Three-body recombination of cold fermionic atoms

H Suno\textsuperscript{1}, B D Esry\textsuperscript{1} and Chris H Greene\textsuperscript{2}

\textsuperscript{1} Department of Physics, Kansas State University, Manhattan, KS 66506, USA
\textsuperscript{2} Department of Physics and JILA, University of Colorado, Boulder, CO 80309, USA
E-mail: esry@phys.ksu.edu

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Abstract. Recombination of identical, spin-polarized fermions in cold three-body collisions is investigated. We parametrize the mechanisms for recombination in terms of the ‘scattering volume’ $V_p$ and another length scale $r_0$. Model two-body interactions were used within the framework of the adiabatic hyperspherical representation. We examine the recombination rate $K_3$ as a function of the collision energy $E$ for various values of $V_p$. Not only do we consider the dominant $J^{\pi}=1^+$ case, but also the next-leading order contributions from $J^{\pi}=1^-$ and $3^-$. We discuss the behaviour near a two-body resonance and the expected universality of fermionic recombination. Comparisons with boson recombination are considered in detail.

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1. Introduction

Three-body recombination is a three-body collision process in which two atoms form a molecular bound state and the third one carries away the binding energy. This process limits the achievable density and lifetime in ultracold dilute gases such as degenerate Fermi gases [1] and Bose–Einstein condensates (BECs) (for example [2]). Three-body recombination and the time-reversed process of collision-induced dissociation are also important in nuclear physics, atmospheric chemistry and combustion chemistry. Several theoretical investigations have been carried out for ultracold bosons: Fedichev et al [3] predicted that the three-body recombination rate \( K_3 \) grows with the two-body s-wave scattering length \( a_s \), namely \( K_3 \propto a_s^4 \) for \( a_s > 0 \). This scaling was later confirmed by Nielsen and Macek [4] who also pointed out that it should hold for negative \( a_s \). The scaling law for both signs of \( a_s \) was indeed obtained by Esry et al [5], then again by Bedaque et al [6] for \( a_s > 0 \) and Braaten and Hammer [7] for \( a_s < 0 \). Three-body recombination of fermions, however, has not yet been considered [8].

The purpose of this paper is to study the recombination of three identical, spin-polarized fermionic atoms in cold collisions. This study is important since experimentalists are increasingly working with trapped fermions such as \(^{40}\text{K} \) [9] and \(^{6}\text{Li} \) [10, 11] with the aim of observing pairing of fermions, hopefully leading to a state analogous to superconductivity. In the case of identical fermions, the relevant low-energy scattering parameter is the two-body p-wave ‘scattering volume’ defined as

\[
V_p = -\lim_{k \to 0} \frac{\tan \delta_p(k)}{k^3},
\]

where \( \delta_p(k) \) is the p-wave scattering phase shift and \( k \) is the wavenumber. We choose \( V_p \) rather than the p-wave scattering length \( a_p (\equiv V_p^{1/3}) \) [12] since an artificial nonanalyticity is introduced into \( a_p \) when taking the cube root of the quantity in the right-hand side of equation (1).

We examine the behaviour of the recombination rate \( K_3 \) as a function of the scattering volume \( V_p \) by numerically solving the three-body Schrödinger equation for scattering near zero energy. A generalization of Wigner’s threshold law states that the \( J/\Pi_1 = 1^+ \) symmetry should dominate near threshold [13], where \( J \) is the total nuclear orbital angular momentum and \( \Pi_1 \) is the parity of the system. It follows that the recombination rate \( K_3 \) depends on the collision energy \( E \) as \( E^2 \) near threshold. Dimensional analysis, together with the \( E^2 \) threshold law, suggests a \( |V_p|^{8/3} \) dependence of the recombination rate \( K_3 \) at threshold.

Although the \( E^2 \) threshold law suppresses the three-body recombination rate at ultracold temperatures, it does not vanish. While the rate remains vanishingly small under typical experimental conditions, it can become substantial near a two-body Feshbach resonance. The \( E^2 \) threshold law no longer applies, and the recombination rate approaches the limit imposed by unitarity—often comparable to or larger than for bosons. Since Feshbach resonances are extremely useful tools for experimentalists, it is crucial to understand the behaviour near a resonance. Such resonances have been observed in systems of fermions such as \(^{40}\text{K} \) [15] and \(^{6}\text{Li} \) [10] as well as in a BEC [14].

In this work, we calculate the three-body recombination rate for various values of \( V_p \), emphasizing its energy dependence. We revisit the dominant 1\( ^+ \) symmetry considered in \[8\], but we also present results for the next contributing symmetries, i.e. \( J/\Pi_1 = 1^- \) and 3\( ^- \). We describe our method and give all necessary formulae for calculating the three-body recombination rate in section 2. The results are presented in section 3. A summary of this work is given in section 4. We use atomic units throughout except where explicitly stated otherwise.

