Low-energy three-body dynamics in binary quantum gases

O I Kartavtsev and A V Malykh
Joint Institute for Nuclear Research, Dubna 141980, Russia
E-mail: oik@nasun.jinr.ru and maw@theor.jinr.ru

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Abstract
The universal three-body dynamics in ultra-cold binary Fermi and Fermi–Bose mixtures is studied. Two identical fermions of mass $m$ and a particle of mass $m_1$ with the zero-range two-body interaction in states of total angular momentum $L = 1$ are considered. Using the boundary condition model for the $s$-wave interaction of different particles, both eigenvalue and scattering problems are treated by solving hyper-radial equations, whose terms are derived analytically. The dependences of the three-body binding energies on the mass-ratio $m/m_1$ for the positive two-body scattering length are calculated; it is shown that the ground and excited states arise at $m/m_1 \geq \lambda_1 \approx 8.17260$ and $m/m_1 \geq \lambda_2 \approx 12.91743$, respectively. For $m/m_1 \ll \lambda_1$ and $m/m_1 \ll \lambda_2$, the relevant bound states turn to narrow resonances, whose positions and widths are calculated. The 2 + 1 elastic scattering and the three-body recombination near the three-body threshold are studied, and it is shown that a two-hump structure in the mass-ratio dependences of the cross sections is connected with the rise of the bound states.

1. Introduction
In the last few years, investigations of multi-component ultra-cold quantum gases have attracted much interest. Properties of binary Fermi–Bose [1, 2] and Fermi [3–5] mixtures and of impurities embedded in a quantum gas [6, 7] are under experimental and theoretical study. Different aspects of the few-body dynamics of two-species compounds are of interest both from the general point of view and for many-body applications. For example, there is an infinite number of three-body bound states of two-component fermions (Efimov effect) if their mass ratio exceeds the critical value [8]. Recently, an infinite number of 1* bound states has been predicted [9] for three identical fermions with the resonant $p$-wave interaction. A more detailed study of the energy spectrum of three two-component particles is of interest to shed light on the role of trimer molecules in the many-body dynamics, and provides an insight into...
the few-body processes. Concerning the low-energy scattering, one of the interesting features is a two-hump structure in the isotopic dependence of the three-body recombination rate of two-component fermions [10, 11]. Note that the low-energy three-body recombination rate of two-component fermions scales as the first power of the collision energy and the sixth power of the two-body scattering length [10, 12, 13].

The aim of the present paper is to study the three-body energy spectrum and the low-energy (2 + 1)-scattering for two identical fermions of mass $m$ and a third different particle of mass $m_1$. Here one considers the unit total angular momentum $L = 1$ and the $s$-wave interaction between different particles, which is most important for a description of the low-energy processes. Note that the $s$-wave interaction takes place only in binary mixtures, whereas only the $p$-wave interaction is possible in a one-component Fermi gas. The description of the three-body properties turns out to be universal and depends on a single parameter $m/m_1$ in the limit of the zero interaction range. For the interaction given within the framework of the boundary condition model (BCM), a solution of hyper-radial equations (HREs) provides an efficient approach to treat both the eigenvalue and the scattering problem [14–16]. An important advantage of the BCM is that all the terms of HREs are derived in analytical form; the method of derivation and the analytical expressions are similar to those obtained for three identical bosons in three and two dimensions [14, 17]. The calculations reveal that two three-body bound states arise while the mass ratio $m/m_1$ increases from zero to the critical $\lambda_c$, beyond which the number of bound states becomes infinite [8]. A two-hump structure is found for the mass-ratio dependences of the elastic and inelastic (2 + 1)-scattering cross sections near the three-body threshold. The structure of the isotopic dependencies is qualitatively related to the rise of the bound states as a common origin is an increase of the potential-well depth in the (2 + 1)-channel.

2. Outline of the approach

In the universal low-energy limit, the short-range two-body interaction is described by a single parameter, a natural choice for which is the two-body scattering length $a$. For the vanishing range of interaction, the two-body interaction is defined within the framework of the BCM by imposing the boundary condition at the zero inter-particle distance $r$:

$$\lim_{r \to 0} \frac{\partial \ln(r \Psi)}{\partial r} = -\frac{1}{a}. \quad (1)$$

The two-body interaction introduced in this way is known in the literature as the zero-range potential [18], the Fermi pseudo-potential [19], the Fermi–Huang pseudo-potential [20, 21], and an equivalent approach is used in the momentum-space representation [22].

