Atom-Dimer Scattering for Confined Ultracold Fermion Gases

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We solve the three-body problem of a quasi-one-dimensional ultracold Fermi gas with parabolic confinement length $a_\perp$ and 3D scattering length a. On the two-body level, there is a Feshbach-type resonance at $a_\perp/a \approx 1.46$, and a dimer state for arbitrary $a_\perp/a$. The three-body problem is shown to be universal, and described by the atom-dimer scattering length a_{ad} and a range parameter b_{ad}. In the dimer limit $a_\perp/a \gg 1$, we find a repulsive zero-range atom-dimer interaction. For $a_\perp/a \ll -1$, however, the potential has long range, with $a_{ad} > 0$ and $b_{ad} \gg a_{ad}$. There is no trimer state, and despite $a_{ad} = 0$ at $a_\perp/a \approx 2.6$, there is no resonance enhancement of the interaction.

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The recent experimental observation of the formation of dimers (molecules) in ultracold binary Fermi gases [1] has sparked intense excitement and activity among both atomic and condensed-matter physicists. Experiments are now able to probe in detail the BEC-BCS crossover regime by using magnetic-field tuned Feshbach resonances [2–4], where the 3D scattering length a describing the s-wave interaction strength among different fermion species can be tuned almost at will. This crossover remains a difficult and long-standing challenge to theory, as there is no small parameter in the problem [5]. Here we discuss the related but simpler problem of an ultracold two-species ($\uparrow, \downarrow$) Fermi gas confined in a 1D trap potential. On the two-body level, there is always a bound state (dimer), and one has a confinement-induced resonance (CIR) in the 1D atom-atom scattering length a_{aa} [6,7], similar to a Feshbach resonance. Such a scenario appears to be experimentally feasible [1–4,8,9] and could reveal interesting new physics. In this Letter, we analytically solve the three-body problem for confined ultracold fermions, and compute the atom-dimer scattering length a_{ad} and the potential range b_{ad} [see Eq. (13) below]. Our results also determine parameters entering models that may be solved exactly by powerful many-body techniques in 1D [10]; see also Refs. [11,12].

For simplicity, we assume the two fermion species to have the same mass m_0. Under the harmonic transverse confinement potential $U_c(\mathbf{r}) = \frac{1}{2} m_0 \omega_\perp^2 (x^2 + y^2)$, with associated length scale $a_\perp = (2\hbar/m_0\omega_\perp)^{1/2}$, there is a two-body bound state (dimer) with dimensionless binding energy

$$\Omega_B = (\hbar\omega_\perp - E_B)/2\hbar\omega_\perp \tag{1}$$

determined by the condition [6,7]

$$\zeta(1/2, \Omega_B) + a_\perp/a = 0. \tag{2}$$

Since the zeta function $\zeta(1/2, \Omega)$ is monotonic in Ω, there is exactly one bound state for any given $a_\perp/a$, although the 3D problem has a bound state only for $a > 0$. For $a_\perp/a \to -\infty$, the "BCS limit" is reached, where $\Omega_B \simeq (a/a_\perp)^2 \ll 1$, and the dimer size is large, of the order $a_\perp^2/|a|$. In the tightly bound "dimer limit", $a_\perp/a \to +\infty$, the dimer size is small, of the order a, and $\Omega_B \simeq (a_\perp/2a)^2 \gg 1$. The analogue of the Feshbach resonance is then realized by the CIR. Solving the two-body scattering problem with just one open channel, the 1D scattering length is [6,7]

$$a_{aa} = -\frac{a_\perp}{2}\left[\frac{a_\perp}{a} - C\right], \quad C = -\zeta(1/2) \simeq 1.4603. \tag{3}$$

At low energies, this implies that one can use the 1D atom-atom interaction potential $V_{aa}(z, z') = g_{aa}\delta(z - z')$ with $g_{aa} = -2\hbar^2/m_0 a_{aa}$. The CIR then occurs for $a_{aa} = 0$, corresponding to $\Omega_B = 1$, and can be reached by tuning $a_\perp$ or a.