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2. Method

We solve the Schrödinger equation for three interacting atoms using a combination of the adiabatic hyperspherical representation [16, 17] and the R-matrix method [18]. In the adiabatic hyperspherical representation, we calculate eigenfunctions and eigenvalues of the fixed-hyperradius Hamiltonian in order to construct a set of coupled radial equations. The R-matrix method is then used to extract the scattering matrix from these coupled equations.

After separation of the centre-of-mass motion, any three-particle system (in the absence of an external field) can be described by six coordinates. Three of these can be chosen to be the Euler angles $\alpha$, $\beta$, and $\gamma$ that specify the orientation of the body-fixed frame relative to the space-fixed frame. The remaining three internal coordinates can be represented by a hyperradius $R$ and two hyperangles $\theta$ and $\varphi$. We use a modified version of the Smith–Whitten hyperspherical coordinates [19]–[22]. The details of the modifications are given in [17]. These coordinates allow us to easily impose the correct permutation symmetry on the wavefunctions. The hyperradius $R$ is the only length coordinate and can thus be thought of as characterizing the overall size of the system. The hyperangles $\theta$ and $\varphi$ characterize the shape of the system, and span the ranges $[0, \pi/2]$ and $[0, 2\pi]$, respectively. Taking into account the indistinguishability of these three particles, the hyperangle $\varphi$ can be further restricted to the range $[0, 2\pi/3]$.

We rewrite the Schrödinger equation in terms of a rescaled wavefunction $\psi$, which is related to the usual Schrödinger solution $\Psi$ by $\psi = R^{5/2}\Psi$. The volume element relevant to integrals over $|\psi|^2$ then becomes $2\,dR\sin 2\theta\,d\theta\,d\varphi\,d\alpha\sin \beta\,d\beta\,d\gamma$. The Schrödinger equation for three identical particles now takes the form

$$\left[-\frac{1}{2\mu} \frac{\partial^2}{\partial R^2} + \frac{\Lambda^2 + \frac{15}{4}}{2\mu R^2} + V(R, \theta, \varphi)\right] \psi_E = E \psi_E, \tag{2}$$

In this expression, $\Lambda^2$ is the squared ‘grand angular momentum operator’ [17, 20, 22], and $\mu$ is the three-body reduced mass (in the case of identical particles, $\mu = m/\sqrt{3}$). When considering fully spin-polarized atoms that collide in a quartet electronic state, the interaction potential can be modelled as a sum of triplet two-body potentials [5, 8] for the present purposes, i.e.

$$V(R, \theta, \varphi) = v(r_{12}) + v(r_{23}) + v(r_{31}), \tag{3}$$

where $r_{ij}$ are the interparticle distances. For the dimer potential $v(r)$, we use model potentials for simplicity.

The first step that must be carried out is the solution of the fixed-$R$ adiabatic eigenvalue equation for a given symmetry $J^\Pi$ to determine the channel functions $\Phi_v(R; \Omega)$ (we will use $\Omega \equiv (\theta, \varphi, \alpha, \beta, \gamma)$) and potential curves $U_v(R)$ [16, 17]. In the adiabatic representation the wavefunction $\psi_E(R, \Omega)$ is written in terms of the complete, orthonormal set of angular wavefunctions $\Phi_v$ and radial wavefunctions $F_{vE}$,

$$\psi_E(R, \Omega) = \sum_v F_{vE}(R) \Phi_v(R; \Omega). \tag{4}$$

The channel functions $\Phi_v$ are eigenfunctions of the adiabatic equation, a five-dimensional partial differential equation

$$\left[\Lambda^2 + \frac{15}{4} \frac{1}{2\mu R^2} + V(R, \theta, \varphi)\right] \Phi_v(R; \Omega) = U_v(R) \Phi_v(R; \Omega), \tag{5}$$
and depend parametrically on $R$. Insertion of $\psi_E$ from equation (4) into the Schrödinger equation from equation (2) results in a set of coupled ordinary differential equations

$$\left[ -\frac{1}{2\mu} \frac{d^2}{dR^2} + U_\nu(R) \right] F_{\nu E}(R) - \frac{1}{2\mu} \sum_{\nu'} \left[ 2P_{\nu\nu'}(R) \frac{d}{dR} + Q_{\nu\nu'}(R) \right] F_{\nu' E}(R) = EF_{\nu E}(R). \quad (6)$$

The nonadiabatic coupling elements $P_{\nu\nu'}(R)$ and $Q_{\nu\nu'}(R)$ involve partial first and second derivatives of the channel function $\Phi_\nu$ with respect to $R$.

