Three-body problem in Fermi gases with short-range interparticle interaction

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We discuss 3-body processes in ultracold two-component Fermi gases with short-range intercomponent interaction characterized by a large and positive scattering length $a$. It is found that in most cases the probability of 3-body recombination is a universal function of the mass ratio and $a$, and is independent of short-range physics. We also calculate the scattering length corresponding to the atom-dimer interaction.

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In the search for fermionic superfluidity, ultracold Fermi gases with strong interactions and high densities are produced routinely. In current experiments with $^{40}$K [1] and $^6$Li [2–5], the scattering length $a$, corresponding to the interaction between different fermionic species, has been modified using a powerful tool of Feshbach resonances. Reaching high densities is limited by 3-body recombination – the process in which two atoms form a bound state and a third one carries away the binding energy $\varepsilon$. In the case of a two-component Fermi gas the 3-body process requires at least two identical fermions to approach each other to a distance of the order of the size of the final bound state. Therefore, in the ultracold limit the recombination probability acquires an additional small factor $K/\varepsilon$, where $K$ is the relative kinetic energy of identical fermions (cf. [6]). One may speculate that limitations on achieving high densities are not as severe as in Bose gases, where the recombination rate is independent of the kinetic energy of particles.

Theoretical studies of the 3-body problem have revealed the existence of two universality classes for the case where $a$ greatly exceeds the characteristic radius of interatomic interaction, $R_e$ [7,8]. For the first class, short-range physics is not important and the 3-body problem can be described in terms of 2-body scattering lengths and masses of particles. One can then use the zero-range approximation for the interatomic potential, which has been successfully demonstrated, e.g. in the calculations of neutron-deuteron scattering with the total spin $S = 3/2$ [9]. For the second class, where short-range behavior is important, the description of the 3-body problem requires at least one parameter coming from short-range physics [10]. For two identical fermions ($\uparrow \uparrow$) interacting with a third particle ($\downarrow$), the presence of two universality classes has been shown by Efimov [7,8]. For a large $a$, the pair interaction between distinguishable particles leads to the appearance of an attractive $1/r^2$ interaction in the 3-body system [11]. If the mass ratio $m_\uparrow/m_\downarrow$ is smaller than approximately 13, then this attraction is not sufficient to overcome the centrifugal barrier $l(l+1)/r^2$ ($l = 1$ due to the symmetry). In this case the probability of all three particles being in the volume $R_e^3$ vanishes and short-range physics drops out of the problem. However, the effective attraction increases with the mass ratio and for $m_\uparrow/m_\downarrow \gtrsim 13$ we have a well-known phenomenon of the fall of a particle into the center in an attractive $r^{-2}$ potential [12]. The shape of the wavefunction at distances of the order of $R_e$ then significantly influences the large-scale behavior and short-range parameters of the interaction potential are required to describe the 3-body system.

In this paper we discuss a 3-body system ($\uparrow \uparrow \downarrow$) containing two identical fermions and belonging to the first universality class. In the ultra-cold limit we find universal functions of $a$ and $m_\uparrow/m_\downarrow$ for the probability of 3-body recombination and for the amplitude of atom-dimer scattering. As expected, the recombination to comparatively deep bound states is much slower than in the Bose case. However, despite the suppression factor of $K/\varepsilon$, the recombination to a weakly bound $s$-level ($a > 0$ and $a \gg R_e$) for realistic parameters of a two-component Fermi gas can be as important as in a Bose gas with the same density and scattering length.

In the center of mass reference frame the state of the 3-body system ($\uparrow \uparrow \downarrow$) with total energy $E$ is described by the Schrödinger equation

$$[-\nabla^2_X - E] \Psi = -\sum_\pm V\left(\frac{\hbar(x \tan \theta \pm y)}{2\sqrt{m_\uparrow}}\right) \Psi, \quad (1)$$

where $\hbar y/\sqrt{m_\uparrow}$ is the distance between identical $\uparrow$-fermions, $\hbar x/\sqrt{2\mu}$ is the distance between their center of mass and the $\downarrow$-particle, $\mu = 2m_\uparrow m_\downarrow/(2m_\uparrow + m_\downarrow)$ is the corresponding reduced mass, and $\theta = \arctan(1 + 2m_\uparrow/m_\downarrow)$. The vector $X = \{x, y\}$ describes the rescaled 6D configuration space for the 3-body problem. The potential of interaction between distinguishable particles is $V$ and the interaction between identical fermions is omitted.

