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Publication date
2004

Published in
Physical Review Letters

[Link to publication](#)

Citation for published version (APA):

Petrov, D. S., Salomon, C., & Shlyapnikov, G. V. (2004). Weakly Bound Dimers of Fermionic Atoms. *Physical Review Letters*, 93, 090404.

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Weakly Bound Dimers of Fermionic Atoms

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(Received 1 September 2003; published 24 August 2004)

We discuss the behavior of weakly bound bosonic dimers formed in a two-component 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.

DOI: 10.1103/PhysRevLett.93.090404

PACS numbers: 03.75.Ss, 05.30.Fk

The last few 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) [1–8]. 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 $T \lesssim 1 \mu\text{K}$ and densities $n \sim 10^{13} \text{ cm}^{-3}$, 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 of two different components 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 for $k_F|a| > 1$, 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 crossover to the BEC regime has been discussed in literature in the context of superconductivity [12–14].

For the BEC regime of the bosonic dimers, 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 collisional relaxation of the dimers to deep bound states. The relaxation 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 $a \sim 100 \text{ \AA}$ [18], undergo a rapid collisional decay. On the other hand, recent observations [19–22] indicate the existence of long-lived weakly bound Li_2 and K_2 dimers at densities $\sim 10^{13} \text{ cm}^{-3}$.

In this Letter we present an exact solution for the dimer-dimer elastic scattering, assuming that the (positive) atom-atom scattering length a for the interspecies interaction greatly exceeds the characteristic radius of interatomic potential R_e . Then, as in the case of the 3-body problem with fermions (see [23,24] and references in [24]), the amplitude of elastic interaction is determined only by a and can be found in the zero-range approximation for the interatomic potential. Our findings lead to a positive dimer-dimer scattering length $a_{\text{dd}} = 0.6a$ [25]. This is quite different from the assumption of earlier studies, $a_{\text{dd}} = 2a$ [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 wave functions 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 indicate a remarkable collisional stability of the weakly bound bosonic dimers, which is consistent with recent experiments.

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

$$-[\nabla_{\mathbf{r}_1}^2 + \nabla_{\mathbf{r}_2}^2 + \nabla_{\mathbf{R}}^2 + mE/\hbar^2]\Psi = -(m/\hbar^2) \times [U(r_1) + U(r_2) + U(\mathbf{r}_+) + U(\mathbf{r}_-)]\Psi. \quad (1)$$

The internal states of atoms are labeled by the symbols \uparrow and \downarrow . In Eq. (1), \mathbf{r}_1 is the distance between two given \uparrow and \downarrow fermions, and \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, $\mathbf{r}_{\pm} = (\mathbf{r}_1 + \mathbf{r}_2 \pm \sqrt{2}\mathbf{R})/2$, and U is the interatomic potential [26]. The total energy is $E = -2\varepsilon_0 + \varepsilon$, with ε being the collision energy.

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

$$\begin{aligned} \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{R}) &= \Psi(\mathbf{r}_2, \mathbf{r}_1, -\mathbf{R}) \\ &= -\Psi[\mathbf{r}_{\pm}, \mathbf{r}_{\mp}, \pm(\mathbf{r}_1 - \mathbf{r}_2)/\sqrt{2}]. \end{aligned} \quad (2)$$

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 wave function is given by

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

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 wave function of a weakly bound dimer.

The characteristic de Broglie wavelength of atoms is $\sim a$, and it greatly exceeds the radius R_e of the potential U . Hence, for finding the scattering amplitude one can replace U by a pseudopotential providing proper boundary conditions for Ψ at vanishing distances between \uparrow and \downarrow fermions. For $\mathbf{r}_1 \rightarrow 0$ the boundary condition reads:

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

and it is readily written for $\mathbf{r}_2 \rightarrow 0$ and $\mathbf{r}_{\pm} \rightarrow 0$ by using Eqs. (2). The function f carries the information about the second pair of particles when the first two sit on top of each other. The knowledge of this function is sufficient for describing all of the four boundaries. In the following, we derive and solve the equation for f . The value of a_{dd} is then deduced from the behavior of f at large R , where from Eqs. (3), (4), and (5) we obtain:

$$f = (2/ra) \exp(-r/a)(1 - \sqrt{2}a_{\text{dd}}/R), \quad R \gg a. \quad (6)$$

In the pseudopotential approach the interaction potential can be written as $U(r) = (4\pi\hbar^2 a/m)\delta(\mathbf{r})(\partial/\partial r)r$. Then, making use of Eq. (5) we express the right hand side of Eq. (1) in terms of the function f and, putting $E = -2\varepsilon_0$, transform Eq. (1) into an inhomogeneous Poisson equation

$$\hat{P}\Psi \equiv -[\nabla_{\mathbf{r}_1}^2 + \nabla_{\mathbf{r}_2}^2 + \nabla_{\mathbf{R}}^2 - 2/a^2]\Psi = \delta(\mathbf{r}_1)f(\mathbf{r}_2, \mathbf{R}) + \delta(\mathbf{r}_2)f(\mathbf{r}_1, -\mathbf{R}) - \sum_{\pm} \delta(\mathbf{r}_{\pm})f[\mathbf{r}_{\mp}, \pm(\mathbf{r}_1 - \mathbf{r}_2)/\sqrt{2}].$$

The Green function of the operator \hat{P} is unique ($E < 0$) and, as the free-motion equation $\hat{P}\Psi = 0$ has no nontrivial solutions that are regular at vanishing distances between \uparrow and \downarrow fermions, Ψ is expressed through f as:

$$\Psi(S) = \int_{\mathbf{r}', \mathbf{R}'} \left[\sum_{i=1,2} G(|S - S_i|) - \sum_{\pm} G(|S - S_{\pm}|) \right] f(\mathbf{r}', \mathbf{R}'), \quad (7)$$

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. For $R \gg a$, due to exponential decay of the Green function, the distance R' in Eq. (7) is also much larger than a . Then, using Eq. (6) for $f(\mathbf{r}', \mathbf{R}')$, one obtains Ψ in the form (3) which is a required superposition of the incident and scattered waves.

The equation for the function f is obtained from Eq. (7) by taking the limit $r_1 \rightarrow 0$ and using Eq. (5). The singular terms proportional to $1/r_1$ cancel each other automatically, and matching the regular parts yields

$$\int_{\mathbf{r}', \mathbf{R}'} \{G(|\bar{S}_1 - S_1|)[f(\mathbf{r}', \mathbf{R}') - f(\mathbf{r}, \mathbf{R})] + [G(|\bar{S}_1 - S_2|) - \sum_{\pm} G(|\bar{S}_1 - S_{\pm}|)]f(\mathbf{r}', \mathbf{R}')\} = (\sqrt{2} - 1)f(\mathbf{r}, \mathbf{R})/4\pi a, \quad (8)$$

where $\bar{S}_1 = \{0, \mathbf{r}, \mathbf{R}\}$. 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. At $R \gg a$, fitting Eq. (6) with $f(\mathbf{r}, \mathbf{R})$ obtained numerically from Eq. (8) for all distances \mathbf{R} and \mathbf{r} , we find with 2% accuracy:

$$a_{\text{dd}} = 0.6a > 0. \quad (9)$$

Our calculations show the absence of 4-body weakly bound states, and the behavior of f suggests a soft-core repulsion between molecules, with a range $\sim a$. The result of Eq. (9) indicates the stability of molecular BEC with respect to collapse. Compared to earlier studies which were assuming $a_{\text{dd}} = 2a$ [14], Eq. (9) gives 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 their collisional relaxation into deep bound states. The released binding energy of a deep state is $\sim \hbar^2/mR_e^2$. It is transformed into the kinetic energy of particles in the outgoing collisional channel and they escape from the sample. We 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. It is assumed that the inelastic amplitude of relaxation is much smaller than the amplitude of elastic scattering. Then the dependence

of the relaxation rate on a is related only to the a -dependence of the initial-state wave function 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 $r \sim R_e$. As at distances $r \ll a$ the 3-body wave function $\tilde{\Psi}$ is determined by the Schrödinger equation with $\varepsilon_0 = 0$, 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. The goal then is to find the coefficient $A(a)$, which determines the dependence of the relaxation rate on a .