The rigid-body motion represented by the Euler angles $(\alpha, \beta, \gamma)$ is treated by expanding the channel functions $\Phi_\nu$ onto Wigner $D$ functions. The resulting complex coupled equations in $\theta$ and $\varphi$ are solved by expanding the wavefunctions onto a direct product of fifth-order basis splines in $\theta$ and $\varphi$. The identical particle symmetry is built into the adiabatic equations via the boundary conditions

$$\Phi_\nu(R; \theta, \varphi = 0, \alpha, \beta, \gamma) = \pm \Phi_\nu(R; \theta, \varphi = \frac{2\pi}{3}, \alpha, \beta, \gamma) \quad \text{for } \Pi = \pm 1, \quad (7)$$

which ensure that each solution is either totally symmetric or totally antisymmetric with respect to the exchange of any two particles. The antisymmetric wavefunctions appropriate for identical fermions are identified using a postsymmetrization procedure as the solutions that satisfy

$$\left( \langle \Phi_\nu(R; \Omega) | \frac{1 - P_{23}}{2} | \Phi_\nu(R; \Omega) \rangle \right) = 1, \quad (8)$$

where $P_{23}$ is a permutation operator of two particles. Since the channel functions are complex quantities, one has to be careful when choosing their phases in order for the derivative couplings $P_{\nu\nu'}(R)$ and $Q_{\nu\nu'}(R)$ to be continuous in $R$ [17].

In the adiabatic hyperspherical representation for short-range potentials, the three-body continuum is rigorously discretized since the adiabatic Hamiltonian in equation (5) depends only on the bounded coordinates $\Omega$. In the asymptotic region ($R \to \infty$), the potential curves approach either the dimer binding energies for the recombination (or two-body) channels or the three-body break-up threshold ($U = 0$) for the three-body continuum channels. For potential curves with the maximum physics content we must include the diagonal nonadiabatic correction $Q_{\nu\nu}(R)$ yielding the effective channel potential

$$W_\nu(R) = U_\nu(R) - \frac{1}{2\mu} Q_{\nu\nu}(R). \quad (9)$$

In the three-body continuum when the interparticle distances $r_{ij}$ are all large—giving also a large hyperradius—the interaction potential vanishes, leaving only the kinetic energy term in the adiabatic Hamiltonian. The eigenfunctions of $\Lambda^2$ are just the hyperspherical harmonics whose eigenvalues are $\lambda(\lambda + 4)$, so the effective potential approaches

$$W_\nu(R) \to \frac{\lambda(\lambda + 4) + \frac{15}{4}}{2\mu R^2}, \quad (10)$$

where $\lambda$ takes only the non-negative integer values allowed by symmetry. Asymptotically, the recombination channels approach

$$W_\nu(R) \to E_{el} + \frac{l'(l' + 1)}{2\mu R^2}, \quad (11)$$

where $E_{el}$ is the rovibrational energy of the molecule in the vibrational state $v$ with angular momentum $l'$; $l'$ is the two-body angular momentum between the molecule and the atom.
Note that the two-body angular momenta \( \vec{l} \) and \( \vec{l}' \) are related to the total angular momentum \( \vec{J} = \vec{l} + \vec{l}' \), while the parity of the three-body system is \( \Pi = (-1)^{l+l'} \).

Three-body recombination can be pictured as a transition from a three-body continuum channel to a recombination channel driven by their nonadiabatic coupling. In order to characterize the magnitude of this coupling, we define the dimensionless quantity called the ‘nonadiabatic coupling strength’,

\[
f_{\nu\nu'}(R) = \frac{P_{\nu\nu'}(R)^2}{2\mu[U_{\nu}(R) - U_{\nu'}(R)]}.
\]

(12)

The coupled equations in equation (6) are solved using the finite element method [23], and the scattering matrix \( S \) is extracted using an \( R \)-matrix approach [17, 23, 24]. The total event rate constant for three-body recombination is then expressed as

\[
K_3 = \frac{k}{\mu} = \sum_{J,\Pi} K_{3J/\Pi},
\]

(13)

where \( K_{3J/\Pi} \) is the partial recombination rate corresponding to the \( J/\Pi \) symmetry

\[
K_{3J/\Pi} = \sum_{\lambda,f} \frac{192(2J + 1)}{\mu k^4} |S_{f\lambda}^{J/\Pi}|^2.
\]

(14)

Here, \( \lambda \) and \( f \) label the incident (three-body continuum) and outgoing (three-body recombination) channels, respectively, and \( k = (2\mu E)^{1/2} \) is the hyperradial wavenumber in the incident channels.

As pointed out in [4]–[8], we expect that the three-body recombination rate depends on one additional parameter. We can choose it as a length parameter \( r_0 \), coming into play in the two-body potential in the form

\[
v(r_{ij}) = Df\left(\frac{r_{ij}}{r_0}\right)
\]

(15)

where \( D \) is the overall coefficient used to control the scattering volume \( V_p \). Then, because of the analytical form of the Schrödinger equation (2), the three-body reduced mass \( \mu \) and the length parameter \( r_0 \) can be used to define scaled quantities. By defining the scaled hyperradius and the scaled energy as \( \tilde{R} = R/r_0 \) and \( \tilde{E} = \mu r_0^2 E \), the Schrödinger equation (2) can be written in the form

\[
\left[-\frac{1}{2} \frac{\partial^2}{\partial \tilde{R}^2} + \Lambda^2 + \frac{15}{4} \frac{1}{2\tilde{R}^2} + \tilde{V}(\tilde{R}, \theta, \varphi)\right] \psi_{\tilde{E}} = \tilde{E} \psi_{\tilde{E}},
\]