A natural question then concerns the scattering properties of the atom-dimer system, for instance, the scattering length a_{ad}. This problem has recently been solved for the unconfined 3D case by Petrov [13], where $a_{ad} \approx 1.2a$. In the confined geometry, it is then interesting to ask (i) whether the scattering length a_{ad} also shows CIR-related resonant behavior, (ii) whether a trimer state could be possible in the confined geometry, and (iii) whether a universal description in terms of simple two-body physics is always applicable. For the unconfined case, Efimov [14] showed that this three-body problem is universal. Moreover, there is no bound trimer state. Below we shall answer these questions in detail.

We study the three-body problem ($\uparrow\uparrow\downarrow$) with two identical fermions, and denote by $\mathbf{x_1}$ ($\mathbf{x_{2,3}}$) the position of the $\downarrow$ (the two $\uparrow$) particles. Next we perform an orthogonal transformation to variables $(\mathbf{x}, \mathbf{y}, \mathbf{z})$ in order to decouple the center-of-mass coordinate $\mathbf{z}$ [13]. Since the confinement is harmonic, U_c remains diagonal in the positions. The three-body problem then reduces to

$$\left[-\frac{\hbar^2}{m_0}\nabla^2_{\mathbf{X}} + U_c(\mathbf{X}) - E\right]\Psi(\mathbf{X}) = -\sum_{\pm} V(\mathbf{r}_{\pm})\Psi(\mathbf{X}), \quad (4)$$

where $\mathbf{X} = (\mathbf{x}, \mathbf{y})$ is a six-dimensional vector, $\mathbf{x} = (2\mathbf{x}_1 - \mathbf{x}_2 - \mathbf{x}_3)/2$ and $\mathbf{y} = \mathbf{x}_3 - \mathbf{x}_2$. With these definitions, the distances between the $\downarrow$ particle and each $\uparrow$ particle are $\mathbf{r}_{\pm} = \sqrt{3}\mathbf{x}/2 \pm \mathbf{y}/2$. We adopt the pseudopotential approximation for the 3D interaction, $V(\mathbf{r}) = (4\pi\hbar^2 a/m_0)\delta(\mathbf{r})\frac{\partial}{\partial r}(r\cdot)$, which allows us to incorporate interactions via boundary conditions imposed for vanishing distances between $\uparrow$ and $\downarrow$ atoms. For $\mathbf{r}_{\pm} \to 0$, this implies the singular behavior

$$\Psi(\mathbf{X}) \simeq \mp \frac{f(\mathbf{r}_{\perp,\pm})}{4\pi r_{\pm}}(1 - r_{\pm}/a), \quad (5)$$

where the $\mathbf{r}_{\perp,\pm} = \mathbf{x}/2 \mp \sqrt{3}\mathbf{y}/2$ are orthogonal to $\mathbf{r}_{\pm}$. We consider $E < 0$ and write

$$E = -2\Omega_B\hbar\omega_{\perp} + \hbar^2\bar{k}^2/m_0,$$

where the relative momentum $\hbar\bar{k}$ of the atom-dimer complex is sent to zero later.

The boundary conditions (5) allow us to write Eq. (4) in the form

$$m_0\Psi(\mathbf{X}) = \sum_{\pm} \mp \int d\mathbf{x}' d\mathbf{y}' G_E^{(2)}(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}') f(\mathbf{r}'_{\perp,\pm})\delta(\mathbf{r}'_{\pm}), \quad (6)$$

where the two-particle Green function is

$$G_E^{(2)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = \sum_{\lambda_1,\lambda_2} \frac{\psi_{\lambda_1}(\mathbf{r}_1)\psi_{\lambda_2}(\mathbf{r}_2)\psi^*_{\lambda_1}(\mathbf{r}_3)\psi^*_{\lambda_2}(\mathbf{r}_4)}{E_{\lambda_1} + E_{\lambda_2} - E}.$$