We assume that the range $R_e$ of the interatomic potential $V$ is much smaller than the (positive) scattering length $a$, which in the rescaled coordinates equals $1/\sqrt{\varepsilon}$. Therefore, in the 6D space the rhs of Eq.(1) van-

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ishes everywhere except in the close vicinity to 3D subspaces \( S_+ \) and \( S_- \), which we define parametrically as \( X_\pm(r) = \{ r \cos \theta, \pm r \sin \theta \} \), where the 3D vector \( r \) is a parameter. Near the subspace \( S_+ (S_-) \) the \( \downarrow \)-particle is close to one of the \( \uparrow \)-fermions and is separated by the distance \( r \) from the other. The distance to the first \( \uparrow \)-fermion we denote by \( r_\perp \), which is then a parameter in a 3D subspace orthogonal to \( S_+ (S_-) \). The subspace \( S_- \) differs from \( S_+ \) by the permutation of the \( \uparrow \)-fermions \((y \rightarrow -y)\). We thus face a typical boundary-value problem for the Poisson equation \(-\nabla^2 S = -E \) \( \Psi = 0 \), with a boundary condition given by

\[
\Psi \sim 1 - 1/(\sqrt{\pi |r_\perp|}) + O(r_\perp).
\]  

(2)

Introducing functions \( f_+(r) \) and \( f_-(r) \) we can write a general solution of Eq.(1), which is valid everywhere except the narrow vicinity of \( S_+ \) and \( S_- \):

\[
\Psi = \Psi_0(X) + \sum \int G_E(|X - X_\pm(r)|) f_\pm(r) d^3r.
\]  

(3)

Here \( \Psi_0 \) is a solution of the Poisson equation and has no singularities at \( S_+ \) or \( S_- \). We restrict \( \Psi_0 \) to be finite everywhere and, hence, for \( E < 0 \) we have \( \Psi_0 \equiv 0 \). The Green’s function \( G_E \) is a solution of Eq.(1) with the rhs \( \delta^3(X) \delta^3(y) \) and is given by

\[
G_E(X) = \begin{cases} 
\frac{E K_2(\sqrt{\pi |E|})}{\sqrt{\pi |E|}}, & E < 0 \\
\frac{i E H_2(\sqrt{\pi |E|})}{16 \pi^2 X^2}, & E > 0 \quad \text{as} \quad E \rightarrow 0 \rightarrow \frac{1}{4 \pi^2 X^4}.
\end{cases}
\]

Here \( K_2 \) is an exponentially decaying Bessel function and \( H_2 \) is a Hankel function representing the outgoing wave.

In order to satisfy the symmetry with respect to permutation of identical fermions we set \( f_+(r) = -f_-(r) = f(r) \) and require \( \Psi_0(x,y) = -\Psi_0(x,-y) \). Eqs. (2) and (3) then give the integral equation for the function \( f(r) \)

\[
\left( \hat{L}_E - \sqrt{\varepsilon} + \sqrt{-E} \right) f(r) = 4\pi \Psi_0(X_+(r)),
\]  

(4)

where the hermitian operator \( \hat{L}_E \) is given by

\[
\hat{L}_E f(r) = 4\pi \int \left[ G_E(|r-r'|) f(r) - f(r') \right] + G_E \left( \sqrt{r^2 + r'^2 - 2rr' \cos 2\theta} \right) f(r') d^3r'.
\]  

(5)

This operator conserves angular momentum, and we can expand the solution of Eq.(4) in spherical harmonics and deal only with a set of uncoupled integral equations for functions of a single variable \( r \). Eq.(4) is a particular case of the Faddeev equations [13] and in the momentum representation it was first obtained in [9] for \( m_1 = m_2 \).

The method presented above allows us to solve the problem of atom-molecule scattering for an arbitrary mass ratio. Let us assume that the relative kinetic energy of a \( \uparrow\downarrow \)-dimer and \( \uparrow \)-fermion is much less than the di
er binding energy \( \varepsilon \). The total energy of the system is then negative \( E \approx -\varepsilon \) and, consequently, \( \Psi_0 \equiv 0 \). As the size of the dimer is much smaller than the inverse relative momentum, the \( s \)-wave contribution dominates and Eq.(4) becomes

\[
\hat{L}_{L=0} f(r) = 0.
\]  

(6)

Here \( \hat{L}_{L=0} \) is an integral operator which is obtained from \( \hat{L}_{L=0} \) by integrating over angles.