(16)

with

\[
\tilde{V}(\tilde{R}, \theta, \varphi) = \tilde{v}(\tilde{r}_{12}) + \tilde{v}(\tilde{r}_{23}) + \tilde{v}(\tilde{r}_{31})
\]

(17)

and

\[
\tilde{v}(\tilde{r}_{ij}) = \tilde{D} f(\tilde{r}_{ij}),
\]

(18)

where \( \tilde{D} = \mu r_0^2 D \) and \( \tilde{r}_{ij} = r_{ij}/r_0 \). Here, the scaled coefficient \( \tilde{D} \) is used to control the scaled scattering volume \( \tilde{V}_p = V_p/r_0^3 \). Finally, the scaled three-body recombination rate is expressed as

\[
\tilde{K}_3 = \frac{\mu}{r_0^4} K_3 = \sum_{J,\Pi} \frac{192(2J + 1)}{\tilde{k}^4} |S_{f\lambda}^{J/\Pi}|^2.
\]

(19)
where the scaled wavenumber is given by $\tilde{k} = \sqrt{2\tilde{E}}$. Once the rate is calculated as a function of $V_p$ at a constant $\tilde{E}$ and for given $\mu$ and $r_0$, we can obtain the rate for any other value of $\mu$ and $r_0$ by means of the above scaling. Similarly, the rate for a different $r_0$ can be obtained. In practice, we use the values $r_0 = 15$ au and $\mu = m/(40K)/\sqrt{3}$.

### 3. Results and discussion

Since we do not expect the result to depend sensitively on the exact form of the two-body potential at threshold temperatures, we use a model potential of the form

$$v(r_{ij}) = D \text{sech}^2 \left( \frac{r_{ij}}{r_0} \right)$$

(20)

since it has proven convenient in previous calculations [5, 8]. The coefficient $D$ controls the scattering volume $V_p$ and can be used to economize the calculations substantially since we can reduce the number of two-body bound states without sacrificing the ultracold physics. To check this dependence, we also used

$$v(r_{ij}) = \frac{D}{1 + \left( \frac{r_{ij}}{r_0} \right)^6}.$$  

(21)

This potential more realistically models neutral atom interactions in that it has a van der Waals’ tail with the coefficient $C_6 = Dr_0^6$. In our calculations, however, $D$ must be small to keep the number of channels manageable, so $C_6$ is much smaller than would be found for atoms of current experimental interest. Nevertheless, it is qualitatively different from the sech$^2$ potential, offering a check on the universality of our results. We also performed calculations using a Morse potential

$$v(r_{ij}) = De^{-\alpha(r_{ij}-r_{\text{min}})}(e^{-\alpha(r_{ij}-r_{\text{min}})} - 2),$$

(22)

with $\alpha = 0.35$ au$^{-1}$ and $r_{\text{min}} = 11.65$ au, which has the final feature of a realistic potential that is missing from our model potentials—a repulsive core at $r_{ij} = 0$.

Figure 1 shows the dependence of $V_p$ on $D$ using the sech$^2$ potential with $r_0 = 15$ au. The two-body p-wave scattering volume $V_p$ behaves qualitatively like the typical s-wave scattering length as a function of the parameter $D$, displaying a tangent-like structure. As $D$ becomes more negative and the potential becomes more attractive, the scattering volume passes through a pole and changes sign each time the potential becomes deep enough to support one additional p-wave bound state. For computational simplicity, we consider the parameter range for which there exists only one two-body bound state. In the following sections, we consider each of the partial waves $J^{\Pi} = 1^+, 1^-$ and $3^-$ in turn. In particular, we present representative potential curves and couplings and discuss the physical mechanisms of recombination within this framework.

#### 3.1. $J^{\Pi} = 1^+$

We first consider $J^{\Pi} = 1^+$ since we expect it to dominate in the zero-energy limit $E \rightarrow 0$ [8]. In this symmetry, three-body recombination is suppressed and has an $E^2$ threshold behaviour. Figures 2(a) and (b) show the generic features of the lowest two potential curves (solid curve) and the nonadiabatic coupling strength (dashed curve) respectively for positive and negative values of the scattering volume, i.e. $V_p = +10^6$ and $-10^6$ au$^3$. In each case the lowest potential curve $\nu = 0$ corresponds to the recombination (two-body) channel and approaches asymptotically the
Figure 1. Two-body p-wave scattering volume as a function of the potential depth $D$, for the potential $v(r) = D \text{sech}^2(r/15)$. The dotted lines enclose the parameter range considered in our numerical calculations. Here, we use $m(^{40}\text{K}) = 72\,849 \text{ au}$.

dimer binding energy with the centrifugal term characterized by $l' = 1$ in equation (11). The molecule itself is also in a p-wave $l = 1$ bound state to satisfy the Pauli principle. The second lowest potential $v = 1$ represents the lowest three-body continuum channel, whose asymptotic behaviour is characterized by $\lambda = 2$ in equation (10) [13]. Higher potential curves, which we do not show here, asymptotically correspond to $\lambda = 6, 8, 10, \ldots$ as determined by symmetry requirements. In the case of $V_p > 0$, the important feature is the broad avoided crossing that extends over several thousands of atomic units as indicated by the large coupling strength. We identify this as an ‘avoided crossing’ based only upon the behaviour of the coupling strength—the potentials do not obviously show the crossing. For $V_p < 0$ the potential barrier in the lowest three-body continuum channel (shown in the inset of (b)) plays an important role in the recombination process.

