Three-Boson Problem near a Narrow Feshbach Resonance

D. S. Petrov

ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA
Harvard-MIT CUA, Physics Department, Harvard University, Cambridge, Massachusetts 02138, USA
Russian Research Center, Kurchatov Institute, Kurchatov Square, 123182 Moscow, Russia

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We consider a three-boson system with resonant binary interactions and show that for sufficiently narrow resonances three-body observables depend only on the resonance width and the scattering length. The effect of narrow resonances is qualitatively different from that of wide resonances revealing novel physics of three-body collisions. We calculate the rate of three-body recombination to a weakly bound level and the atom-dimer scattering length and discuss implications for experiments on Bose-Einstein condensates and atom-molecule mixtures near Feshbach resonances.

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The creation of strongly interacting atomic BEC's by increasing the scattering length, a, is impeded by inelastic processes [1], the most important of which is three-body recombination to molecular states (see [2], and references therein). For several years this process has been the primary motivation to study three-body physics in the context of ultracold gases. Recent observations of weakly bound dimers and their mixtures with atoms [3–5] stimulate a strong interest in atom-dimer collisions and in peculiar weakly bound trimer states (Efimov states) [6], which have been extensively studied in theory but have never been observed experimentally.

In the case of a potential resonance when the scattering length is much larger than the radius, R_e, of interatomic forces, low-energy observables in a three-boson system are universal functions of a and the three-body parameter r_0. In particular, for $a > 0$ the rate constant of three-body recombination of atoms of mass m to a weakly bound state is given by $\alpha_{\rm rec} = C\hbar a^4/m$, where C is a periodic function of $\log(a/r_0)$ and can have any value between 0 and approximately 68 [7,8]. The atom-dimer scattering length is periodic in $\log(a/r_0)$ and goes through infinity each time a new Efimov state is at the atom-dimer threshold [9,10]. The three-body parameter r_0 may be determined from the three-body wave function at distances of the order of R_e. For realistic interatomic potentials an *ab initio* calculation of r_0 is difficult and it is usually considered as a parameter of the theory. The related uncertainty makes an exact determination of the three-body observables impossible. Moreover, application of these results to three-body systems near a narrow Feshbach resonance should be done with care as the two-body scattering then depends strongly on energy.

Feshbach resonances occur when the energy, E, of a pair of colliding atoms in the open channel is close to the energy, $E_{\rm res}$, of a quasidiscrete molecular state in the closed channel [11]. In the limit when both E and $E_{\rm res}$ are much smaller than the spacing, $D \sim \hbar^2/mR_e^2$, between molecular levels, and the detuning $E - E_{\rm res}$ is sufficiently small to neglect the background scattering [12], the scattering amplitude is given by [13]:

$$F(E) \approx -\frac{\hbar\gamma/\sqrt{m}}{E - E_{\rm res} + i\gamma\sqrt{E}} = -\frac{1}{1/a + R^* q^2 + iq}, \quad (1)$$

where $q = \sqrt{mE}/\hbar$, $a = -\hbar\gamma/\sqrt{m}E_{\rm res}$, and we introduce the length R^* related to the width of the resonance by $R^* = \hbar/\sqrt{m}\gamma > 0$ [14].

In this Letter we show that the resonant dependence of the scattering amplitude on E is of fundamental importance for the three-body problem and develop a method for its solution near a narrow resonance in the case $R^* \gg R_e$, $|a| \gg R_e$. The three-body recombination rate, the positions of Efimov states, and the atom-dimer scattering length are shown to be functions only of the two-body observables, a and R^*. We identify two physically distinct regimes of the three-body scattering. In the regime of small detuning, $|a| \gg R^*$, the physics of a three-body collision is the same as near a wide resonance. However, r_0 is unambiguously determined by the parameter R^*. The regime of intermediate detuning, $|a| \ll R^*$, is qualitatively different. There are no Efimov states for three bosons and for $a > 0$ neither the atom-dimer scattering length nor the three-body recombination rate shows the periodic dependence on $\log(a)$. The rate constant of three-body recombination to a weakly bound level is proportional to $a^{7/2}R^{*1/2}$ and by far exceeds the maximum value expected from the a^4 law [7,8]. Our result for $\alpha_{\rm rec}$ agrees with the experimental observation at MIT [1].

First, we analyze the consequences of the finite resonance width for binary collisions. Although the validity of Eq. (1) does not require $qR^* \ll 1$, the amplitude (1) formally corresponds to a truncated effective range expansion with the range $R = -2R^*$. In the case $R^* \gg R_e$ this range exceeds the actual radius of interatomic forces and the interaction acquires unusual *long-range* properties. Two examples of such resonances are the 907 G Feshbach resonance in Na ($\Delta_B \approx 1$ G, $R_e \approx 45$ Å, $R^* \approx 260$ Å) [1] and the 1007.4 G resonance in ^{87}Rb ($\Delta_B \approx 0.17$ G, $R_e \approx 85$ Å, $R^* \approx 320$ Å) [15,16]. The amplitude

(1) is also a feature of optically induced resonances. A pair of free atoms can be coupled to an electronically excited molecular level [17] or, through a two-photon Raman transition reducing the spontaneous emission, to a vibrational state of the ground-state potential [18]. In contrast to magnetic resonances, the width of an optical one can be modified by changing laser intensities.