For definiteness, one supposes that particle 1 is of mass $m_1$ and particles 2 and 3 are two identical fermions of mass $m$. The wavefunction $\Psi$ satisfies the equation

$$[\Delta_x + \Delta_y + E] \Psi = 0, \quad (2)$$

where the scaled Jacobi variables $x = \sqrt{2\mu} (r_2 - r_1)$ and $y = \sqrt{2\tilde{\mu}} (r_3 - \frac{m_1 r_1}{m_1 + m_2 + m_3} - \frac{m_2 r_2}{m_1 + m_2 + m_3})$ are defined via the position vectors $r_i$ and the reduced masses $\mu = \frac{m m_1}{m + m_1}$ and $\tilde{\mu} = \frac{m_1 m_2 m_3}{m_1 + m_2 + m_3}$, respectively. The total interaction is expressed by imposing two boundary conditions of the form (1) at zero distances between the different particles in two pairs 1–2 and 1–3. One demands that the wavefunction should be antisymmetric under permutation of identical fermions 2 and 3; under this condition only a single boundary condition of the form (1) should be imposed at the zero distance between particles 1 and 2, $x \to 0$. The unit total angular momentum $L = 1$ is considered, which is most important for the low-energy processes [10, 12, 13].
\( \hbar = 2\mu = |a| = 1 \) will be used hereafter; thus, any three-body property depends only on the single remaining parameter \( m/m_1 \).

The three-body bound and resonance states and the low-energy scattering are conveniently treated by solving a system of HREs [23]. The eigenfunctions \( \Phi_n(\rho, \Omega) \) are defined as regular solutions on the hyper-sphere at the fixed hyper-radius \( \rho \),

\[
\frac{1}{\sin^2 2\alpha} \left( \sin^2 2\alpha \frac{\partial}{\partial \alpha} + \frac{1}{\sin^2 \alpha} \Delta \delta + \frac{1}{\cos^2 \alpha} \Delta \delta + \gamma_n^2(\rho) - 4 \right) \Phi_n(\rho, \Omega) = 0, \tag{3}
\]

\[
\lim_{\alpha \to 0} \left[ \frac{\partial \ln (\alpha \Phi_n)}{\partial \alpha} \pm \rho \right] = 0, \tag{4}
\]

where \( \Omega \) is a brief notation for the hyper-angles \( \alpha, \hat{x} \) and \( \hat{y} \). The hyper-spherical variables are defined by the relations \( x = \rho \sin \alpha, y = \rho \cos \alpha, \hat{x} = x/x \) and \( \hat{y} = y/y \). The ± sign in (4), which corresponds to the positive and negative scattering length \( a \), hereafter will be incorporated into the parameter \( \rho \). Thus, the eigenvalue problem will be considered for an arbitrary \(-\infty < \rho < \infty \). For each value of \( \rho \), the solution of (3) and (4) determines a set of discrete eigenvalues \( \gamma_n^2(\rho) \), which are enumerated in an ascending order by an index \( n = 1, 2, 3, \ldots \), and corresponding eigenfunctions \( \Phi_n(\rho, \Omega) \). The expansion of the total wavefunction in a set of eigenfunctions \( \Phi_n(\rho, \Omega) \) normalized by the condition \( \langle \Phi_n | \Phi_m \rangle = \delta_{nm} \),

\[
\Psi = \rho^{-5/2} \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\rho, \Omega), \tag{5}
\]

leads to an infinite set of coupled HREs

\[
\left[ \frac{d^2}{d\rho^2} - \frac{\gamma_n^2(\rho) - 1/4}{\rho^2} + E \right] f_n(\rho) - \sum_{m=1}^{\infty} \left[ P_{nm}(\rho) - Q_{nm}(\rho) \frac{d}{d\rho} - \frac{d}{d\rho} Q_{nm}(\rho) \right] f_m(\rho) = 0, \tag{6}
\]

where

\[
Q_{nm}(\rho) = \left\{ \Phi_n \frac{\partial \Phi_m}{\partial \rho} \right\}, \quad P_{nm}(\rho) = \left\{ \frac{\partial \Phi_n}{\partial \rho} \frac{\partial \Phi_m}{\partial \rho} \right\}, \tag{7}
\]

and the notation \( \langle \cdot | \cdot \rangle \) stands for integration over the invariant volume on the hyper-sphere \( d\Omega = \sin^2 2\alpha d\alpha d\hat{x} d\hat{y} \).

The eigenfunctions \( \Phi_n(\rho, \Omega) \) inherit the antisymmetry of the wavefunction under permutation of the identical fermions 2 and 3. The solutions of the eigenvalue problem (3) and (4), which satisfy the permutational symmetry and belong to the total angular momentum \( L = 1 \) and its projection \( M \), are expressed as

\[
\Phi_n(\rho, \Omega) = (1 - \hat{P}) \frac{\psi_n(\alpha, \rho)}{\sin 2\alpha} Y_{1M}(\hat{y}), \tag{8}
\]

where \( Y_{1M}(\hat{y}) \) is the spherical function and \( \hat{P} \) denotes the permutation of particles 2 and 3. The action of \( \hat{P} \) in terms of the Jacobi variables is given by

\[
\hat{P}x = -\sin \omega x + \cos \omega y, \quad \hat{P}y = -\cos \omega x - \sin \omega y, \tag{9}
\]

where the angle of the kinematic rotation \( \omega \) is expressed via the mass ratio as \( \cot \omega = (m_1/m)\sqrt{1 + 2m/m_1} \). Given the representation (8), the eigenvalue problem (3) and (4) is reduced to the equation