Figure 3 shows the nonadiabatic coupling strength for various positive values of the scattering volume $V_p$. The peak position is essentially independent of $V_p$ at $R \approx 80 \text{ au}$. In the region just past the peak, a ‘shoulder’ appears that behaves roughly like $R^{-1/2}$ and eventually gives way to a ‘tail’ that decreases like $R^{-5}$ as expected [25]. We empirically find that the inflection point between shoulder and tail occurs at roughly $R = 12V_p^{1/3}$. For $V_p \to +\infty$, we speculate that the $R^{-1/2}$ behaviour holds even asymptotically. In this case, it can be expected that the larger the scattering volume, the easier it is for atoms to recombine at large hyperradii. It is worth noting again that the lowest potential curve has a centrifugal barrier for all values of the scattering volume $V_p$. When the scattering volume $V_p$ is positive and large, the two-body threshold moves towards the three-body breakup threshold, eventually pushing the top of this barrier above the collision energy for ultracold collisions. It might be expected, then, that recombination will be suppressed by this extra barrier, except possibly at energies matching three-body shape resonances behind this barrier. However, we have not observed any such resonances.

For $V_p < 0$ (figure 2(b)), the nonadiabatic coupling strength is localized with a peak near $R = 40 \text{ au}$ and is essentially independent of $V_p$. Here, the recombination takes place primarily
Figure 2. The lowest two adiabatic potential curves (solid curve) along with their nonadiabatic coupling strength (dashed curve) for (a) $V_p > 0$ and (b) $V_p < 0$. The inset in (a) shows the behaviour of the nonadiabatic coupling strength for large hyperradii $R$. The inset in (b) shows the potential barrier in the three-body recombination channel.

Figure 3. Nonadiabatic coupling strength for several positive values of the scattering volume $V_p$ using the sech$^2$ potential with $r_0 = 15$ au. The inset focuses on the asymptotic behaviour.
by tunnelling through the potential barrier that exists in the lowest three-body entrance channel to reach the region of large coupling. Figure 4 shows the potential barrier for several negative values of the scattering volume $V_p$. (The conversion from $\mu K$ to au is $1 \mu K = 3.166 \times 10^{-12}$ au.) When $V_p$ becomes large and negative, such that the barrier maximum is below the collision energy, recombination is greatly enhanced since the incoming atoms can now pass freely above the barrier and reach the large coupling region. When the energy is over the barrier, the system is certainly not in the threshold regime—no matter the collision energy—and the recombination rate will be large. Stated another way, at a fixed collision energy there is always a negative $V_p$ with large enough magnitude that recombination proceeds via over-the-barrier collisions. In these cases the recombination probability approaches one so that the rate is determined primarily by unitarity and falls off as $E^2$. In addition, when $V_p$ becomes negative and large, there appears a two-body p-wave shape resonance. Figure 5 shows that such a resonance produces a series of avoided crossings in the three-body potential curves at energies near the position of the resonance [26, 27, 29]. The figure shows only five continuum channels, but there are actually an infinity of them producing an infinity of crossings. Interestingly, a two-body Feshbach resonance seems to produce a nearly identical series of crossings [26, 27], increasing our confidence that understanding the three-body physics near a two-body shape resonance will help us to understand the physics near a Feshbach resonance. As might be expected, though, this infinity of crossings causes difficulties in an adiabatic representation with a finite number of channels. We have not fully resolved this difficulty, but are working on reformulating the problem. In analogy to equation (11), a potential curve of the form

$$U_{\text{diabatic}}(R) = E_{\text{res}} + \frac{l'(l' + 1)}{2\mu R^2}$$

(with $l' = 1$) can be plotted and is shown in figure 5 with a dashed curve. It can be seen that this diabatic curve traces through these crossings suggestively. The two-body p-wave resonance energy—and thus the position of these avoided crossings—approaches the three-body breakup threshold $U = 0$ when $V_p \to -\infty$. So, at a fixed collision energy, there always exists a value of $V_p$ at which the collision energy is above this series of avoided crossings and out of the threshold regime. Note that the dashed curve is for illustration only and was not used for the calculation.

Figure 6(a) shows the three-body recombination rate $K_3$ as a function of the collision energy $E$ for positive values of the scattering volume $V_p$. The dashed curve shown in figure 6 represents the unitarity limit. In the zero-energy limit, $K_3$ indeed increases like $E^2$, as is predicted from the threshold law in [13]. At higher collision energies, $K_3$ decreases as $E^{-2}$, required by unitarity. For the smallest $V_p$ in figure 6(a), the energy-dependent recombination rate presents a pronounced minimum at higher collision energies. This minimum results from a destructive interference between two indistinguishable pathways—a St"uckelberg oscillation.

