

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

D. S. Petrov

*FOM Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands
and Russian Research Center, Kurchatov Institute, Kurchatov Square, 123182 Moscow, Russia*

(Received 17 September 2002; published 29 January 2003)

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

DOI: 10.1103/PhysRevA.67.010703

PACS number(s): 34.50.-s, 05.30.Fk

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

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

at distances of the order of R_e then significantly influences the large-scale behavior and short-range parameters of the interaction potential are required to describe the three-body system.

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

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

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

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

We assume that the potential V supports a weakly bound s state with the binding-energy ε and with the size determined by the scattering length $a > 0$. The latter greatly exceeds the range R_e of the potential V . We also assume the condition $|E| < \varepsilon$ which means that wavelengths of particles are at least as large as a . Then, neglecting corrections of the order of R_e/a we can take the interaction potential into account by imposing the boundary condition on the wave function Ψ for vanishing distance between two unlike particles:

$$\Psi \xrightarrow{r_\perp \rightarrow 0} \frac{f(\mathbf{r})}{4\pi} \left(\frac{1}{r_\perp} - \sqrt{\varepsilon} \right). \quad (2)$$

Here $\mathbf{r}_\perp = \mathbf{x} \sin \theta - \mathbf{y} \cos \theta$ is the rescaled distance from the \downarrow particle to the first of the two \uparrow fermions, $1/\sqrt{\varepsilon}$ is the rescaled scattering length, and the unknown function f depends only on the distance $\mathbf{r} = \mathbf{x} \cos \theta + \mathbf{y} \sin \theta$ to the second \uparrow fermion. Under permutation ($\mathbf{y} \rightarrow -\mathbf{y}$) of the \uparrow fermions the function Ψ should change sign due to the symmetry, and we then require $f \rightarrow -f$.

Let us first construct the wave function Ψ such that it satisfies the Poisson equation $[-\nabla_X^2 - E]\Psi = 0$ and the symmetry conditions. Then, the general form reads

$$\Psi = \Psi_0(X) + \sum_{\pm} \int \pm G_E(|X - X_{\pm}(\mathbf{r})|) f(\mathbf{r}) d^3\mathbf{r}, \quad (3)$$

where $X_{\pm}(\mathbf{r}) = \{\mathbf{r} \cos \theta, \pm \mathbf{r} \sin \theta\}$, and $\Psi_0(\mathbf{x}, \mathbf{y}) = -\Psi_0(\mathbf{x}, -\mathbf{y})$ is a solution of the Poisson equation without singularities. We restrict Ψ_0 to be finite everywhere and, hence, for $E < 0$ we have $\Psi_0 = 0$. The Green's function G_E is a solution of Eq. (1) with the rhs $\delta^6(X) = \delta^3(\mathbf{x})\delta^3(\mathbf{y})$ and is given by

$$G_E(X) = \begin{cases} \frac{-EK_2(\sqrt{-E}|X|)}{8\pi^2 X^2}, & E < 0 \\ \frac{iEH_2(\sqrt{E}|X|)}{16\pi^3 X^2}, & E > 0 \end{cases} \xrightarrow{E \rightarrow 0} \frac{1}{4\pi^3 X^4}.$$

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

The function f is defined by the condition that Eqs. (2) and (3) give the same result at $r_\perp \rightarrow 0$. Direct calculations show that the parts proportional to $1/r_\perp$ coincide automatically for any f , and the comparison of the regular parts gives the integral equation

$$(\hat{L}_E - \sqrt{\varepsilon} + \sqrt{-E})f(\mathbf{r}) = 4\pi\Psi_0(X_+(\mathbf{r})), \quad (4)$$

where the Hermitian operator \hat{L}_E is given by

$$\hat{L}_E f(\mathbf{r}) = 4\pi \int [G_E(|\mathbf{r} - \mathbf{r}'|)[f(\mathbf{r}) - f(\mathbf{r}')] + G_E(\sqrt{\mathbf{r}^2 + \mathbf{r}'^2 - 2\mathbf{r}\mathbf{r}'\cos 2\theta})f(\mathbf{r}')] d^3\mathbf{r}'. \quad (5)$$

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

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

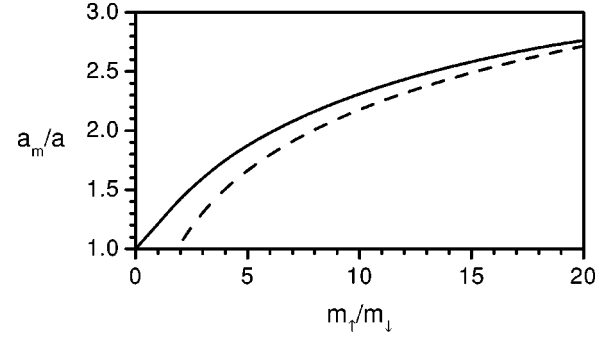


FIG. 1. The ratio a_m/a versus m_\uparrow/m_\downarrow calculated from Eq. (6) (solid line) and from the Born-Oppenheimer approximation (dashed line).

$$\hat{L}_{-\varepsilon}^{l=0} f(r) = 0. \quad (6)$$

Here $\hat{L}_{-\varepsilon}^{l=0}$ is an integral operator which is obtained from $\hat{L}_{-\varepsilon}$ by integrating over angles.