\[
\left[ \frac{\partial^2}{\partial \alpha^2} - \frac{2}{\cos^2 \alpha} + \gamma_n^2(\rho) \right] \psi_n(\alpha, \rho) = 0 \tag{10}
\]
complemented by the boundary conditions \( \varphi(\alpha, \rho) = 0 \) at \( \alpha = \pi/2 \) and
\[
\lim_{\alpha \to 0} \left( \frac{\partial}{\partial \alpha} + \rho \right) \varphi_n(\alpha, \rho) + \frac{2}{\sin 2\omega} \varphi_n(\omega, \rho) = 0,
\]
(11)
at the singular point \( \alpha = 0 \) of the eigenfunctions \( \Phi_n(\rho, \Omega) \). The boundary condition (11) is deduced from equations (4), (8) and (9) by observing that \( \tilde{P} \alpha \to \pi/2 - \omega \) and \( \tilde{P} Y_{1M}(\Omega) \to -Y_{1M}(\Omega) \) as \( \alpha \to 0 \).

The zero-valued at \( \alpha = \pi/2 \) unnormalized solutions to equation (10) are straightforwardly written as
\[
\varphi_n(\alpha, \rho) = \gamma_n(\rho) \cos[\gamma_n(\rho)(\pi/2 - \alpha)] - \tan \alpha \sin[\gamma_n(\rho)(\pi/2 - \alpha)].
\]
(12)
Substituting (12) into the boundary condition (11), one eventually finds the transcendental equation
\[
\rho = \frac{1 - \gamma^2}{\gamma} \tan \frac{\pi}{2} - \frac{2}{\sin 2\omega} \cos \gamma \omega \gamma \sin^2 \omega \cos \frac{\pi}{2} + \sin \gamma \omega \gamma \sin^2 \omega \cos \frac{\pi}{2},
\]
(13)
which determines the infinitely multivalued function \( \gamma^2(\rho) \) of an arbitrary complex-valued variable \( \rho \) at various mass ratios \( m/m_1 \) given by the parameter \( \omega \). Different branches of this unique function for the real-valued \( \rho \) form a set of real-valued eigenvalues \( \gamma_n^2(\rho) \); thus, the solution of the eigenvalue problem is accomplished by means of expressions (12) and (13).

An advantage of the BCM is that the eigenvalues \( \gamma_n^2(\rho) \) entering into HREs are expressed in a simple analytical form [15–17], which is helpful both for qualitative analysis and in the numerical calculations. Moreover, the coupling terms \( Q_{nm}(\rho) \) and \( P_{nm}(\rho) \) can be determined in the analytical form via \( \gamma_n^2(\rho) \) and their derivatives as was done in [14, 17]; the derivation is outlined in the appendix.

Properties of the eigenvalues \( \gamma_n^2(\rho) \) are deduced by analysing equation (13), in particular, all \( \gamma_n^2(\rho) \) monotonically decrease within the intervals \( 9 > \gamma_1^2(\rho) > -\infty \) and \( (2n + 1)^2 > \gamma_n^2(\rho) > (2n - 1)^2 \) for \( n \geq 2 \) as the hyper-radius runs the interval \( -\infty < \rho < \infty \). The effective potentials in the upper channels for \( n \geq 2 \) contain the repulsive term \( \gamma_n^2(\rho)/\rho^2 \), which means a dominant role of the lowest channel for the low-energy solutions. Furthermore, the first-channel potential at small \( \rho \) is approximately determined by \( \gamma_1^2(0) \) so that \( V_1(\rho) \approx \left[ \gamma_1^2(0) - 1/4 \right]/\rho^2 \), which entails that the number of the bound states is finite for \( \gamma_1^2(0) > 0 \) and infinite for \( \gamma_1^2(0) < 0 \). As follows from equation (13), \( \gamma_1^2(0) \) decreases with increasing \( \omega \) and crosses zero at the critical value \( \omega_c \approx 1.198\,623\,76 \), which satisfies the equation
\[
\frac{\pi}{2} \sin^2 \omega_c - \tan \omega_c = 0,
\]
(14)
and corresponds to the critical mass ratio \( \lambda_c \approx 13.606\,9657 \). Thus, one concludes that a number of three-body bound states is either finite or infinite if the mass ratio \( m/m_1 \) is below or above \( \lambda_c \). An infinite energy spectrum of three fermions for the mass ratio above the critical value, \( m/m_1 > \lambda_c \), was first discovered in [8]. Note that the unambiguous description of the three-body properties for \( m/m_1 > \lambda_c \) requires an additional parameter which determines the wavefunction in the vicinity of the triple-collision point.

