previously shown that a simple WKB approximation to the tunneling probability through the potentials given by Eqs. (3) – (5) is sufficient to determine both the threshold and the scattering length scaling laws for equal mass three-body collisions [10]. For heteronuclear systems, a_{δ} , s_0 , s_{ν} , p_0 , and p_{ν} generate the only nontrivial mass dependence in the threebody rates and follow directly from Efimov's analysis.

For systems and symmetries from our first category with an attractive potential (4)], relaxation for $a > 0$ is

$$
V_{\rm rel} \propto \mu^{l-1} E_{\rm coll}^{l} \frac{\sinh(2\,\eta)}{\sin^{2}[s_{0} \ln(a \, s/r_{0}) + \Phi] + \sinh^{2}(\eta)} a_{\delta}^{2l+1};\tag{6}
$$

and for $a < 0$, $V_{rel} \propto \mu^{l-1} E_{coll}^l r_0^{2l+1}$. $E_{coll} = E - E_{vl'}$ is the collision energy, Φ is an unknown short-range phase [10], and η labels parameters related to the inelastic transition probability at small distances [17]. These parameters can depend on the masses nontrivially and can lead to resonance effects, depending upon details of the interactions. Recombination for $a>0$ and $a<0$ is given by

$$
K_3 \propto \mu^{\lambda - 1} E^{\lambda} \Big[\sin^2 \Big[s_0 \ln \Big(\frac{a_{\delta}}{r_0} \Big) + \Phi \Big] + A_{\eta} \Big(\frac{r_0}{a_{\delta}} \Big)^{2s_{\nu}} \Big] a_{\delta}^{2\lambda + 4},
$$

$$
K_3 \propto \mu^{\lambda - 1} E^{\lambda} \frac{\sinh(2\eta)}{\sin^2[s_0 \ln(|a_{\delta}|/r_0) + \Phi] + \sinh^2(\eta)} |a_{\delta}|^{2\lambda + 4}, \qquad (7)
$$

For systems and symmetries from our second category [with a repulsive potential (5)], relaxation for $a > 0$ is

$$
V_{\rm rel} \propto \mu^{l-1} E_{\rm coll}^l (r_0/a_\delta)^{2p_0} a_\delta^{2l+1},\tag{8}
$$

while it is $V_{\text{rel}} \propto \mu^{l-1} E_{\text{coll}}^l r_0^{2l+1}$ for $a < 0$. Recombination for $a > 0$ and $a < 0$ is given by

$$
K_3 \propto \mu^{\lambda - 1} E^{\lambda} \left[1 + A_{\eta} \left(\frac{r_0}{a_{\delta}} \right)^{2p_0} + B_{\eta} \left(\frac{r_0}{a_{\delta}} \right)^{2p_{\nu}} \right] a_{\delta}^{2\lambda + 4},
$$

$$
K_3 \propto \mu^{\lambda - 1} E^{\lambda} (r_0 / |a_{\delta}|)^{2p_0} |a_{\delta}|^{2\lambda + 4}.
$$
 (9)

The mass dependence of s_0 and p_0 can substantially modify the *a* dependence of the three-body rates. The coefficients s_{ν} and p_{ν} , however, do not affect the scaling laws. Figure 1 shows s_0 and p_0 for systems with two identical bosons *(BBX,* $\delta = m_X/m_B$ *)* and with two identical fermions $(FFX, \delta = m_X/m_F)$. These coefficients are determined analyti-

FIG. 1. Mass dependence of s_0 and p_0 , for (a) two identical boson and (b) two identical fermion systems.

cally following Ref. [14] after proper symmetrization. It is important to notice that for $J>0$ the effective potentials can change from attractive to repulsive and vice versa, changing the category in which the system is classified, and thus modifying its collisional properties. It happens, for instance, for 2⁺ *BBX* systems at $\delta_c \approx 0.0259$ [Fig. 1(a)] and for 1[−] *FFX* systems at $\delta_c \approx 0.0735$ [Fig. 1(b)].

For bosonic systems *BBX*, the dominant contribution for relaxation and recombination is $J^{\pi}=0^+$ with $l=0$ and $\lambda=0$, and is described by Eqs. (6) and (7) due to the presence of an attractive dipole potential. In this case, the variations of s_0 with δ [Fig. 1(a)] changes the number of Efimov states. These variations manifest themselves in the three-body rates through the locations of the minima and peaks in Eqs. (6) and (7). We note that the mass dependence in this case does not modify the scaling laws.

In contrast, for fermionic systems *FFX*, the power-law behavior does change with mass for the dominant contributions to relaxation $(J^{\pi}=0^+$ with $l=0$) and recombination $(J^{\pi} = 1^-$ with $\lambda = 1$). These changes follow from the mass dependence of the repulsive dipole potential due to p_0 [Fig. $1(b)$] combined with Eqs. (8) and (9). It follows that relaxation for $FX + F$ collisions scales as a^{1-2p_0} for $a > 0$ and is suppressed for all δ since $2 \le p_0 \le 4$ [Fig. 1(b)], approaching its greatest suppression, a^{-7} , as $\delta \rightarrow 0$ and its least, a^{-3} , as $\delta \rightarrow \infty$. Suppression of *FX*+*F* collisions can thus be much stronger than $a^{-3.33}$, found for $\delta=1$ *FF'* +*F* collisions of fermionic atoms in different spin states $[10,12]$. Extremely long-lived heteronuclear molecules in ultracold boson-

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fermion and fermion-fermion mixtures might thus be possible. The modifications to the recombination scaling law occurs for *a* < 0 and $\delta \ge 0.0735$ where it scales as *a*^{6−2*p*₀ with} $0 \le p_0 \le 2$ [Fig. 1(b)]; otherwise it scales as a^6 , leading to an asymmetry between $a>0$ and $a<0$. The strongest asymmetry is obtained when $\delta \rightarrow \infty$, where recombination scales as a^6 and $|a|^2$, respectively, so that greater collisional stability against recombination might be expected for $a < 0$.

