Weakly bound dimers of fermionic atoms

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We discuss the behavior of weakly bound bosonic dimers formed in a cold Fermi gas at a large positive scattering length a for the interspecies interaction. We find the exact solution for the dimer-dimer elastic scattering and obtain a strong decrease of their collisional relaxation and decay with increasing a. The large ratio of the elastic to inelastic rate is promising for achieving Bose-Einstein condensation of the dimers and cooling the condensed gas to very low temperatures.

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The last years were marked by remarkable achievements in the physics of cold Fermi gases. Several groups succeeded in cooling trapped fermionic atoms to well below the temperature of quantum degeneracy (Fermi temperature T_F) [1–7], and the ratio $T/T_F = 0.05$ has been reached in the recent MIT experiment [8]. One of the main goals of these studies is achieving a transition to a superfluid Cooper-paired state. Trapped Fermi gases are very cold and dilute, with temperatures $T \lesssim 1$ μK and densities $n \sim 10^{13}$ cm^{-3}, and for an attractive interspecies interaction (negative s-wave scattering length a) the most efficient will be the superfluid s-wave pairing between atoms of different components. However, the superfluid transition temperature T_c is exponentially small compared to the Fermi temperature T_F and is beyond experimental reach for ordinary small values of a.

At present, actively discussed ideas to circumvent this difficulty rely on superfluid pairing between fermionic atoms via a Feshbach resonance [9–11]. In the vicinity of the resonance the scattering length is very large, being negative on one side of the resonance and positive on the other side. On approach to the resonance, the gas enters a strong-coupling regime. This occurs when the parameter $k_F|a| > 1$, with $k_F = \sqrt{2mT_F}/\hbar$ being the Fermi momentum and m the atom mass. Crossing the resonance and making the scattering length positive, the formation of weakly bound dimers of two different fermions becomes energetically favorable. Sufficiently far from resonance on the positive side, one has a weakly interacting gas of these composite bosons and encounters the problem of their Bose-Einstein condensation (BEC). This cross-over to the BEC regime has been discussed in literature in the context of superconductivity [12–14].

The BEC regime of the bosonic dimers is interesting from a fundamental point of view as it couples the problem of superfluidity in Fermi gases to the problem of molecular condensates. Here the most important questions are the stability of the condensate with regard to elastic dimer-dimer interactions, and the decay of the gas due to relaxation of the dimers to deep bound states. The relaxation occurs in dimer-dimer collisions and in collisions of dimers with remaining unbound atoms. It is a crucial process as these dimers are diatomic molecules in the highest rovibrational state. Several experiments show that such molecules consisting of bosonic ^{87}Rb [15,16] and ^{133}Cs atoms [17], or fermionic ^{40}K atoms with a scattering length $a \sim 100$Å [18], undergo a rapid collisional decay. On the other hand, recent observations [19–21] indicate the existence of long-lived weakly bound Li_2 dimers at densities $\sim 10^{13}$ cm^{-3}.

In this Letter we present an exact solution for the dimer-dimer elastic scattering, assuming that the (positive) scattering length greatly exceeds the characteristic radius of interaction between atoms, R_e. Then, as in the case of the 3-body problem with fermions (see [22,23] and references in [23]), the amplitude of elastic interaction is determined by a single parameter, the two-body scattering length a, and can be found in the zero-range approximation for the interatomic potential. Our findings lead to a positive dimer-dimer scattering length $a_{dd} = 0.6a$ [24]. This is quite different from the assumption of earlier studies, $a_{dd} = 2a$ [14], and has serious consequences for the low-temperature behavior of the system.

We then discuss the collisional relaxation of the weakly bound dimers to deep bound states and show that it is *suppressed* due to *Fermi statistics* for the atoms. The binding energy of the dimers is $\varepsilon_0 = \hbar^2/ma^2$ and their size is close to a. The size of deep bound states is of the order of $R_e \ll a$. Hence, the relaxation requires the presence of at least three fermions at distances $\sim R_e$ from each other. As two of them are necessarily identical, due to the Pauli exclusion principle the relaxation probability acquires a small factor proportional to a power of (kR_e), where $k \sim 1/a$ is a characteristic momentum of the atoms in the weakly bound molecular state. The inequality $a \gg R_e$ allows us to obtain the dependence of the atom-dimer and dimer-dimer wavefunctions at short interparticle distances on the two-body scattering length a and thus to establish a strong decrease of the relaxation rate with increasing a. Our results show that the

rate constant is proportional to a^{-s}, where s is close to 3. This indicates a remarkable collisional stability of the weakly bound bosonic dimers at a large positive a, which is consistent with recent observations at ENS [19], Innsbruck [20], and Rice [21]. Note that the elastic collisional rate is proportional to a^2, and for large a we obtain a very large ratio of this rate to the inelastic rate of relaxation.