A more detailed analysis is needed to describe the energy spectrum for the mass ratio below the critical value, \( m/m_1 \leq \lambda_c \). The description is quite simple for the negative two-body scattering length \( a < 0 \), in which case all \( \gamma_n^2(\rho) \) are non-negative for \( m/m_1 \leq \lambda_c \); therefore, there are no three-body bound states. Considering the positive two-body scattering length \( a > 0 \), one finds that there are no bound states for the mass ratio roughly below 5 because the first-channel diagonal term is strictly above the two-body threshold \( (\gamma_1^2(\rho)/\rho^2 > -1) \)
for \( m/m_1 \lesssim 5 \). To estimate the number of the bound states which occur as \( m/m_1 \) increases up to the critical mass ratio \( \lambda_c \), one should consider the small-\( \rho \) behaviour of the eigenvalue \( \gamma_1^2(\rho) \approx -q_c/\rho \) at \( m/m_1 = \lambda_c \). Correspondingly, the first-channel diagonal term is of the form 
\[-1/4 \rho^2 - q_c/\rho, \]
where
\[ q_c = \left[ \frac{\pi}{2} \left( 1 + \frac{\pi^2}{24} - \frac{\omega_c^2}{2} \right) - \frac{\omega_c^3}{3 \sin^3 \omega_c} \right]^{-1} \approx 2.34253823. \]

As the energy of the \( n \)th level in this potential is \( E_n = -q_c^2 / (2n - 1)^2 \), one can roughly estimate that at least one and not more than two bound states exist for \( m/m_1 = \lambda_c \). To illustrate the above-described properties, the two lowest terms \( \gamma_n^2(\rho)/\rho^2 \) of HREs are depicted in figure 1 for different values of the mass ratio.

The asymptotic expressions for the channel potentials \( V_n(\rho) = \gamma_n^2(\rho) + P_{nn}(\rho) \) and the coupling terms \( P_{nn}(\rho) \) and \( Q_{nn}(\rho) \) are of interest for a solution of both the eigenvalue and the scattering problem. In this respect, one should emphasize that the exact analytical expressions for all the terms of the hyper-radial equations provide an easy way to determine the asymptotic expansions with a desired accuracy. Note that a direct derivation of the asymptotic expressions for the channel potentials and the coupling terms is a comparatively difficult problem, as one can see from the estimates of [24]. The asymptotic form of \( \gamma_n^2(\rho) \) at a large hyper-radius is determined by the expansion of equation (13) for \( \gamma \to \infty \) and \( \gamma \to 2n - 1 \), which gives
\[\gamma_n^2(\rho) = \begin{cases} -\rho^2 + 2 + 1/\rho^2 + O(\rho^{-2}), & n = 1, \\ (2n - 1)^2 + c_n/\rho + O(\rho^{-2}), & n > 1, \end{cases}\]
where
\[ c_n = \frac{4}{\pi} \left[ \frac{4n(n - 1)}{2n - 1} - 2 \frac{(-1)^n \cos(2n - 1)\omega}{\sin 2\omega} + \frac{(-1)^n \sin(2n - 1)\omega}{(2n - 1) \sin^2 \omega} \right]. \]

Substituting equation (15) in the exact expressions (A.7), (A.9) and (A.13), one obtains a large-\( \rho \) expansion for the coupling terms
\[ Q_{n1}(\rho) = \frac{\sqrt{2} c_n}{\rho^{5/2}} + O(\rho^{-7/2}). \]
Table 1. Mass ratios $\lambda_c$ for which the three-body bound states arise and energies $E_{ic}$ of these states for $m/m_1 = \lambda_c$ calculated with $N$ HREs.

| $N$ | $\lambda_1$   | $\lambda_2$ | $E_{ic}$ 1 | $E_{ic}$ 2 |
|-----|---------------|--------------|------------|------------|
| 1   | 8.183 854     | 12.929 430  | −5.894 05  | −1.136 32  |
| 2   | 8.175 776     | 12.921 084  | −5.895 25  | −1.137 30  |
| 3   | 8.173 692     | 12.918 879  | −5.895 37  | −1.137 52  |
| 4   | 8.173 003     | 12.918 061  | −5.895 40  | −1.137 59  |
| 5   | 8.172 771     | 12.917 712  | −5.895 41  | −1.137 62  |
| 6   | 8.172 688     | 12.917 564  | −5.895 42  | −1.137 63  |
| 7   | 8.172 651     | 12.917 500  | −      | −          |
| 8   | 8.172 633     | 12.917 473  | −      | −          |
| 9   | 8.172 633     | 12.917 457  | −      | −          |
| 12  | 8.172 608     | 12.917 436  | −      | −          |
| $\infty$ | 8.172 60  | 12.917 43  | −      | −          |

$P_{11}(\rho) = \frac{1}{4\rho^2} + O(\rho^{-6}),$ (17)

$P_{n1}(\rho) = \frac{\sqrt{c_n/2}}{\rho^{7/2}} + O(\rho^{-9/2}),$ (18)

and

$Q_{nn}(\rho) = \frac{\sqrt{c_n c_m}}{4\rho^2(n-m)(n+m-1)} + O(\rho^{-3}),$ (19)

$P_{nm}(\rho) = \frac{\sqrt{c_n c_m(c_n + c_m)}}{16\rho^4(n-m)^2(n+m-1)^2} + O(\rho^{-5})$ (20)

for $n, m \neq 1$. The channel potentials take the asymptotic form

$V_1(\rho) = -1 + \frac{2}{\rho^2} + \frac{1}{\rho^3} + O(\rho^{-6})$ (21)

and

$V_n(\rho) = \frac{(2n-1/2)(2n-3/2)}{\rho^2} + \frac{c_n}{\rho^3} + O(\rho^{-4}), \quad n \geq 2,$ (22)

which corresponds to the long-range interaction of a dimer with the third particle for $n = 1$ and of three asymptotically free particles for $n \geq 2$.