From Eq.(3) we find that far from the origin \((r \gg 1/\sqrt{\varepsilon})\) and in the region of \( S_\pm \) the wavefunction \( \Psi \approx \pm f(r) \exp(-\sqrt{\pi} r_\perp)/4\pi r_\perp \). Therefore, at these distances the function \( f(r) \) describes the atom-molecule relative motion and behaves as \( 1 - \beta/r \). The atom-molecule scattering length is then given by \( a_m = a\beta\sqrt{\varepsilon} \sin 2\theta \). The ratio \( a_m/a \) is plotted in Fig.1 as a function of \( m_1/m_2 \). In the limit of \( m_1/m_2 \gg 1 \) one can use the Born-Oppenheimer approximation. In this case the heavy \( \uparrow \)-fermions move slowly in a field produced by the exchange of the fast light \( \downarrow \)-particle. The adiabatic behavior assumes decomposition of the wavefunction into two parts. The first part describes \( s \)-wave scattering of the heavy fermions. The motion of the light particle is, therefore, described by a wavefunction antisymmetric with respect to their permutation. At large distances \((y \gg 1/\sqrt{\varepsilon})\) the effective interaction has the form of a repulsive Yukawa potential \( U(y) = \cos \theta(m_1/m_2)\beta\varepsilon \exp(-\varepsilon r_\perp)/y \). The corresponding scattering length is plotted in Fig.1 as a dashed line. We estimate \( a_m/a \sim \ln(m_1/m_2) \).

![FIG. 1. The ratio \( a_m/a \) versus \( m_1/m_2 \) calculated from Eq.(6) (solid line) and from the Born-Oppenheimer approximation (dashed line).](image-url)
\(~1/\sqrt{\varepsilon}\). Therefore at these distances the shapes of the functions \(\Psi\) and \(f\) are independent of \(E\). The normalization coefficient, however, depends on the large scale behavior and, therefore, on energy \(E\). We can illustrate this by writing the wavefunction for free motion in the form \(\Psi_0(x,y) = \sin(k \cdot y) \exp(i q \cdot x)\), where the momenta \(k\) and \(q\) satisfy the equation \(E = k^2 + q^2\). At distances comparable with \(1/\sqrt{\varepsilon}\) the function \(\Psi_0\) reduces to \(k \cdot y\), giving rise to the \(k^2\) threshold law for the probability of 3-body recombination \([6]\). Considering the limit \(E \to 0\) we keep the term \(4\pi k \cdot r \sin \theta\) in the rhs of Eq.(4).

We now search for the solution of Eq.(4) in the form \(f(r) = f(r)k \cdot r/kr\), which corresponds to the angular part of \(f(r)\).

The operator \(\hat{L}_0^{\nu=1}\) has remarkable properties which allow us to solve Eq.(7) analytically. Firstly, for \(f(r) = r^\nu\), where \(\nu\) is in the region \(-4 < \text{Re}(\nu) < 2\), the action of the operator reduces to \(\hat{L}_0^{\nu=1}r^\nu = \lambda(\nu)r^{\nu-1}\), and the function \(\lambda(\nu)\) is given by

\[
\lambda(\nu) = \frac{\nu(\nu+2)}{\nu+1} \cot \frac{\pi \nu}{2} - \frac{\nu \cos 2\theta \cos [(\nu+1)(2\theta - \pi/2)] + \sin [\nu(2\theta - \pi/2)]}{(\nu+1) \cos^2 2\theta \sin(\pi \nu/2)}.
\]

In the specified interval of \(\nu\) the function \(\lambda\) has two roots: \(\nu_0\) and \(-\nu_0-2\). With \(m_\uparrow/m_\downarrow\) increasing from 0 to approximately 13.6 the root \(\nu_0\) decreases from 1 to -1 approaching the second root. At larger mass ratios the roots are complex conjugates with the real part equal to -1. Zeros of \(\lambda(\nu)\) are important to understand the behavior of \(f(r)\) at short distances.