Here ψ_λ denotes the eigenfunctions to the single-particle problem for eigenenergy E_λ. The quantum numbers λ include the 1D momentum k, the (integer) angular momentum m, and the radial quantum number $n = 0, 1, 2\ldots$, which gives $E_\lambda = \hbar\omega_{\perp}(2n + |m| + 1) + \hbar^2k^2/m_0$ and $\psi_\lambda = e^{im\phi}R_{nm}(\rho)e^{ikz}$ with radial functions R_{nm} [6]. Using the fact that $G_E^{(2)}$ and the integration measure are both invariant under orthogonal transformations, we find from Eq. (6)

$$m_0\Psi(\mathbf{r}, \mathbf{r}_{\perp}) = \int d\mathbf{r}'_{\perp} f(\mathbf{r}'_{\perp})[G_E^{(2)}(\mathbf{r}, \mathbf{r}_{\perp}; 0, \mathbf{r}'_{\perp}) - G_E^{(2)}(\mathbf{r}/2 + \sqrt{3}\mathbf{r}_{\perp}/2, \sqrt{3}\mathbf{r}/2 - \mathbf{r}_{\perp}/2; 0, \mathbf{r}'_{\perp})],$$

where $\mathbf{r} \equiv \mathbf{r}_-$ and $\mathbf{r}_{\perp} \equiv \mathbf{r}_{\perp,-}$. Next we implement the $\mathbf{r} \to 0$ limit according to Eq. (5) to obtain a closed equation for $f(\mathbf{r}_{\perp})$. This limit can be directly taken for the nonsingular second term in the integral above, while the first term contains the singular behavior necessary from Eq. (5). Once this singular behavior is removed, one obtains a regular integral equation for $f(\mathbf{r}_{\perp})$ [13,15,16]. It is convenient to transform from real space into the complete basis $\{\psi_\lambda\}$, implying

$$\mathcal{L}(\Omega_\lambda) f_\lambda = \sum_{\lambda'} A_{\lambda,\lambda'} f_{\lambda'}, \quad (7)$$

where we use [see also Eq. (2)],

$$\mathcal{L}(\Omega) = \zeta(1/2, \Omega) - \zeta(1/2, \Omega_B),$$
$$\Omega_\lambda = \Omega_B - (a_{\perp}\bar{k}/2)^2 + E_\lambda/2\hbar\omega_{\perp},$$

and the matrix $A_{\lambda,\lambda'}$ is given by

$$\frac{4\pi a_{\perp}}{m_0}\int d\mathbf{r}_{\perp}\psi^*_\lambda(\mathbf{r}_{\perp})\psi_{\lambda'}(-\mathbf{r}_{\perp}/2)G_{E-E_\lambda}(\sqrt{3}\mathbf{r}_{\perp}/2, 0).$$

Using the integral representation of Ref. [11] for the two-body Green function $G_E(\mathbf{r}, \mathbf{r}')$, $A_{\lambda,\lambda'}$ can be evaluated explicitly. Before analyzing Eq. (7) further, however, it is useful to perform a rescaling. So far, f has been taken as a function of $\mathbf{r}_{\perp} = (\rho, z)$. However, for the asymptotic solution consisting of a dimer and a free atom, the atom-dimer distance $\mathbf{d}$ does not coincide with $\mathbf{r}_{\perp}$. With the dimer wave function $\Phi_0(\mathbf{r})$ [6], we expect

$$\Psi(\mathbf{r}, \mathbf{r}_{\perp}) \simeq \Phi_0(\mathbf{r})\chi(\mathbf{d}),$$
$$\mathbf{d} = (\mathbf{x}_1 + \mathbf{x}_3)/2 - \mathbf{x}_2 = \mathbf{r}_+ - \mathbf{r}_-.$$

In the $r \to 0$ limit, $\Psi \simeq \chi(\sqrt{3}\mathbf{r}_{\perp}/2)/4\pi r$, which establishes a connection between $\mathbf{d}$ and $\mathbf{r}_{\perp}$ from Eq. (5). After the rescaling $\mathbf{r}_{\perp} \to \sqrt{3}\mathbf{r}_{\perp}/2$, f coincides with the scattering solution χ. Therefore, from now on, all wave vectors are rescaled by the factor $2/\sqrt{3}$.