In addition to the above-described qualitative conclusions, a detailed quantitative description of the three-body properties will be given for the non-trivial case $\alpha > 0$ and $m/m_1 \leq \lambda_c$. In the following sections, both the energy spectrum and the scattering characteristics are obtained by the numerical solution of HREs (6) complemented by the natural zero boundary conditions $f_n(\rho) \to 0$ as $\rho \to 0$ and the specified asymptotic boundary conditions as $\rho \to \infty$. All the terms of HREs are calculated by using the eigenvalue equation (13) and the exact expressions (A.7), (A.9) and (A.13) for the coupling terms, which provide a high accuracy of the numerical results. The numerical solution of HREs is basically the same as in [17]. For all the values calculated in section 3, the parameters of the numerical procedure were adjusted to reach an accuracy given in table 1. In particular, the integration was carried out up to $\rho_{\text{max}} \approx 150$. For the scattering characteristics near the three-body threshold, an accuracy of the numerical integration about 3–4 significant digits was obtained with the range of integration extended up to $\rho_{\text{max}} \approx 3000$. 


3. Three-body bound states and near-threshold resonances

The dependences of the three-body binding energies on the mass ratio are determined by solving a system of HREs with the zero asymptotic boundary conditions, \( f_n(\rho) \to 0 \) as \( \rho \to \infty \). The results of the calculations are shown in figure 2 and in table 1; it turns out that there are zero, one and two bound states for \( 0 < m/m_1 < \lambda_1, \lambda_1 \leq m/m_1 < \lambda_2 \) and \( \lambda_2 \leq m/m_1 \leq \lambda_c \), respectively. The binding energies increase as the mass ratio increases to the critical value \( \lambda_c \); in the limit \( m/m_1 \to \lambda_c \) the energies tend to the finite values \( E_{ic} (i = 1, 2) \) following a square-root dependence \( E_i - E_{ic} \propto \sqrt{\lambda_c - m/m_1} \), which is demonstrated in figure 3. Note that this mass-ratio dependence comes from the expansion \( \gamma_i^2(0) \propto \lambda_c - m/m_1 \) as \( m/m_1 \to \lambda_c \).

For the mass ratios \( \lambda_i \), at which the three-body bound states arise, there are true bound states at the threshold energy \( E = -1 \), whose wavefunctions are square integrable with a power fall-off at large distances. Thus, to calculate the precise values \( \lambda_i \), a system of HREs is solved for \( E = -1 \) by using the power dependence of the first-channel function, \( f_1(\rho) \sim \rho^{-2} \).
as $\rho \to \infty$. The calculated $\lambda_i$ rapidly converge with an increasing number of HREs $N$, being fairly well fitted to the power dependence $a + b/N^c$ with $c \approx 4$; the dependences of $\lambda_i$ on $N$ and the fitted values in the limit $N \to \infty$ are presented in table 1. If the mass ratio slightly exceeds $\lambda_i$, the separation of the loosely bound state from the two-body threshold is proportional to the mass ratio excess, namely, $|E_i+1| \propto m/m_1 - \lambda_i$. For the mass ratio just below $\lambda_i$, the relevant bound state turns to a narrow resonance, whose position $E_{ri}$ continues a linear mass-ratio dependence of the bound-state energy, $E_{r1} + 1 \propto \lambda_i - m/m_1$, whereas the width $\Gamma_1$ depends quadratically on the mass ratio excess, $\Gamma_1 \propto (\lambda_i - m/m_1)^2$. The above-described threshold features are connected with the presence of the long-range term $2/\rho^2$ in the $(2 + 1)$-channel effective potential (illustrated in the inset of figure 1).

To calculate the positions and widths of two narrow resonances for $m/m_1 \lesssim \lambda_i$, a system of HREs is solved for $E > -1$. In view of equation (21), the asymptotic boundary condition for $\rho \to \infty$ imposed to allow for the incoming and outgoing waves in the first channel is taken in the form

$$f_1(\rho) \to \rho [j_1(k\rho) - \tan \delta(k)y_1(k\rho)],$$

where the wave number $k$ is given by $E = -1 + k^2$, $\delta(k)$ is the $(2 + 1)$-scattering phase shift and $j_1(x)$ and $y_1(x)$ are the spherical Bessel functions. The resonance position $E_r$ and the width $\Gamma_1$ are determined by fitting $\delta(k)$ to the Wigner dependence,

$$\cot[\delta(k) - \delta_{bg}] = \frac{2}{\Gamma_1(E_r - E)},$$

where $\delta_{bg}$ is the non-resonant phase shift. Near-threshold mass-ratio dependences of the bound-state energies $E_i$ and the resonance parameters $E_{ri}$ and $\Gamma_1$ are shown in figure 4.