Secondly, any eigenfunction \(\chi(r)\) of the operator \(\hat{L}_0^{\nu=1}\) corresponding to the eigenvalue 1 can be rescaled to generate an eigenfunction corresponding to a new eigenvalue \(\epsilon\) for any \(p > 0\)

\[
\hat{L}_0^{\nu=1}\chi(p r) = p \chi(p r).
\]

Strictly speaking this process is described by the linear combination \(f_{\text{mol}}(r) = A\chi_1(\sqrt{\varepsilon}r) + B\chi_2(\sqrt{\varepsilon}r)\). The determination of the coefficients \(A\) and \(B\) involves short-range physics, i.e. the knowledge of the 3-body wavefunction \(\Psi\) at distances of the order of \(R_e\), and is beyond the scope of this paper. However, the matching procedure implies that at these distances both terms in \(f_{\text{mol}}(r)\) are of the same order of magnitude, so \(B/A \sim (\sqrt{\varepsilon}R_e)^{2n_0+2}\). In the case of \(m_\uparrow/m_\downarrow < 13.6\), the exponent \(2n_0+2\) is real and positive, and at distances \(r \gg R_e\) one has \(f_{\text{mol}}(r) \approx A\chi_1(\sqrt{\varepsilon}r)\). Hence, short-range 3-body parameters are unnecessary.

Fortunately, the discussed case of \(m_\uparrow/m_\downarrow < 13.6\) covers almost all practical situations. Using the function \(\chi_1(r)\) and the scaling property \((8)\) we can construct a complete orthonormal set of functions \(f_\nu(r) = p\chi_1(pr)\). Completeness follows from the equality \(rf_\nu(r) = \int f_\nu(r) \delta(r') dr\) and from the normalization condition \(\int f_\nu(r) f_\nu(r') r^2 dr = 2\pi \delta(p - p')\). The operator \(\hat{L}_0^{\nu=1} - \sqrt{\varepsilon}\) in Eq.(7) can now be inverted and after some manipulation we obtain

\[
f(r) = -\frac{4\pi k \sin \theta}{\varepsilon} \left( \sqrt{\varepsilon}r + \lambda(1) + \frac{\lambda(0) \lambda(1)}{\varepsilon} \sqrt{r} \right) - \frac{\lambda(0) \lambda(1)}{2\pi} \int_0^\infty \frac{\chi_1(z) dz}{z - \sqrt{\varepsilon}r}.
\]

The integral in Eq.(9) is taken as a principal value. The solution \(f\) is not singular at short distances. The terms containing \(r^{-1}\), \(r^0\) and \(r\) vanish as expected except in situations where \(\lambda(1)\), \(\lambda(0)\) or \(\lambda(-1)\) are equal to 0. At distances \(r \ll 1/\sqrt{\varepsilon}\) we have \(f(r) \approx r^2\) and the short-range physics does not come into play.

For large distances the asymptotic behavior \(\chi_1(r) \approx 2\sin(r + \delta_1)/r\) gives

\[
\int_0^\infty \frac{\chi_1(z) dz}{z - \sqrt{\varepsilon}r} = 2\pi \cos(\sqrt{\varepsilon}r + \delta_1) + O\left(\frac{1}{\sqrt{\varepsilon}r}\right).
\]

Obviously, this describes the molecule-atom channel responsible for 3-body recombination. An outgoing wave of the form \(\exp(i\sqrt{\varepsilon}r)/r\) describing the dimer and atom flying apart, is obtained by adding a general solution of the homogeneous form of Eq.(7), which is proportional to \(f_{\text{mol}}(r)\), to \(f(r)\).

Eqs. (9), (10) and (3) provide the 3-body wavefunction \(\Psi(X)\) at distances \(1/\sqrt{\varepsilon} \ll |X| \ll 1/\sqrt{E}\), where the inelastic dimer-atom channel is well separated from the elastic one, and give the amplitude of recombination. Then for the number of recombination events \((\uparrow + \downarrow + \downarrow \to \downarrow + \downarrow + \downarrow)\) per unit time and unit volume in a gas we obtain

\[
\Omega_{\uparrow\downarrow\downarrow} = \alpha_\uparrow(\varepsilon r/n_\uparrow) n_\downarrow n_\uparrow^2,
\]

where \(n_\downarrow\) and \(n_\uparrow\) are the densities of the fermionic components. The rate constant \(\alpha_\uparrow(\varepsilon r/n_\uparrow)\) is proportional to the average kinetic energy of \(\uparrow\)-particles \(\varepsilon r\), which equals
$3T/2$ in a nondegenerate gas, and $3T_F/5$ in a deeply degenerate gas. The coefficient $\alpha_\uparrow$ is given by

$$\alpha_\uparrow = \frac{8 \pi^3}{3} \frac{\hbar^5}{m^2} \lambda^2(1) \lambda^2(-1) \sin^2 \theta \sin^3 \theta.$$  \hspace{1cm} (12)