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

It can be shown analytically that $f(r) \sim r^\gamma$ near the origin. The exponent γ increases monotonically from 1 to 3, with m_\uparrow/m_\downarrow growing from 0 to ∞ indicating an effective repulsion in the system [7]. In the case of $m_\uparrow = m_\downarrow$ we obtain $a_m/a \approx 1.2$ (cf. Ref. [9]).

We now turn to the problem of three-body recombination just above the threshold $0 < E \ll \varepsilon$. This process ($\uparrow + \uparrow + \downarrow \rightarrow \uparrow + \uparrow\downarrow$) takes place at interparticle distances comparable with the size of a $\uparrow\downarrow$ -dimer ($\sim 1/\sqrt{\varepsilon}$). At these distances the shapes of the functions Ψ and f are independent of E . The normalization coefficient, however, depends on the large scale behavior and, therefore, on energy E . In terms of plain waves the wave function of free motion is $\Psi_0(\mathbf{x}, \mathbf{y}) = \sin(\mathbf{k} \cdot \mathbf{y}) \exp(i\mathbf{q} \cdot \mathbf{x})$, where the momenta \mathbf{k} and \mathbf{q} satisfy the equation $E = k^2 + q^2$. At distances comparable with $1/\sqrt{\varepsilon}$ the quantity $|\Psi_0|^2$ is equal to $(\mathbf{k} \cdot \mathbf{y})^2 [1 + O(E/\varepsilon)]$, giving rise to the k^2 threshold law for the probability of three-body recombination [6]. Higher-order terms lead to small correc-

tions to the recombination probability. Considering the limit $E \rightarrow 0$ we keep only the leading term $4\pi\Psi_0(X_+(\mathbf{r})) \approx 4\pi\mathbf{k} \cdot \mathbf{r} \sin\theta$ in the rhs of Eq. (4).

Accordingly, the solution of Eq. (4) has the form $f(\mathbf{r}) = f(r)\mathbf{k} \cdot \mathbf{r}/kr$ corresponding to the angular momentum $l = 1$, and Eq. (4) transforms to

$$(\hat{L}_0^{l=1} - \sqrt{\varepsilon})f(r) = 4\pi kr \sin\theta. \quad (7)$$

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

In the specified interval of ν the function λ has two roots: ν_0 and $-\nu_0 - 2$. With m_\uparrow/m_\downarrow increasing from 0 to ≈ 13.6 the root ν_0 decreases from 1 to -1 approaching the second root. At larger mass ratios the roots are complex conjugates with the real part equal to -1 . Zeros of $\lambda(\nu)$ are important to understand the behavior of $f(r)$ at short distances.

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

$$\hat{L}_0^{l=1}\chi(pr) = p\chi(pr). \quad (8)$$

As λ has two roots, the spectrum of $\hat{L}_0^{l=1}$ is two-fold degenerate, and for $p=1$ there are only two linearly independent eigenfunctions which behave as $\chi_1 \sim r^{\nu_0}$ and $\chi_2 \sim r^{-\nu_0-2}$ at small r . The complex exponents ν_0 and ν_0^* at larger mass ratios imply that the function $\chi_1 = \chi_2^*$ rapidly oscillates as $r \rightarrow 0$ and the Efimov effect takes place. In both cases we choose two real eigenfunctions which at large distances ($r \gg 1$) have the asymptotes $\chi_{1,2}(r) \approx 2 \sin(r + \delta_{1,2})/r$. The phases δ_1 and δ_2 can be determined from a numerical calculation of Eq. (8).

The case $p = \sqrt{\varepsilon}$ corresponds to the collision of a molecule with an atom just below the three-body recombination threshold ($E = -0$), where the function Ψ_0 is zero. Strictly speaking this process is described by the linear combination $f_{mol}(r) = A\chi_1(\sqrt{\varepsilon}r) + B\chi_2(\sqrt{\varepsilon}r)$. The determination of the coefficients A and B involves short-range physics, i.e., the knowledge of the three-body wave function Ψ at distances of the order of $R_e' \sim \sqrt{m_\uparrow}R_e/\hbar \ll 1/\sqrt{\varepsilon}$, and is beyond the scope of this paper. However, the matching procedure implies that at these distances both terms in $f_{mol}(r)$ are of the same order of magnitude, so $B/A \sim (\sqrt{\varepsilon}R_e')^{2\nu_0+2}$. In the case of $m_\uparrow/m_\downarrow < 13.6$, the exponent $2\nu_0+2$ is real and positive, and at distances $r \gg R_e'$ one has $f_{mol}(r) \approx A\chi_1(\sqrt{\varepsilon}r)$. Hence, short-range three-body parameters are unnecessary.