4. Low-energy scattering near the three-body threshold

The scattering problem at small energies near the three-body threshold is solved in the two-channel approximation for the mass ratio within the range $0 \leq m/m_1 \leq \lambda_c$. The $K$-matrix is calculated by using two independent solutions $f^{(1)}$ and $f^{(2)}$, respectively, which satisfy, in view of equations (21) and (22), the following asymptotic boundary conditions:

$$[f^{(1)}, f^{(2)}] = \sqrt{\rho} \begin{bmatrix} Y_{3/2}(k\rho) & 0 \\ 0 & Y_3(\sqrt{k^2 - 1}\rho) \end{bmatrix} + K \begin{bmatrix} J_{3/2}(k\rho) & 0 \\ 0 & J_3(\sqrt{k^2 - 1}\rho) \end{bmatrix} \begin{bmatrix} Y_{3/2}(k\rho) & 0 \\ 0 & Y_3(\sqrt{k^2 - 1}\rho) \end{bmatrix}$$

as $\rho \to \infty$. The elastic $(2 + 1)$-scattering phase shift is defined by $\cot \delta(k) = -K_{11}(k)$ and the inelastic scattering amplitude is determined by the non-diagonal element of the $T$-matrix given

Figure 4. Near-threshold mass-ratio dependences of the bound-state energies $E_i$ (solid lines), resonance positions $E_{ri}$ (dashed lines) and resonance widths $\Gamma_1$ (dash-dotted lines).
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Figure 5. Mass-ratio dependences of the elastic (2+1)-scattering cross section at the three-body threshold $\sigma_{th}$ (solid line) and the low-energy leading-order term $A^2 = \lim_{E \to 0} |T_{21}(E)\rangle^2 E^{-3}$ of the three-body recombination rate $\alpha_r \sim A^2 E$ (dashed line).

by $T = 2(1 - iK)^{-1}$. The elastic-scattering phase shift at the three-body threshold $\delta_{th} \equiv \delta(1)$ is a smooth increasing function of $m/m_1$, which takes the value $3\pi/2 < \delta_{th} \approx 5\pi/2 < 2\pi$ for the mass ratio $m/m_1 = \lambda_c$. Correspondingly, the elastic-scattering cross section at the three-body threshold, which is determined in the dimensional units as $\sigma_{th} = 12\pi a_1^2 (1 + 2m/m_1) (1 + m/m_1)^2 \sin^2 \delta_{th}$, has two maxima located near those values $m/m_1$ at which $\delta_{th}$ passes through $\pi/2$ and $3\pi/2$.

A two-hump structure of $\sigma_{th}(m/m_1)$ is shown in figure 5. The mass-ratio dependence of the leading-order term $A^2$, which determines the three-body recombination rate at low energy, is shown in figure 5. A two-hump structure of $A^2(m/m_1)$ with two maxima and three zeros within the interval $0 \leq m/m_1 \leq \lambda_c$ is in agreement with the result of [10]. One should note that the next-order term in the low-energy expansion $B(m/m_1)$ oscillates with increasing mass ratio, passing through zero at the points $m/m_1 \approx 7, 12.5$.

A similar structure of both mass-ratio dependences $\sigma_{th}(m/m_1)$ and $A^2(m/m_1)$ originates from the interference of the incoming and outgoing waves in the lowest (2+1)-channel, being closely connected with the potential-well deepening as $m/m_1$ increases. Qualitatively, with increasing potential-well depth, the (2+1)-channel function $f_1(\rho)$ acquires additional oscillations in the region of small hyper-radius $\rho \lesssim 5$, which leads to an oscillating mass-ratio dependence of both elastic and inelastic scattering amplitudes. As seen in figure 5, $A^2(m/m_1)$ passes through maxima and zeros at smaller values of $m/m_1$ than $\sigma_{th}(m/m_1)$, which reflects a complicated dependence of the inelastic amplitude on the oscillating function $f_1(\rho)$. For a better understanding, one could consider the matrix element of the inelastic scattering within the framework of the perturbation theory, $A(m/m_1) \propto \int d\rho f_1(\rho) [P_{12}(\rho) - Q_{12}(\rho) \frac{d}{d\rho} - \frac{d}{d\rho} Q_{12}(\rho)] f_2(\rho)$. On the other hand, the potential-well deepening with increasing $m/m_1$ leads to the rise of the three-body bound states, which is connected with the occurrence of oscillations of the first-channel function $f_1(\rho)$ calculated at the two-body threshold $E = -1$. A similar oscillating behaviour of the first-channel function $f_1(\rho)$ for $E = -1$ and $E = 0$ within the potential-well range allows one to link the rise of the three-body bound states with the zeros of the scattering amplitudes.
5. Discussion

The universal low-energy description for two identical fermions interacting with the third different particle in the states of the total angular momentum \( L = 1 \) is given within the framework of the approach based on the solution of hyper-radial equations, whose terms are derived in the analytical form. It is found that there are no three-body bound states for the negative scattering length and \( m/m_1 \leq \lambda_c \), whereas for the positive scattering length there are exactly zero, one and two bound states for \( m/m_1 < \lambda_1 \), \( \lambda_1 \leq m/m_1 < \lambda_2 \) and \( \lambda_2 \leq m/m_1 \leq \lambda_c \), respectively. For \( m/m_1 \) just below \( \lambda_1 \) or \( \lambda_2 \), the bound states disappear and turn to narrow resonances, whose positions and widths are calculated.