The key idea behind these studies is twofold. First, a large ratio of the elastic to inelastic rate is promising for evaporative cooling of the dimers, achieving their BEC, and further cooling of the Bose-condensed gas to very low temperatures. Molecular BEC is a great challenge and many ongoing studies are directed to reaching this goal. Second, adiabatically crossing the Feshbach resonance and reaching a negative value of the scattering length a, the molecules are converted into fermionic atoms at extremely low temperatures $T \sim 0.01T_F$ which can be below the BCS transition temperature T_c [25]. Remarkably, at these temperatures the strong Pauli blocking of elastic collisions provides the collisionless regime for the atomic Fermi gas even for a large negative a. This opens up the possibility of identifying the BCS-paired state via the asymmetric expansion of the cloud released from a cylindrical trap [26].

We start with the dimer-dimer elastic scattering which is a 4-body problem described by the Schrödinger equation

$$-\left[\nabla^2_{\mathbf{r}_1}+\nabla^2_{\mathbf{r}_2}+\nabla^2_{\mathbf{R}}+mE/\hbar^2\right]\Psi=-(m/\hbar^2) \times\Big[U(r_1)+U(r_2)+\sum_{\pm}U\left((\mathbf{r}_1+\mathbf{r}_2\pm\sqrt{2}\,\mathbf{R})/2\right)\Big]\Psi. \quad (1)$$

Here $\mathbf{r}_1$ is the distance between two given distinguishable fermions, $\mathbf{r}_2$ is the distance between the other two, $\mathbf{R}/\sqrt{2}$ is the distance between the centers of mass of these pairs, and U is the interatomic potential. The total energy is $E=-2\varepsilon_0+\varepsilon$, with ε being the collision energy.

The wavefunction Ψ is symmetric with respect to the permutation of the dimers and antisymmetric with respect to permutations of identical fermions:

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{R})=\Psi(\mathbf{r}_2,\mathbf{r}_1,-\mathbf{R}) \quad (2)$$
$$=-\Psi\left(\frac{\mathbf{r_1}+\mathbf{r_2}\pm\sqrt{2}\mathbf{R}}{2},\frac{\mathbf{r_1}+\mathbf{r_2}\mp\sqrt{2}\mathbf{R}}{2},\frac{\pm(\mathbf{r_1}-\mathbf{r_2})}{\sqrt{2}}\right).$$

At energies $\varepsilon \ll \varepsilon_0$ the scattering is dominated by the contribution of the s-wave channel and can be analyzed from the solution of Eq. (1) with $E=-2\varepsilon_0$. For large R the corresponding wavefunction is given by

$$\Psi \approx \varphi_0(r_1)\varphi_0(r_2)(1-\sqrt{2}a_{dd}/R), \quad (3)$$

where a_{dd} is the dimer-dimer scattering length, and

$$\varphi_0(r)=(r\sqrt{2\pi a})^{-1}\exp(-r/a) \quad (4)$$

is the wavefunction of a weakly bound dimer.

The characteristic de Broglie wavelength of atoms is of the order of a and it greatly exceeds the radius R_e of the interatomic potential U. Hence, for finding the scattering amplitude one can use the well known method of pseudopotentials, that is, to replace the potential U by a pseudopotential providing proper boundary conditions for Ψ at vanishing distances between two distinguishable fermions. For $\mathbf{r_1}\to 0$ the boundary condition reads:

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{R})\to f(\mathbf{r}_2,\mathbf{R})(1/4\pi r_1-1/4\pi a), \quad (5)$$

where the function $f(\mathbf{r}_2,\mathbf{R})$ carries the information about the second pair of particles when the first two sit on top of each other. The boundary conditions for $\mathbf{r}_2\to 0$, and for $\mathbf{r}_1+\mathbf{r}_2\pm\sqrt{2}\mathbf{R}\to 0$ are readily written using Eqs. (2). The knowledge of the function f is sufficient for describing all of the four boundaries. Combining Eqs. (3) and (5) one can deduce the value of a_{dd} from the behavior of f at large R. It is important that in contrast to Ψ, the function f depends only on three variables: the absolute values of $\mathbf{r}_2$ and $\mathbf{R}$, and the angle between them. In the following, we derive and solve the equation for f.