For $V_p < 0$ in figure 6(b), the recombination rate does not show such a feature in this energy range. As for positive $V_p$ above, the rate first increases from threshold according to $E^2$ until the energy is near the top of the barrier, then decreases as $E^{-2}$ due to the unitarity limit. In fact, at collision energies high compared to the barrier, the rate does not depend on the scattering volume, and takes a value about a factor of 3 smaller than that limit. We empirically find that for $V_p < 0$, the peak position in the rate occurs at an energy slightly higher than the barrier maximum in the lowest three-body entrance channel. Unphysical oscillations are seen near the maximum of $K_3$ for $V_p = -8 \times 10^6$ au$^3$, because the six channels included are not sufficient to achieve the convergence near the barrier maximum of the three-body entrance channel. Including more channels reduces the amplitude of the oscillation, but does not eliminate it.
Figure 4. Potential barrier in the three-body entrance channel for several negative values of the scattering volume $V_p$, using the sech$^2$ potential with $r_0 = 15$ au. When $V_p$ becomes negative and large, the barrier maximum lowers leading to an explosive enhancement of recombination.

Figure 5. Adiabatic hyperspherical potential curves for $V_p = -8 \times 10^6$ au$^3$. They show a series of avoided crossing near the two-body shape resonance $E_{\text{res}} = 4.56 \times 10^{-11}$ au = 14.4 $\mu$K. The dashed curve shows the diabatic curve of the form $E_{\text{res}} + 1/(\mu R^2)$.

We show in figure 7 the three-body recombination rate $K_3$ as a function of $V_p$ for a collision energy equivalent to a temperature of 2 $\mu$K as well as the thermally averaged recombination rate,

$$\langle K_3 \rangle(T) = \frac{\int K_3(E)E^2e^{-E/k_B T}dE}{\int K_3(E)e^{-E/k_B T}dE} = \frac{2}{(k_BT)^3} \int K_3(E)E^2e^{-E/k_B T}dE, \quad (24)$$

at a temperature of 2 $\mu$K. We plot $K_3^{3/8}$ to best reveal whether the predicted $|V_p|^{8/3}$ scaling holds for the calculated rate [8]. The figure shows that this scaling holds quite well for $|V_p|/r_0^3$ less than
Figure 6. Three-body recombination rate $K_3$ as a function of the collision energy $E$ for several values of (a) $V_p > 0$ and (b) $V_p < 0$. The dotted line indicates the unitarity limit. For $V_p < 0$, the short vertical lines indicate the height of the barrier in the entrance channel. Note also that the scattering volume $V_p = -2.0 \times 10^3$ au$^3$ corresponds to the position of the local peak of $K_3$ in figure 7.

about 3000 for $K_3(E)$, but for $\langle K_3 \rangle (T)$ it only holds over the region $|V_p/r_0^3|$ below approximately 1000. Since this scaling is based on the threshold behaviour of the rate, it is not surprising that it breaks down sooner for the thermally averaged rates as they include contributions from energies not near threshold. The scaling breaks down for $K_3(E)$ when the fixed collision energy passes out of the threshold regime as a function of $V_p$, which can be expected to happen when $|V_p|$ becomes large. In particular, the scaling will break down when there is a two-body resonance at or below the collision energy. At large negative $V_p$, for instance, there will be a p-wave resonance. In this limit, it is also possible to pass out of the threshold scaling regime if the barrier in the entrance channel becomes lower than the collision energy. As can be seen in figure 7, the scaling does not hold for very small $V_p$ since $K_3$ is finite (but small) when $V_p = 0$. We observed a small peak in the rate located at about $V_p/r_0^3 = -60$. This peak is another manifestation of a St"uckelberg oscillation, this time from a constructive interference. It disappears and reappears as a function of the collision energy, since the phase difference between these two pathways varies with the collision energy. It should be noted that there is no Efimov effect [31] for fermions in the limit $|V_p| \to \infty$ as there is for the boson case in the limit $|a_s| \to \infty$. As
Figure 7. The scaled recombination rate $\mu K_3/r_0^4$ at $E = 2 \mu K$ (a) and scaled thermal averaged rate $\mu \langle K_3 \rangle/r_0^4$ at $T = 2 \mu K$ (b) as functions of $V_p/r_0^3$. The solid curve, circles and squares show the results for the potentials from (20), (21) and (22), respectively. The inset focuses on the region with small $|V_p|$ showing a St"uckelberg oscillation.

a consequence, we do not expect to see the series of three-body shape resonances found for bosons [5] as $n \rightarrow -\infty$ in the present calculations. Indeed, we have seen no evidence of such resonances as $V_p \rightarrow -\infty$. The rates from the three potentials (20)–(22)—which are qualitatively very different—show reasonable quantitative agreement, especially for the more experimentally relevant thermally averaged rate. The poorest agreement occurs at small $|V_p|$ where the rates are also small.