The above-described universal picture should be observed in the limit \( |a| \to \infty \), i.e. if the potential is tuned to produce the loosely bound two-body state. In this limit, one expects to observe simultaneously the loosely bound two-body and three-body states, whose binding energies scale as \( a^{-2} \) and their ratio depends on \( m/m_1 \). A similar threshold behaviour of the binding energies was discussed in [17, 25. 26] for three two-dimensional bosons.

Both the elastic \((2 + 1)\)-scattering cross sections and the three-body recombination rate near the three-body threshold manifest a two-hump structure of their mass-ratio dependences for \( m/m_1 \leq \lambda_c \). The structure of both isotopic dependences stems from the interference of the incoming and outgoing waves due to deepening of the effective potential in the \((2 + 1)\)-channel; in this respect, the interference is connected with the rise of two three-body bound states with increasing \( m/m_1 \).

As the present paper describes the universal three-body properties in the idealized limit of the zero interaction range, it is of interest to discuss briefly the effect of the finite, though small enough interaction radius \( r_0 \ll a \). For the mass ratio below the critical value \( \lambda_c \), the binding energies depend smoothly on the interaction radius \( r_0 \) and on the interaction in the vicinity of the triple-collision point provided \( r_0 \ll a \), whereas for \( m/m_1 > \lambda_c \) the infinite energy spectrum is extremely sensitive to these parameters. Furthermore, an abrupt transition from two to an infinite number of bound states at \( m/m_1 = \lambda_c \) will be smeared off if either the interaction range is not zero or the three-body force is present. One can roughly estimate that the number of three-body bound states \( N_b = 2 \) for the mass ratio within the range \( m/m_1 - \lambda_c \lesssim r_0/a \) and increases as \( N_b \propto \sqrt{m/m_1 - \lambda_c} \ln \frac{a}{r_0} \) with increasing \( m/m_1 \).

Finally, it is worth noting that the \( p \)-wave molecule containing two heavy fermions and the light third particle could be observed in the ultra-cold mixtures of \( ^{87}\text{Sr} \) with lithium isotopes. For the mixtures of \( ^{87}\text{Sr} \) with \( ^{7}\text{Li} \), the mass ratio \( m/m_1 \approx 12.4 \) falls into the interval \([\lambda_1, \lambda_2]\), which entails existence of exactly one bound state of the bosonic molecule \( ^{7}\text{Li}^{87}\text{Sr}_2 \), whose binding energy is about 0.793 times the binding energy of the \( ^{7}\text{Li}^{87}\text{Sr} \) molecule. For the mixtures of \( ^{87}\text{Sr} \) with \( ^{6}\text{Li} \), the mass ratio \( m/m_1 = 14.5 \) exceeds the critical value \( \lambda_c \), which entails existence of at least two bound states of the fermionic molecule \( ^{6}\text{Li}^{87}\text{Sr}_2 \), whose binding energies are expected to be slightly above 4.895 and 0.138 times the binding energy of the \( ^{6}\text{Li}^{87}\text{Sr} \) molecule. As \( m/m_1 > \lambda_c \), one could expect that there are more bound states of \( ^{6}\text{Li}^{87}\text{Sr}_2 \); however, a number of these states and their binding energies essentially depend on details of the inter-atomic two-body and three-body interactions.

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Appendix. Analytical expressions for the coupling terms

Although the direct calculation of the coupling terms $Q_{nm}(R)$ and $P_{nm}(R)$ via the definition (7) is quite involved, one can circumvent this problem and obtain the analytical expressions for $Q_{nm}(\rho)$ and $P_{nm}(\rho)$ via $\gamma^2_n(\rho)$ and their derivatives by using the explicit dependence on $\rho$ in the boundary condition (4). Similar analytical expressions were derived for a number of problems based on the BCM; more details are given in [17].