In the pseudopotential approach the interaction potential can be written as $U(r)=(4\pi\hbar^2a/m)\delta(\mathbf{r})(\partial/\partial r)r$. Then, making use of Eq.(5) we express the rhs of Eq.(1) in terms of the function f. The first term reads $-mU(r_1)\Psi/\hbar^2=\delta(\mathbf{r_1})f(\mathbf{r}_2,\mathbf{R})$, and similarly for the other terms. The resulting inhomogeneous Poisson equation can be solved by inverting the differential operator. The Green function of this operator is unique ($E=-2\varepsilon_0<0$), and Ψ is expressed through f as:

$$\Psi(S)=\int_{\mathbf{r}',\mathbf{R}'}\Big[\sum_{i=1,2}G(|S-S_i|)-\sum_{\pm}G(|S-S_\pm|)\Big]f(\mathbf{r}',\mathbf{R}'), \quad (6)$$

where $S=\{\mathbf{r}_1,\mathbf{r}_2,\mathbf{R}\}$, $S_1=\{0,\mathbf{r}',\mathbf{R}'\}$, $S_2=\{\mathbf{r}',0,-\mathbf{R}'\}$, $S_\pm=\{\mathbf{r}'/2\pm\mathbf{R}'/\sqrt{2},\mathbf{r}'/2\mp\mathbf{R}'/\sqrt{2},\mp\mathbf{r}'/\sqrt{2}\}$, and the Green function is $G(x)=(2\pi)^{-9/2}(xa/\sqrt{2})^{-7/2}K_{7/2}(\sqrt{2}\,x/a)$, with $K_{7/2}$ being the decaying Bessel function.

The equation for the function f is obtained from Eq. (6) by taking the limit $r_1\to 0$ and using Eq. (5). The singular terms proportional to $1/r_1$ cancel each other automatically, and matching the regular parts yields

$$\int_{\mathbf{r}',\mathbf{R}'}\Big\{G(|\bar{S}_1-S_1|)[f(\mathbf{r}',\mathbf{R}')-f(\mathbf{r},\mathbf{R})]+\big[G(|\bar{S}_1-S_2|) -\sum_{\pm}G(|\bar{S}_1-S_\pm|)\big]f(\mathbf{r}',\mathbf{R}')\Big\}=(\sqrt{2}-1)f(\mathbf{r},\mathbf{R})/4\pi a, \quad (7)$$

where $\bar{S}_1=\{0,\mathbf{r},\mathbf{R}\}$. Note that the only length scale in Eq. (7) is a. Solving this equation numerically we obtain the function f for all distances $\mathbf{R}$ and $\mathbf{r}$. According to Eqs. (3), (4) and (5), at $R\to\infty$ one has $f=(2/ra)\exp(-r/a)(1-\sqrt{2}a_{dd}/R)$. Fitting our results with this expression we find with 2% accuracy:

$$a_{dd} = 0.6a > 0. \quad (8)$$

Our calculations show the absence of 4-body weakly bound states, and the behavior of f at small R suggests a soft-core repulsion between molecules, with a range $\sim a$. The result of Eq. (8) indicates the stability of molecular BEC with respect to collapse. Compared to earlier studies which were assuming $a_{dd} = 2a$ [14], Eq. (8) gives almost twice as small a sound velocity of the molecular condensate and a rate of elastic collisions smaller by an order of magnitude.

The lifetime of the Bose gas of weakly bound dimers is determined by the process of their collisional relaxation into deep bound states. The released binding energy of a deep state is of the order of $\hbar^2/mR_e^2$. It is transformed into the kinetic energy of particles in the outgoing collisional channel and they escape from the trapped sample. We will establish a dependence of the relaxation loss rate on the scattering length a, without going into a detailed analysis of the short-range behavior of the systems of three and four atoms. We employ a perturbative scheme assuming that the amplitude of the inelastic process of relaxation is much smaller than the amplitude of elastic scattering. Then the dependence of the relaxation rate on the scattering length a is related only to the a-dependence of the initial-state wavefunction Ψ.