As mentioned above, recombination for *FFX* systems with $\delta \geq 0.0735$ was studied in Ref. [11] and found to scale as a^6 for $a>0$ which agrees with our prediction. It was also predicted that the recombination rate oscillates as a function of δ with zeros at $\delta = 0.0735, 0.1160$, and as $\delta \rightarrow \infty$ (note that the mass ratio in [11] is $1/\delta$). These zeros were ascribed to a decoupling of the three-body continuum and bound channels [11], leading to elastic scattering only, and have also been interpreted as interference effects $[17]$. In our formulation, however, no such zeros are predicted. In fact, in this range of δ , the potentials for both continuum and bound channels, Eq. (5), are repulsive and interference effects are expected to be suppressed by tunneling. Further, we have noticed through representative numerical calculations that the continuum and bound channels never decouple and that the nonadiabatic coupling peaks at $R \approx r_0$ and $R \approx a$, in accord with our model [10]. While we have observed minima in our calculations, they do not correspond to the minima discussed in Ref. [11]. They are most likely a consequence ofusing a two-body potential with finite *a*, and we expect them to disappear in the limit $a \rightarrow \infty$ considered in [11]. Preliminary numerical results support this expectation.

Table I summarizes the threshold and scattering length scaling laws for the three-body rates, including dissociation D_3 . The three dominant partial waves (as determined by their energy dependence) are shown for each process. The table thus indicates the terms expected to be important for finite energies or $|a| \rightarrow \infty$. For *BBX* systems, these contributions are not expected to be important for relaxation with $a > 0$ or recombination with $a < 0$. For *FFX* systems, however, the higher partial waves are comparatively more important.

In two-component ultracold atomic gases with resonant interspecies interactions, the important three-body processes are those that involve both atomic species, assuming that intraspecies interactions are not resonant. In this case, there are only two relevant systems and the competition between the collision rates for each system as well as the density of

TABLE I. Threshold and scattering length scaling laws for three-body rates. For 2⁺ *BBX* and 1[−] *FFX* systems the rates are given for $\delta < \delta_c$ and $\delta > \delta_c$. Boldface indicates the leading contribution at threshold.

	J^{π}	$V_{\rm rel}$		$K_3(D_3)$		
		E	a>0	E	a > 0	a<0
BBX	0^+	const	$\mathfrak a$	$\text{const}(E^2)$	a^4	$ a ^4$
	$1 -$	E_{coll}	a^{3-2p_0}	$E(E^3)$	a^6	$ a ^{6-2p_0}$
	2^+	E_{coll}^2	a^5 , a^{5-2p_0}	$E^2(E^4)$	a^8 , a^8	$ a ^8$, $ a ^{8-2p_0}$
FFX	0^+	const	a^{1-2p_0}	$E^2(E^4)$	a^8	$ a ^{8-2p_0}$
	1^{-}	E_{coll}		$E(E^3)$	a^6 , a^6	$ a ^6, a ^{6-2p_0}$
	2^+	E_{coll}^2	a^3 , a^{3-2p_0} a^{5-2p_0}	$E^2(E^4)$	a^8	$ a ^{8-2p_0}$

each species determines the atomic and molecular lifetimes. In boson-fermion mixtures, for instance, relaxation for *BF* +*F* collisions decreases with *a* while for *BF*+*B* it increases. In this case, if all bosons are bound in *BF* molecules, the molecules are expected to be long lived. Otherwise, the molecules will be rapidly quenched by collisions with the bosonic atoms.

Vibrational relaxation, as we have shown, can be controlled by choosing the atomic species according to their mass, and consequently, the molecular lifetime can be substantially modified. We show in Table II the suppression predicted for *BF*+*F* collisions of commonly used alkali-metal atoms. The table includes systems used in recent experiments: $^{23}Na-^{6}Li$ and $^{87}Rb-^{40}K$ [2], as well as $^{7}Li-^{6}Li$. [6]. We have included H due to the prospects for using it for sympathetic cooling [18]. Molecule-molecule collisions also contribute to the molecular lifetime $[12]$, but in bosonfermion mixtures the molecules are composite fermions so that only *p*-wave molecule-molecule collisions occur. In this case, molecule-molecule collisions are suppressed for ultracold temperatures, and atom-molecule collisions are expected to be dominant.

In this paper, we have explored the mass dependence of the ultracold three-body collision rates and derived its energy and scattering length dependence for all cases relevant for two-component quantum gases with resonant interspecies interactions, assuming nonresonant intraspecies interactions. In the process, we have demonstrated that the mass dependence in three-body collisions is intimately related with Efimov physics. In bosonic systems, the mass dependence affects the

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TABLE II. Scattering length scaling laws for relaxation $(a>0)$ of *BF*+*F* collisions in boson-fermion mixtures based solely on mass.

features due to Efimov physics, but leaves the dominant scattering length scaling laws unchanged. In fermionic systems, however, the mass dependence modifies the scattering length scaling laws substantially from the equal mass results. The stronger suppression found for relaxation of weakly bound heteronuclear molecules in boson-fermion mixtures, suggests the possibility of long-lived heteronuclear fermionic molecules.

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