Let us then proceed by projecting the integral Eq. (7) to the lowest transverse state ($n = m = 0$). Explicit calculations [17] show that the higher states are negligible in the BCS limit and affect a_{ad} only slightly in the dimer limit, see below. Taking into account the above rescaling, noting that only $m = 0$ modes have nonzero overlap with the lowest state we find

$$\mathcal{L}(\Omega_k) f_k = \int_{-\infty}^{+\infty} \frac{dk'}{2\pi} A_{k,k'} f_{k'},$$
$$\Omega_k = \Omega_B + \frac{3a_{\perp}^2(k^2 - \bar{k}^2)}{16} \quad (8)$$

with the kernel given by

$$A_{k,k'} = \sum_{p=0}^{\infty} \frac{4^{-p}}{p + \Omega_B + (a_{\perp}/2)^2[-3\bar{k}^2/4 + k^2 + k'^2 + kk']}. \quad (9)$$

Following Ref. [15], we now make an *ansatz* for the solution of the integral equation,

$$f(k) = 2\pi\delta(k - \bar{k}) + i\tilde{f}(k, \bar{k})\sum_{\pm} \frac{1}{\bar{k} \pm k + i0^+}, \quad (10)$$

with a regular function $\tilde{f}(k, \bar{k})$. This ansatz gives the expected scattering state after Fourier transforming to real space,

$$f(z) = e^{i\bar{k}z} + \tilde{f}(\mathrm{sgn}(z)\bar{k}, \bar{k})e^{i\bar{k}|z|}.$$

In the low-energy limit $k, \bar{k} \to 0$, on general grounds [18], the expansion

$$\tilde{f}(k, \bar{k}) = -1 + ikb_{ad} + i\bar{k}a_{ad} + \mathcal{O}(k^2, \bar{k}^2, k\bar{k}) \quad (11)$$

applies, where a_{ad} is the atom-dimer scattering length. From the analysis of model potentials, the length b_{ad} is linked to the range of the effective 1D atom-dimer potential. In particular, $b_{ad} \to 0$ if a zero-range δ potential can be used for the effective 1D atom-dimer scattering at low-energy scales.

Inserting the ansatz (10) into Eq. (8), we obtain

$$\frac{\mathcal{L}(\Omega_k)}{\bar{k}^2 - k^2} 2i\bar{k}\,\tilde{f}(k, \bar{k}) - i\mathcal{P}\sum_{\pm}\int_{-\infty}^{+\infty}\frac{dk'}{2\pi}\frac{A_{k,k'}}{\bar{k} \pm k'}\tilde{f}(k', \bar{k}) - \frac{1}{2}\left[\tilde{f}(\bar{k}, \bar{k})A_{k,\bar{k}} + \tilde{f}(-\bar{k}, \bar{k})A_{k,-\bar{k}}\right] = A_{k,\bar{k}}, \quad (12)$$

where $\mathcal{P}$ denotes a principal value integration. Finally, the analysis can be simplified considerably by letting $\bar{k} \to 0$, i.e., by expanding Eq. (12) in $\bar{k}$ and keeping only the lowest order. At that stage, we switch to dimensionless momenta u, u' by writing $k = (2\sqrt{\Omega_B}/a_\perp)u$. Some algebra gives, with the weakly Ω_B-dependent functions

$$G(u, u') = \sum_{p=0}^{\infty}\frac{4^{-p}}{1 + u^2 + u'^2 + uu' + p/\Omega_B}, \qquad H(u) = \sum_{p=0}^{\infty}\frac{4^{-p}u}{2(1 + u^2 + p/\Omega_B)^{-2}},$$

the following integral equation for $h(u) \equiv \tilde{f}(u, 0)$:

$$\int_{-\infty}^{+\infty}\frac{du'}{2\pi u'^2}[G(u, u')h(u') - G(u, 0)h(0)] - \frac{\sqrt{\Omega_B}}{2u^2}\mathcal{L}\left(\Omega_B[1 + \frac{3u^2}{4}]\right)h(u) = \frac{a_{ad}\sqrt{\Omega_B}}{a_\perp}G(u, 0) + iH(u). \quad (13)$$

Note that the real (imaginary) part of $h(u)$ is even (odd) in u. The scattering length a_{ad} finally follows from the real part of Eq. (13) and the condition $h(0) = -1$ [see Eq. (11)], while b_{ad} can be extracted from the imaginary part of Eq. (13). The integral Eq. (13) shows, in particular, that $a_{ad}/a_\perp$ depends only on Ω_B, and hence only on the binding energy of the dimer.