We first discuss the relaxation of weakly bound dimers to a deep bound state in their collisions with atoms. This process occurs when all of the three atoms approach each other to distances $\sim R_e$. As at all interparticle distances $r \ll a$ the three-body wavefunction $\tilde{\Psi}$ is determined by the Schrödinger equation with zero collision energy, it depends on a only through a normalization coefficient: $\tilde{\Psi} = A(a)\tilde{\psi}$. In the region where $R_e \ll r \ll a$, the a-independent function $\tilde{\psi}$ can be found in the zero-range approximation. Then the coefficient $A(a)$, which determines the dependence of the relaxation rate on a, is obtained by matching $\tilde{\Psi}$ with the solution at large interparticle distances.

This requires us to find $\tilde{\Psi}$ at distances $\sim a$, which we do using the zero-range approximation described in Ref. [23]. As in the case of four particles, we introduce the corresponding function $\tilde{f}(\mathbf{r})$. The correctly symmetrized wavefunction $\tilde{\Psi}(\mathbf{x}, \mathbf{y})$ is expressed through $\tilde{f}$ as:

$$\tilde{\Psi} = \sum_{\pm} \int_{\mathbf{r}} \pm \tilde{G}\left(\sqrt{(\mathbf{x} - \mathbf{r}/2)^2 + (\mathbf{y} \mp \sqrt{3}\mathbf{r}/2)^2}\right) \tilde{f}(\mathbf{r}), \quad (9)$$

where $\mathbf{y}$ is the distance between identical fermions, $\sqrt{3}\mathbf{x}/2$ is the distance between their center of mass and the third atom, and the Green function $\tilde{G}(z) = (8\pi^2 z^2 a^2)^{-1} K_2(z/a)$. At a vanishing distance between two given distinguishable fermions $\mathbf{r}_\pm = (\sqrt{3}\mathbf{x} \pm \mathbf{y})/2 \to 0$, the function $\tilde{\Psi}$ (9) should have a correct asymptotic behavior in analogy with Eq. (5). This gives an equation for the function $\tilde{f}(\mathbf{r})$:

$$\int_{\mathbf{r}'} \tilde{G}(|\mathbf{r} - \mathbf{r}'|)[\tilde{f}(\mathbf{r}') - \tilde{f}(\mathbf{r})] - \tilde{G}\left(\sqrt{\mathbf{r}^2 + \mathbf{r}'^2 + \mathbf{r}\mathbf{r}'}\right)\tilde{f}(\mathbf{r}') = 0. \quad (10)$$

For small separations between all three fermions, Eqs. (10) and (9) give the same result as the method of hyperspherical harmonics [28]: $\tilde{\Psi} \approx A(a)\rho^\gamma \Phi_\gamma(\Omega)$, where Ω is a set of hyperangles and the hyperradius $\rho = \sqrt{x^2 + y^2}$ satisfies the inequality $\rho \ll a$. The parameter γ depends on the symmetry of the wavefunction and on the orbital angular momentum of the atom-dimer motion. For the s-wave atom-dimer scattering we have $\tilde{f}(\mathbf{r}) = \tilde{f}(|\mathbf{r}|)$ and obtain $\gamma = \gamma_1 \approx 0.1662$. At large atom-dimer distances y we have $\Psi \approx \pm\varphi_0(r_\pm)(1 - a_{ad}/y)$, where φ_0 is given by Eq. (4), and $a_{ad} = 1.2a$ is the atom-dimer scattering length [27,23]. Solving Eqs. (10) and (9) at distances of the order of a and thus matching the two asymptotic solutions, we find $A(a) = const \times a^{-3/2-\gamma_1}$. This result is explained extending the wavefunction Ψ to interparticle distances $\sim a$ from the region of small distances. This gives $\Psi \sim A(a)a^{\gamma_1}$, whereas being extended to distances $\sim a$ from large separations, the wavefunction is $\Psi \sim 1/a^{3/2}$. Equalizing the two expressions leads to the obtained coefficient $A(a)$. The numerical constant is not needed as the absolute value of the relaxation rate is determined by the contribution of interparticle distances $\sim R_e$, where the zero-range approximation is not valid. It only gives a correct dependence of the rate on a.

As the relaxation rate constant $\alpha_{\rm rel} \propto A^2(a)$, we obtain $\alpha_{\rm rel} \propto a^{-3-2\gamma_1} = a^{-3.33}$. One thus sees that the relaxation rate due to dimer-atom collisions rapidly decreases with increasing two-body scattering length a.