3.2. $J^\pi = 1^-$

Although the $J^\pi = 1^+$ case is predicted to be the dominant symmetry in the limit of zero collision energy, other symmetries may contribute substantially. So, it is interesting to study the energy-dependent partial recombination rates corresponding to various symmetries. We will focus on those predicted to make the main contributions after $1^+—the $J^\pi = 1^-$ and $3^-$ symmetries. Figure 8 shows the potential curves and the nonadiabatic coupling strengths for the $J^\pi = 1^-$ symmetry for (a) $V_p > 0$ and (b) $V_p < 0$. In both cases, the lowest two potential
Figure 8. The three lowest potential curves (solid curve) along with their nonadiabatic coupling strength (dashed curve) belonging to the $J^\pi = 1^-$ symmetry for (a) $V_p > 0$ and (b) $V_p < 0$. The potentials curves are labelled by the two-body angular momentum $l'$ for recombination channels or by the hyperspherical quantum number $\lambda$ for three-body continuum channels. For $V_p = -10^6$ au$^3$, the potential curve corresponding to $\lambda = 5$ is also presented to show its avoided crossing with the channel labelled by $\lambda = 5$. The inset in (a) shows the behaviour of the nonadiabatic couplings strengths in a wide range of $R$. The inset in (b) shows the potential barrier in the three-body recombination channel.

curves correspond to recombination channels that approach the same dimer binding energy but with different centrifugal terms associated with $l' = 0$ and 2 in equation (11) (such that $l = 1$ and $l'$ can combine to $1^-$). The third lowest potential curve represents the lowest three-body entrance channel characterized by $\lambda = 3$ in equation (10) as required by permutation symmetry. Higher channels, that we do not show here, correspond to $\lambda = 5, 7, 9, \ldots$.

Here, the main features are similar to those for $J^\pi = 1^+$: for $V_p > 0$, the long-range nonadiabatic couplings play the key role for the recombination, while for $V_p < 0$ there is again a potential barrier in the lowest three-body continuum channel. For all values of $V_p$, the nonadiabatic coupling strength between the three-body continuum channel $\lambda = 3$ and the lowest recombination channel with $l' = 0$ is larger than that between the channels $\lambda = 3$ and $l' = 2$ as expected intuitively. Further, when the scattering volume $V_p$ becomes positive and increases, the range of large nonadiabatic strength also grows, making it easier for atoms to recombine at
large hyperradii. Finally, just as we have found for both bosons and the $1^+$ fermions above, when $V_p$ becomes negative and large, the barrier maximum in the lowest three-body recombination channel lowers, so that recombination is enhanced.

### 3.3. $J^\Pi = 3^-$

The potential curves and the nonadiabatic coupling strengths for $J^\Pi = 3^-$ case are shown in figures 9(a) for $V_p > 0$ and (b) $V_p < 0$. The lowest two potential curves represent recombination channels that asymptotically approach the dimer binding energy with $l' = 2, 4$ in equation (11). All the higher potential curves (we show here the lowest one) are associated with the three-body continuum, and correspond to $\lambda = 3, 5, 9, 13, \ldots$ in equation (10). For all values of $V_p$, the nonadiabatic coupling strength between the channels $\lambda = 3$ and $l' = 2$ is smaller and broader than that between the channels corresponding to $\lambda = 3$ and $l' = 4$. Just as in the previous cases, the long-range nonadiabatic strengths and the potential barrier in the lowest three-body entrance channel are the key features for $V_p > 0$ and $V_p < 0$, respectively. Note that in the $V_p > 0$ case, the lowest potential curve has a relatively large potential barrier since $l' = 2$. As above, the potential barrier in the lowest entrance channel lowers when $V_p$ becomes large and negative, and recombination is enhanced.

### 3.4. Partial wave comparison

We show in figure 10 the partial recombination rates $K_3$ as functions of the collision energy $E$ for $J^\Pi = 1^+, 1^-$ and $3^-$ with (a) $V_p = +10^6 \text{ au}^3$ and (b) $-10^6 \text{ au}^3$. As expected, the $J^\Pi = 1^+$ partial rate increases like $E^2$ from the threshold while the $1^-$ and $3^-$ rates behave as $E^3$ in that limit. We find a complicated structure for the $J^\Pi = 3^-$, $V_p > 0$ rate. This structure appears to be physical as the calculations are converged with respect to the number of channels as well as the other numerical aspects. The origin of this structure is not completely understood, but a few observations can be made. First, figure 10(c) shows that the structure is entirely in the higher angular momentum state $l' = 4$. Further, the partial rate for recombination into this channel is generally smaller than for $l' = 2$ except near the maxima of the oscillations. Finally, this structure can make the contribution from the $3^-$ channel comparable to the $1^+$ rate already at tens of $\mu$K. In the $V_p < 0$ case, the rates increase smoothly, following the $E^3$ threshold law discussed above, and then decrease as $E^{-2}$ from the unitarity limit. The peak position in each partial recombination rate is always slightly higher than the barrier maximum of the lowest three-body entrance channel.