Hereafter one concisely writes the eigenvalue problem (3), (4) as

\[ \left(\Delta + \gamma_n^2\right) \Phi_n = 0, \]  
\[ \lim_{\alpha \to 0} \left( \frac{\partial}{\partial \alpha} + \rho \right) \sin 2\alpha \Phi_n = 0. \]  

The derivative of the normalized eigenfunction $\Phi_n$ with respect to $\rho$ satisfies the inhomogeneous equation

\[ \left(\Delta + \gamma_n^2\right) \frac{\partial \Phi_n}{\partial \rho} + \frac{d\gamma^2_n}{d\rho} \Phi_n = 0 \]  

and the boundary condition

\[ \lim_{\alpha \to 0} \left[ \left( \frac{\partial}{\partial \alpha} + \rho \right) \sin 2\alpha \frac{\partial \Phi_n}{\partial \rho} + \sin 2\alpha \Phi_n \right] = 0. \]  

By projecting equation (A.3) onto $\Phi_m$ and using the representation (8), one obtains the relation

\[ (\gamma_n^2 - \gamma_m^2) Q_{mn} + \delta_{nm} \frac{d\gamma^2_n}{d\rho} + \phi_n(0, \rho) \phi_m(0, \rho) = 0, \]  

where the integrals over the hyper-sphere are expressed via the integrals over the hypersurfaces surrounding two singularities of the functions $\Phi_n$, namely, one at $\alpha = 0$ and the other given by the permutational symmetry. Here the integration volume is arbitrarily chosen to provide the unit coefficient for the last term in (A.5), and it is taken into account that equal contributions come from two surface integrals around both singularities. The diagonal part of equation (A.5) gives the basic relation

\[ \phi_n^2(0, \rho) = -\frac{d\gamma_n^2}{d\rho}, \]  

which allows one to derive the desired expressions via the derivative of the eigenvalues $\gamma^2_n(\rho)$. Substituting (A.6) in the non-diagonal part of (A.5), one finds

\[ Q_{nm} = (\gamma_n^2 - \gamma_m^2)^{-1} \left[ \frac{d\gamma^2_n}{d\rho} \frac{d\gamma^2_m}{d\rho} \right]. \]  

In a similar way, the projection of equation (A.3) onto $\frac{\partial \Phi_n}{\partial \rho}$ for $n \neq m$ leads to the relation

\[ \frac{d(\gamma_n^2 + \gamma_m^2)}{d\rho} Q_{mn} = (\gamma_n^2 - \gamma_m^2) P_{mn} + \phi_n(0, \rho) \frac{d\phi_m(0, \rho)}{d\rho} - \phi_m(0, \rho) \frac{d\phi_n(0, \rho)}{d\rho}, \]  

which is finally transformed to the expression for the non-diagonal coupling terms

\[ P_{nm} = Q_{nm} \left[ (\gamma_n^2 - \gamma_m^2)^{-1} \frac{d}{d\rho} \left( \gamma_n^2 + \gamma_m^2 \right) + \frac{1}{2} \frac{d^2 \gamma^2_n}{d\rho^2} \left( \frac{d\gamma^2_n}{d\rho} \right)^{-1} - \frac{1}{2} \frac{d^2 \gamma^2_m}{d\rho^2} \left( \frac{d\gamma^2_m}{d\rho} \right)^{-1} \right]. \]
where one uses equation (A.6) and its derivative $\frac{d^2 \gamma^2_{\nu}}{d \rho^2} = -2 \varphi_n(0, \rho) \frac{d \varphi_n(0, \rho)}{d \rho}$.

At last, the second derivative of the eigenfunction $\Phi_n$ with respect to $\rho$ satisfies the equation

$$
\left( \tilde{\Delta} + \gamma^2_{\nu} \right) \frac{\partial^2 \Phi_n}{\partial \rho^2} + 2 \frac{\partial \gamma^2_{\nu}}{\partial \rho} \frac{\partial \Phi_n}{\partial \rho} + \frac{d^2 \gamma^2_{\nu}}{d \rho^2} \Phi_n = 0
$$

(A.10)

and the boundary condition

$$
\lim_{\alpha \to 0} \left[ \left( \frac{\partial}{\partial \alpha} + \rho \right) \sin 2 \alpha \frac{\partial^2 \Phi_n}{\partial \rho^2} + 2 \sin 2 \alpha \frac{\partial \Phi_n}{\partial \rho} \right] = 0.
$$

(A.11)

By projecting equation (A.10) onto $\Phi_n$ and using the identity $P_{nn} = -\langle \Phi_n | \frac{\partial^2 \Phi_n}{\partial \rho^2} \rangle$, one finds that

$$
3 \frac{d^2 \gamma^2_{\nu}}{d \rho^2} P_{nn} = \varphi_n(0, \rho) \frac{d^2 \varphi_n(0, \rho)}{d \rho^2} - 2 \left[ \frac{d \varphi_n(0, \rho)}{d \rho} \right]^2.
$$

(A.12)

The derivatives of $\varphi_n(0, \rho)$ are expressed via the derivatives of $\gamma^2_{\nu}(\rho)$ by using equation (A.6), which allows one to cast the diagonal coupling term in the form

$$
P_{nn} = -\frac{1}{6} \frac{d^2 \gamma^2_{\nu}}{d \rho^2} \left( \frac{d^2 \varphi_n(0, \rho)}{d \rho^2} \right)^{-1} + \frac{1}{4} \left( \frac{d \gamma^2_{\nu}}{d \rho} \right)^2 - \frac{d^2 \gamma^2_{\nu}}{d \rho^2}.
$$

(A.13)

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