Fortunately, the discussed case of $m_\uparrow/m_\downarrow < 13.6$ covers almost all practical situations. Using the function $\chi_1(r)$ and scaling property (8) we can construct a complete orthonormal set of functions $f_p(r) = p\chi_1(pr)$. Completeness follows

An explicit form of the operator $\hat{L}_0^{l=1}$ can be obtained from Eq. (5) by integrating out the angular part of $f(\mathbf{r})$.

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

from the equality $rf_p(r) = pf_p(p)$ and from the normalization condition $\int_0^\infty f_p(r)f_{p'}(r)r^2 dr = 2\pi\delta(p-p')$. The operator $\hat{L}_0^{l=1} - \sqrt{\varepsilon}$ in Eq. (7) can now be inverted and after some manipulation we obtain

$$f(r) = -\frac{4\pi k \sin\theta}{\varepsilon} \left(\sqrt{\varepsilon}r + \lambda(1) + \frac{\lambda(0)\lambda(1)}{\sqrt{\varepsilon}r} - \frac{\lambda(0)\lambda(1)}{\sqrt{\varepsilon}r} \sqrt{\frac{\lambda(-1)}{2\pi}} \int_0^\infty \frac{\chi_1(z)z dz}{z - \sqrt{\varepsilon}r} \right). \quad (9)$$

The integral in Eq. (9) is taken as a principal value. The solution f is not singular at short distances. The terms containing r^{-1} , r^0 , and r vanish as expected except in situations where $\lambda(1)$, $\lambda(0)$, or $\lambda(-1)$ are equal to 0. At distances $r \ll 1/\sqrt{\varepsilon}$ we have $f(r) \sim r^2$ and the short-range physics does not come into play. For large distances the asymptotic behavior $\chi_1(r) \approx 2 \sin(r + \delta_1)/r$ gives

$$\int_0^\infty \frac{\chi_1(z)z dz}{z - \sqrt{\varepsilon}r} = 2\pi \cos(\sqrt{\varepsilon}r + \delta_1) + O\left(\frac{1}{\sqrt{\varepsilon}r}\right). \quad (10)$$

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

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

$$\Omega_{\uparrow\uparrow\downarrow} = \alpha_\uparrow(\bar{\varepsilon}_\uparrow/\varepsilon)n_\downarrow n_\uparrow^2, \quad (11)$$

where n_\downarrow and n_\uparrow are the densities of the fermionic components. The rate constant $\alpha_\uparrow(\bar{\varepsilon}_\uparrow/\varepsilon)$ is proportional to the av-

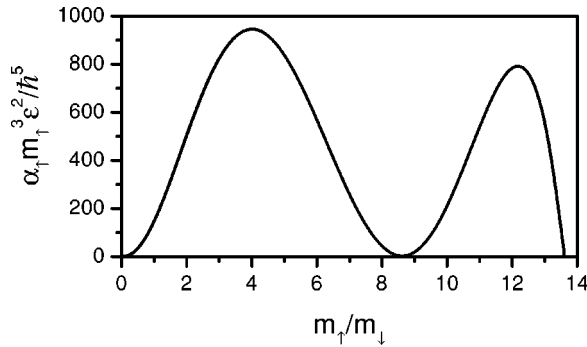


FIG. 2. The parameter $\alpha_1 m_1^3 \epsilon^2 / \hbar^5$ versus m_1 / m_\downarrow .

erage kinetic energy of \uparrow particles $\bar{\epsilon}_\uparrow$, which equals $3T/2$ in a nondegenerate gas, and $3T_F/5 \approx 4.6\hbar^2 n_\uparrow^{2/3} / m_\uparrow$ in a deeply degenerate gas. The coefficient α_1 is given by

$$\alpha_1 = \frac{8\pi^3}{3} \frac{\hbar^5}{m_\uparrow^3 \epsilon^2} \lambda^2(1)\lambda^2(0)\lambda(-1)\sin^2\theta \tan^3\theta. \quad (12)$$

Figure 2 shows the dependence of the dimensionless quantity $\alpha_1 m_1^3 \epsilon^2 / \hbar^5$ on m_1 / m_\downarrow . In the case of $m_\uparrow = m_\downarrow = m$ the quantity $\alpha_1 \approx 148\hbar a^4 / m$.

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

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

$$-\dot{n}/n = Ln^2 \approx 111(na^3)^2 \bar{\epsilon} / \hbar. \quad (13)$$

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

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

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

We thank G. V. Shlyapnikov, J. T. M. Walraven, M. A. Baranov, and M. Olshani for fruitful discussions. This work was financially supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM), by INTAS, and by the Russian Foundation for Basic Studies.

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