The obtained results can be easily generalized to the case of the s-wave dimer-dimer scattering. Indeed, the relaxation process requires only three atoms to approach each other to short distances. The fourth particle does not participate. Let ρ and Ω be the hyperradius and the set of hyperangles of the system of three fermions and $\mathbf{x}$ the distance between their center of mass and the fourth atom. At $\rho \sim R_e$ and $|\mathbf{x}| \gg R_e$ the four-particle wavefunction decomposes into $\rho^{\gamma_2}\Phi_{\gamma_2}(\Omega)\eta(\mathbf{x})$, where the function $\eta(\mathbf{x})$ describes the motion of the fourth particle. Averaging the relaxation probability over the motion of the fourth particle makes the problem similar to the relaxation in atom-dimer collisions, and we arrive at the same result for the rate constant. However, there is a relaxation channel that is more important in the limit of very large a. For the s-wave dimer-dimer scattering, both the fourth particle and the atom bound to this particle can undergo p-wave scattering on the other dimer in such a way that their total angular momentum is equal to zero. This corresponds to an antisymmetric function $\tilde{f}(\mathbf{r})$ in Eqs. (9) and (10) and leads to $\gamma_2 = -0.2273$. For the relaxation rate we then find $\alpha_{\rm rel} \propto a^{-3-2\gamma_2} = a^{-2.55}$.

Assuming that the short-range physics is characterized by the length scale R_e and the energy scale $\hbar^2/mR_e^2$, we can restore the dimensions and write: $\alpha_{\rm rel} =$

$C(\hbar R_e/m)(R_e/a)^s$, where $s \approx 2.55$ for the dimer-dimer collisional relaxation, and $s \approx 3.33$ for the relaxation in atom-dimer collisions. The coefficient C depends on a particular system and is different for dimer-dimer and atom-dimer collisions. Obviously, in the limit $R_e/a \to 0$ the dimer-dimer relaxation should dominate over the atom-dimer one.

The much slower collisional decay of the weakly bound dimers at larger a, following from our results, is consistent with recent observations for Li_2 molecules [19–21], although the experimental data do not yet provide the dependence of $\alpha_{\rm rel}$ on a. Nevertheless, the ENS result $\alpha_{\rm rel} \approx 2 \times 10^{-13}$ cm^3/s for the Li_2 loss rate at $a \approx 1500 a_0$ [19], allows us to establish the coefficient $C \approx 20$.

We emphasize that the remarkable stability of such weakly bound dimers at $a \gg R_e$ is due to *Fermi statistics*. Indeed, two identical fermions participating in the relaxation process have very small relative momenta $k \sim 1/a$ and, hence, the process is suppressed compared to the case of a dimerized gas of bosonic atoms.

The inelastic rate constant $\alpha_{\rm rel}$ is much smaller than the rate constant of elastic collisions $8\pi a_{dd}^2 v_T$, where v_T is the thermal velocity. For the Li_2 weakly bound dimers at a temperature $T \sim 3\mu$K and $a \sim 1500 a_0$, the corresponding ratio is of the order of 10^{-4} or 10^{-5}. This is nearly the same as in a cold gas of Rb atoms at densities $n \sim 10^{14}$ cm^{-3}. For Li_2 the values of both rate constants are larger, and one can expect even a higher efficiency of evaporative cooling. It should be possible to reach BEC of the dimers and cool the Bose-condensed gas to temperatures of the order of its chemical potential.

Then, converting the molecular BEC into fermionic atoms by adiabatically sweeping across the Feshbach resonance to the negative side [29], one obtains the atomic Fermi gas at extremely low temperatures $T \sim 10^{-2} T_F$ which can be below the BCS transition temperature T_c [25]. At these temperatures one has a very strong Pauli blocking of elastic collisions. The collisional rate is suppressed as $15(T/T_F)^2$ [5], i.e. by a factor of 10^3, and one expects the collisionless regime for the Fermi gas. This circumvents the main difficulty for identifying the BCS-paired state via a free expansion of the cloud released from the trap. This difficulty was met in experiments with hydrodynamic Fermi clouds [5] which in cylindrical traps are characterized by the same asymmetry of expansion below and above T_c. Omitting small mean-field effects, the collisionless cloud above T_c expands symmetrically, whereas in the superfluid state the expansion becomes significantly asymmetric [26].

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