For this purpose, we use the zero-range approximation and introduce the corresponding function $\tilde{f}(\mathbf{r})$ [24]. The wave function $\tilde{\Psi}(\mathbf{x}, \mathbf{y})$ is expressed through \tilde{f} as:

$$\tilde{\Psi} = \sum_{\pm} \int_{\mathbf{r}} \pm \tilde{G}(\sqrt{(\mathbf{x} - \mathbf{r}/2)^2 + (\mathbf{y} \mp \sqrt{3}\mathbf{r}/2)^2}) \tilde{f}(\mathbf{r}), \quad (10)$$

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

$$\int_{\mathbf{r}'} \tilde{G}(|\mathbf{r} - \mathbf{r}'|) [\tilde{f}(\mathbf{r}') - \tilde{f}(\mathbf{r})] - \tilde{G}(\sqrt{\mathbf{r}^2 + \mathbf{r}\mathbf{r}'}) \tilde{f}(\mathbf{r}') = 0. \quad (11)$$

Since the only distance scale in Eqs. (10) and (11) is a , the coordinate dependence of $\tilde{\Psi}$ is governed by a function $F(\mathbf{x}/a, \mathbf{y}/a)$ which depends on a only through rescaled coordinates \mathbf{x}/a and \mathbf{y}/a . We thus have $\tilde{\Psi} = B(a)F$. For the hyperradius $\rho = \sqrt{x^2 + y^2} \ll a$, Eqs. (11) and (10) give the same result as the method of hyperspherical harmonics [27]: $\tilde{\Psi} \approx B(a)(\rho/a)^\gamma \Phi_\gamma(\Omega)$, where Ω is a set of hyperangles. So, the coefficient $A(a) = B(a)a^{-\gamma}$. The parameter γ depends on the symmetry of the wave function 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 y we have $\Psi \approx \pm \varphi_0(\tilde{\mathbf{r}}_{\pm})(1 - a_{\text{ad}}/y)$, where φ_0 is given by Eq. (4), and $a_{\text{ad}} = 1.2a$ is the atom-dimer scattering length [24,28]. Using Eq. (4) we find $B \propto a^{-3/2}$ and, hence, $A(a) = \text{const} \times a^{-3/2-\gamma_1}$, where the numerical constant depends on short-range physics.

As the relaxation rate constant is $\alpha_{\text{rel}} \propto A^2(a)$, we obtain $\alpha_{\text{rel}} \propto a^{-3-2\gamma_1} = a^{-3.33}$, rapidly decreasing with an increase in the 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. Let ρ and Ω be the hyper-

radius and hyperangles of the three fermions and \mathbf{x} the distance between their center of mass and the fourth atom. At $\rho \ll |\mathbf{x}| \sim a$ the four-particle wave function 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. 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. (10) and (11) and leads to $\gamma_2 = -0.2273$. For the relaxation rate we then find $\alpha_{\text{rel}} \propto a^{-3-2\gamma_2} = a^{-2.55}$.

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: $\alpha_{\text{rel}} = C(\hbar R_e/m)(R_e/a)^s$, where $s \approx 2.55$ for the dimer-dimer relaxation, and $s \approx 3.33$ for the relaxation in atom-dimer collisions. For $R_e/a \rightarrow 0$ the dimer-dimer relaxation should dominate over the atom-dimer one. However, the coefficient C depends on a particular system and is different for dimer-dimer and atom-dimer collisions.

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 [19,20] and K_2 [22]. The results of Regal *et al.* [22] give $\alpha_{\text{rel}} \propto 1/a^s$ with $s \approx 2.3$, which is close to our value for the dimer-dimer relaxation.

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 relaxation loss rate is usually much smaller than the rate of elastic collisions. For the Li_2 dimers at $T \sim 3 \mu\text{K}$ and $a_0 a \sim 1500a_0$, their ratio is $\sim 10^{-4}$. This opens wide possibilities for reaching BEC of the dimers and cooling 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 [30]. At these temperatures one has a very strong Pauli blocking of elastic collisions. The collisional rate is suppressed as $(T/T_F)^2$ [5], i.e., by a factor of 10^4 , and one expects the collisionless regime for the Fermi gas above T_c . This is promising for identifying the BCS-paired state in trapped gases through the observation of collective oscillations and/or asymmetric free expansion [31].

We acknowledge discussions with M. A. Baranov, C. Lobo, and L. D. Carr. This work was supported by the

Dutch Foundations NWO and FOM, by INTAS, and by the Russian Foundation for Fundamental Research.

Note added.—Since submission of this paper, long-lived Bose-Einstein condensation of weakly bound dimers has been observed for $^{40}\text{K}_2$ [32] and for $^6\text{Li}_2$ [33–35].

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