In the *dimer limit*, $a_\perp/a \gg 1$ and $\Omega_B \gg 1$ [see Eq. (2)], power counting shows that the first term in Eq. (13) is negligible. Using $\zeta(1/2, \Omega \gg 1) \approx -2\sqrt{\Omega}$ and $G(0, 0) = 4/3$ yields from $h(0) = -1$ the result

$$a_{ad} = -\kappa_\infty\sqrt{\Omega_B}a_\perp + \beta a_\perp/\sqrt{\Omega_B} = -\kappa_\infty a_\perp^2/2a + 2\beta a, \quad (14)$$

where $\kappa_\infty = 9/32 = 0.28\,125$. We also specify the subleading order in Eq. (14), where $\beta \approx 0.543$. A similar calculation gives $b_{ad}/a_\perp = (8/9)\Omega_B^{-3/2}$ for $\Omega_B \gg 1$, validating a repulsive zero-range 1D atom-dimer potential in the low-energy limit, $V_{ad}(z) = g_{ad}\delta(z)$ with $g_{ad} > 0$. Because of the presence of higher channels, a_{ad} is renormalized in the dimer limit. This correction can be derived analytically [17] by making explicit contact to the integral equation in the unconfined case [13,15]. We find $\kappa_\infty \approx 0.636$, which gives $a_{ad} = -(a_\perp^r)^2/2(1.2a)$ with the confinement scale $a_\perp^r = (3\hbar/2m_0\omega_\perp)^{1/2}$ for the atom-dimer reduced mass $2m_0/3$. With the 3D atom-dimer scattering length $1.2a$ [13], this result exactly matches the dimer limit of the analogous two-body result (3). Since closed channels do not cause profound changes even in the dimer limit, they are neglected in what follows.

Outside the dimer limit, in general a numerical solution of Eq. (13) is necessary. To ensure regularity of $h(u)$, it is beneficial to Fourier transform back to real space, where the Fourier transformed $h(z)$ is well behaved and allows for a quickly converging solution of the integral equation. The numerical result for $a_{ad}/a_\perp$ as a function of Ω_B is shown in Fig. 1. In the *BCS limit*, where $a_\perp/a \ll -1$ and $\Omega_B \ll 1$, we find

$$a_{ad} = \kappa_0 a_\perp/\sqrt{\Omega_B} = \kappa_0 a_\perp^2/|a|, \quad \kappa_0 \approx 0.75. \quad (15)$$

The solution in Fig. 1 for arbitrary Ω_B nicely matches onto the limits (14) and (15) . Remarkably, around $\Omega_B \approx 2.2$, there is a zero of a_{ad}. At first sight, this behavior seems to be linked to the two-body CIR; see Eq. (3). However, the atom-dimer "resonance" occurs at a different Ω_B, and, more importantly, the assumption of a δ-potential interaction breaks down. This can be seen by computing the range parameter b_{ad} in Eq. (11) [see Fig. 2]. While in the dimer limit, b_{ad} stays small, in accordance with our analytical result, in the BCS limit, it is found to

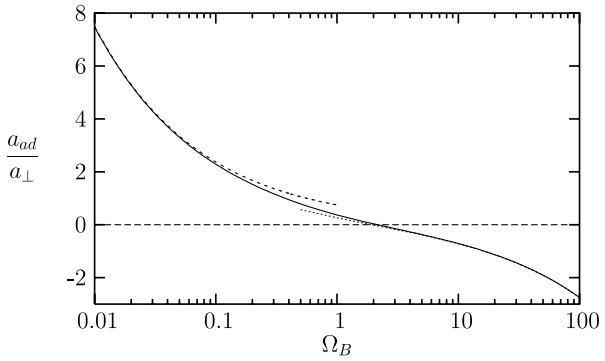

FIG. 1. Scattering length $a_{ad}/a_\perp$ versus dimensionless binding energy Ω_B. The solid curve is the numerical solution to Eq. (13), and the dotted (dashed) curves represent the analytical results in the dimer (BCS) limit, respectively; see Eqs. (14) and (15).