Fig. (2) shows the dependence of the dimensionless quantity $\alpha_\uparrow m_\uparrow^3 \varepsilon^2 / \hbar^5$ on $m_\uparrow / m_\downarrow$. In the case of $m_\uparrow = m_\downarrow$, the quantity $\alpha_\uparrow \approx 148 \hbar a^4 / m$.

The absence of 3-body recombination at the points $\lambda(1) = 0$ ($m_\uparrow / m_\downarrow = 0$), $\lambda(0) = 0$ ($m_\uparrow / m_\downarrow \approx 8.62$) and $\lambda(-1) = 0$ ($m_\uparrow / m_\downarrow \approx 13.6$) is a purely quantum phenomenon. From Eqs. (9) and (10) we see that for these mass ratios the free atom channel is decoupled from the molecular recombination channel and the interparticle interaction leads to elastic scattering only.

The process $(\downarrow + \downarrow + \uparrow \rightarrow \downarrow + \downarrow \uparrow)$ is described in a similar way. The results are given by Eqs. (11) and (12), where one should interchange the subscripts $\uparrow$ and $\downarrow$. In a mixture of two hyperfine components of the same isotope, with equal densities $n_\uparrow = n_\downarrow = n / 2$ and $\tau_\uparrow = \tau_\downarrow = \tau$, the total loss rate of particles is

$$-\dot{n}/n = \frac{8 \pi^3}{3} \frac{\hbar^5}{m^2} \sin^2 \theta \sin^3 \theta.$$  \hspace{1cm} (13)

This formula is valid provided the inequalities $\tau \ll \hbar^2 / ma^2 \ll \hbar^2 / mR_c^2$ are satisfied. In current experiments with $^{40}$K and $^{6}$Li one has $\tau \sim 15 \mu$K, $n \sim 10^{15}$cm$^{-3}$, and the scattering length can be tuned using Feshbach resonances. For $\tau \approx 280 \text{Å}$ we calculate the rate constant $L \sim 10^{-25}$cm$^6$/s and the loss rate (13) is $\sim 10$ s$^{-1}$.

In a trap with a barrier $\varepsilon_{tr}$ higher than the kinetic energy of dimers and fast atoms produced in the recombination process ($\sim \hbar^2 / ma^2$), these particles remain trapped and Eq. (13) overestimates the losses. Actually, the peak loss rate is reached at a finite scattering length $a \sim \sqrt{m \varepsilon_{tr} / \hbar}$, not for $a \rightarrow \infty$. This is consistent with recent observations of particle losses in trapped $^6$Li, where $a$ was tuned by a Feshbach resonance [2-5].

We emphasize the difference between two-component Fermi gases and Bose gases with respect to inelastic processes. Energy dependence of the recombination in Fermi gases leads to decreasing $\tau$ since particles with comparatively high kinetic energies recombine. However, the degeneracy parameter decreases due to a faster particle loss. Eq. (13) gives an estimate of the 3-body loss rate even if $a \sim R_c$ (i.e. deep bound state). In Fermi gases the $a^6$ dependence (13) leads to a substantial suppression of the recombination probability compared to the $a^4$ dependence in Bose gases [14]. Further, in contrast to Bose gases, cold collisions between dimers and atoms have fewer inelastic channels. Indeed, there are no weakly bound Efimov $\uparrow \uparrow \downarrow$-states if $m_\uparrow / m_\downarrow < 13.6$, and the effective repulsion between an atom and a dimer at low energies suppresses the relaxation to deeper molecular states. In the case of a deep trap and large $a$, where products of 3-body recombination stay trapped, one expects a fast creation of weakly bound molecules which can be further cooled. The lifetime of the gas of these Bose dimers is sufficient to observe, for example, a BEC.

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