We should note that although the symmetries $J^\Pi = 1^+, 1^-$, and $3^-$ are the leading contributions at threshold, they need not be near a two-body resonance where $|V_p| \to \infty$. In particular, our results suggest that other $J^\Pi$ can be comparable near the resonance. For any symmetry $J^\Pi$, a p-wave shape resonance produces a series of avoided crossings as in figure 5. Such cases correspond to large and negative values of $V_p$. A two-body resonance associated with a higher angular momentum $l$ (like a d-wave resonance in the boson case [28, 29]) would likely produce the same effect, although our model potentials did not support any such resonances.

### 3.5. Universality

One of the remarkable aspects of the recombination rate for three identical bosons is its universality. Ultracold recombination in this case is parametrized very well using only the
two-body s-wave scattering length and a second length parameter related to the short-range three-body physics. It is interesting, then, to compare and contrast the universality for identical fermion recombination with that for bosons.

In the adiabatic hyperspherical representation, the universality of boson recombination can be understood from the threshold law and the $|a_s| \to \infty$ limit. The former states that the recombination rate is constant at threshold and is proportional to $|a_s|^4$; the latter corresponds to the Effimov limit which allows a description of the modulation of the basic $|a_s|^4$ scaling. Since the rate is constant at threshold, thermal averaging at ultracold temperatures has little effect. Because the above scaling is based upon the threshold law, however, there is no particular reason to expect that it should hold for all values of $a_s$. In other words, at a fixed collision energy, there could be some value of $a_s$ for which the system can no longer be considered to be in the threshold regime. Indeed, we can identify a few such cases. The first is in the limit $a_s \to -\infty$. For some large negative $a_s$, the barrier in the entrance channel shrinks below the collision energy, and recombination occurs with nearly unit probability. This same physics was pointed out for each partial wave in the sections above. The second case for which the scaling will break down is when a two-body shape resonance lies near the collision energy. There are, of course, no s-wave shape resonances, but realistic systems will have resonances for higher partial waves. This

Figure 9. The three lowest potential curves (solid curve) along with their nonadiabatic coupling strength (dashed curve) belonging to the $J^{\pi} = 3^-$ symmetry for (a) $V_p > 0$ and (b) $V_p < 0$. The inset in (a) shows the behaviour of the nonadiabatic couplings strengths in a wide range of $R$. The inset in (b) shows the potential barrier in the three-body continuum channel.
Figure 10. Partial three-body recombination rates \( K_3 \) as functions of the collision energy \( E \) for \( J/\Pi = 1^+, 1^- \) and \( 3^- \) in the cases of (a) \( V_p = 10^6 \) a.u.\(^3\) and (b) \( V_p = -10^6 \) a.u.\(^3\). In (c) and (d), we show the contributions to the particular recombination channels labelled by \( l' \). For \( V_p = -10^6 \) a.u.\(^3\) in (b), the short vertical curves indicate the barrier heights in the lowest entrance channel.

physics was also discussed in previous sections, as was the related physics of a near-threshold two-body Feshbach resonance. In fact, there is some evidence [26] that the recombination rate does not scale as \( |a_\pi|^4 \) near a Feshbach resonance. In each of these cases, however, the \( |a_\pi|^4 \) law is qualitatively correct in predicting enhanced recombination. Moreover, for \( |a_\pi| = \infty \), the Efimov limit is reached, and the entrance channel is known to have the form of an attractive dipole potential. It is further known that the threshold law for superelastic processes from such channels gives an infinite rate at threshold.

The situation for fermions is in many respects the same as for bosons. For instance, the rate appears to be parametrized by two quantities \( V_p \) and \( r_0 \). The primary differences are the threshold law and \( |V_p| \to \infty \) limit. The threshold law for recombination of identical fermions is \( E^2 \). Consequently, thermal averaging has a large effect and folds in rates at energies outside of the threshold regime. The scaling predicted from the threshold law, \( |V_p|^{8/3} \), thus holds only over a relatively small range of \( |V_p| \). For example, for negative \( V_p \), the averaging includes the large rates from over-the-barrier recombination as well as from p-wave (or higher) resonances. The
potential curve obtained in the $|V_p| \to \infty$ limit is not known analytically, so the recombination in this limit is not known with the same confidence as for bosons.

4. Summary

We have investigated the recombination of three identical, spin-polarized fermions in cold collisions and have numerically calculated the recombination rate, focusing on its energy dependence. We have first considered the $J^{\pi} = 1^+$ symmetry that is expected to dominate at threshold, and have also studied its dependence on the scattering volume $V_p$. We have also considered the next-leading symmetries, i.e. $1^-$ and $3^-$. In general, the recombination rate increases following the threshold law and then decreases as $E^{-2}$ imposed by the unitarity limit. The $1^+$ symmetry is indeed dominant in the threshold regime, but $1^-$ and $3^-$ become comparable as the energy passes from this regime. The important point is that this crossover can happen at the energy of a two-body resonance even at what would otherwise be considered ultracold temperatures. Moreover, partial waves higher than wave considered here likely contribute substantially to the recombination rate near the resonance.

Although we have considered three identical fermions, with some slight modifications to our codes, it is possible to treat systems with only two identical particles. Three-body recombination of such systems plays an important role in experiments on mixed-spin state Fermi gases and mixed Bose–Fermi gases.

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