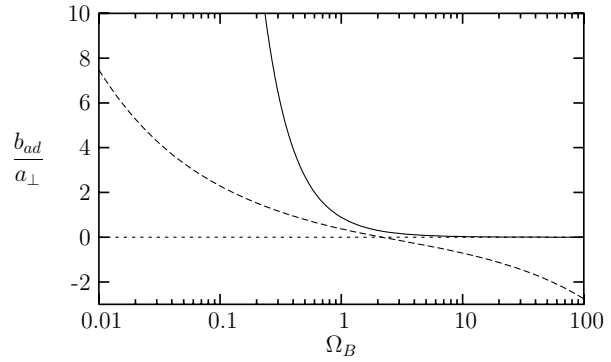

FIG. 2. Range parameter $b_{ad}/a_\perp$ versus Ω_B. The solid curve gives b_{ad} from the numerical solution of Eq. (13), and the dashed line represents a_{ad} from Fig. 1 for comparison.

diverge as $b_{ad} \propto \Omega_B^{-3/2}$. This implies that one cannot use a δ potential to describe atom-dimer scattering outside the dimer limit, but instead more complicated potentials have to be used, e.g., a repulsive square-well potential. Furthermore, the potential becomes nonlocal [19]. An effective 1D potential for low-energy atom-dimer scattering can be constructed directly from Eq. (8). In fact, transforming Eq. (8) back to real space, one gets a Schrödinger equation

$$\left(-\frac{d^2}{dz^2} - \bar{k}^2\right) f(z) = -\int dz' V_{ad}(z, z') f(z') \qquad (16)$$

with the *nonlocal* effective potential

$$V_{ad}(z, z') = -\int \frac{dk}{2\pi} \frac{dk'}{2\pi} e^{ikz - ik'z'} \frac{k^2 - \bar{k}^2}{\mathcal{L}(\Omega_k)} A_{k,k'}, \qquad (17)$$

where $A_{k,k'}$ is given by Eq. (9). It can be easily checked that this potential becomes very wide in the BCS limit, with support given by the dimer size, but it always stays repulsive. Hence there is *no three-body bound state* (trimer) even in the confined problem for arbitrary $a_\perp/a$.

Finally, we have also analyzed the problem of three-body recombination and dissociation, $\uparrow + \uparrow + \downarrow \leftrightarrow \uparrow\downarrow + \uparrow$, see Ref. [13] for the unconfined case, where a nonzero incoming state Ψ_0 has to be taken into account in Eq. (6). Antisymmetry of $\Psi_0(\mathbf{x}, \mathbf{y})$ under $\mathbf{y} \to -\mathbf{y}$ requires that the lowest transverse state (for $\mathbf{y}$) has angular momentum $m = \pm 1$, implying that dissociation processes encounter an energy barrier $\hbar\omega_\perp(1 + \Omega_B)$ not present in the unconfined problem. The three-body recombination problem is therefore simpler, and dimers are rather stable against three-body dissociation.

To conclude, we have solved the three-body problem of a binary cold Fermi gas. The scattering length a_{ad} describing atom-dimer scattering has been extracted for arbitrary confinement and 3D scattering length, and is a universal function of $a_\perp/a$. For $\Omega_B \approx 2.2$, corresponding to $a_\perp/a \approx 2.6$, we find $a_{ad} = 0$. However, this does not imply resonantly enhanced atom-dimer interactions. While in the dimer limit, $a_\perp/a \gg 1$, a standard repulsive zero-range potential is found, in the BCS limit, $a_\perp/a \ll -1$, the situation turns out to be more complicated. The scattering length is positive, $a_{ad} > 0$, but at the same time the range of the effective interaction becomes very large, $b_{ad} \gg a_{ad}$. Therefore it is not possible to employ zero-range potentials in that limit anymore. Nevertheless, it is worth pointing out that also the confined three-body problem is *universal* in the sense that it can be completely expressed in terms of two-body quantities. This is encouraging news for many-body calculations which rely on model parameters extracted only from two-body physics [11,12]. Finally, we mention that the scattering length a_{ad} (and possibly the length b_{ad}) can be extracted experimentally using standard techniques, and thus the scenario put forward above could be checked in detail. Future work should also address the role of Pauli blocking due to the background Fermi sea. For the unconfined case, this was studied by Combescot [20].

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