The poles of the scattering amplitude (1) in the complex energy plane determine the positions of weakly bound molecular states. From the quadratic equation, the inverse size of the bound state is

$$\kappa = \sqrt{m|E_b|}/\hbar = (\sqrt{1 + 4R^*/a} - 1)/2R^*. \quad (2)$$

A true bound level exists only for $a > 0$. In the regime of small detuning we retrieve the well-known result $\kappa \approx 1/a$. In the regime of intermediate detuning, $\kappa \approx 1/\sqrt{aR^*}$ and the binding energy is close to $E_{\rm res} = -\hbar^2/maR^*$. Remarkably, due to the inequality $R^* \gg R_e$ this level remains weakly bound even for $a \sim R_e$.

Outside the radius of the potential the normalized wave function of the bound state is given by

$$\phi_b(r) = (1 + 2\kappa R^*)^{-1/2}\sqrt{\kappa/2\pi}\exp(-\kappa r)/r, \quad (3)$$

where the preexponential factor is determined by the residue of the scattering amplitude at $E = E_b$ [13]. The normalization integral calculated with the wave function (3) tends to 1 in the regime of small detuning. We conclude that atoms in the dimer are well separated and spend most of their time in the open channel. As the bound state becomes deeper the normalization integral decreases that reflects increasing occupation of the quasistationary level. In the regime of intermediate detuning the weakly bound state is this molecular level with a small admixture of the open channel wave function.

To solve the three-body problem we employ the zero-range approximation valid if the binary collision energies are small compared to D. The key idea is to solve the equation for free motion but with the Bethe-Peierls boundary condition on the wave function for vanishing distance, r, between two atoms: $-(r\psi)'/r\psi \to \tilde{a}^{-1}(E_c)$, where the energy-dependent scattering length defined as $\tilde{a}^{-1}(E) = a^{-1} + R^*mE/\hbar^2$ should be evaluated at the collision energy, E_c, of these two atoms. This boundary condition, which can be also rewritten as $\psi \propto 1/r - 1/\tilde{a}(E_c)$, leads to the scattering amplitude (1).

In the center of mass reference frame three bosons with total energy E are described by the equation

$$-[\nabla^2_{\mathbf{x}} + \nabla^2_{\mathbf{y}} + E]\Psi(\mathbf{x}, \mathbf{y}) = 0, \quad (4)$$

where $\mathbf{y}$ is the distance between two bosons, $\sqrt{3}\mathbf{x}/2$ is the distance between their center of mass and the third atom, and $m = \hbar = 1$. Because of the bosonic symmetry Ψ is invariant under the transformations: $\{\mathbf{x} \to (\pm\sqrt{3}\mathbf{y} - \mathbf{x})/2,\ \mathbf{y} \to (\sqrt{3}\mathbf{x} \pm \mathbf{y})/2\}$, and $\{\mathbf{x} \to \mathbf{x},\ \mathbf{y} \to -\mathbf{y}\}$. Therefore, three boundary conditions for $y \to 0$ and for $\sqrt{3}\mathbf{x} \pm \mathbf{y} \to 0$ are dependent and we need to ensure the proper behavior of Ψ only for $y \to 0$:

$$\Psi(\mathbf{x}, \mathbf{y}) \approx [y^{-1} - \tilde{a}^{-1}(E_c)]f(\mathbf{x})/4\pi. \quad (5)$$

The function f contains the information about the relative motion of the third atom with respect to the first two when they are on top of each other. The quantity E_c is the total energy E excluding the energy of this relative motion. Accordingly, E_c can be presented as a differential operator acting on f:

$$E_c = \lim_{\mathbf{y}\to 0}\frac{-\nabla^2_{\mathbf{y}}\Psi}{\Psi} = E + \lim_{\mathbf{y}\to 0}\frac{\nabla^2_{\mathbf{x}}\Psi}{\Psi} = E + \frac{\nabla^2_{\mathbf{x}} f}{f}. \quad (6)$$

Since $\tilde{a}^{-1}(E_c) = a^{-1} + R^*E_c$, Eq. (5) reduces to

$$\Psi \approx [y^{-1} - a^{-1} - R^*(E + \nabla^2_{\mathbf{x}})]f(\mathbf{x})/4\pi. \quad (7)$$

Let us now consider the following solution of Eq. (4):

$$\Psi(\mathbf{x}, \mathbf{y}) = \Psi_0 + \int d^3r' f(\mathbf{r}')[G_E(\sqrt{(\mathbf{x} - \mathbf{r}')^2 + y^2}) + \sum_{\pm} G_E(\sqrt{(\mathbf{x} - \mathbf{r}'/2)^2 + (\mathbf{y} \pm \sqrt{3}\mathbf{r}'/2)^2})], \quad (8)$$

where $\Psi_0(\mathbf{x}, \mathbf{y})$ is a properly symmetrized and finite solution of Eq. (4) without singularities and G_E is the Green function of Eq. (4) given by $G_E(X) = -EK_2(\sqrt{-E}X)/8\pi^3X^2$. For negative energies K_2 is an exponentially decaying Bessel function and for $E > 0$ we use the convention $\sqrt{-E} = -i\sqrt{E}$. A direct examination shows that the wave function (8) is properly symmetrized. In order to ensure that (8) reduces to (7) at $y \to 0$ we add and subtract from Eq. (8) an auxiliary quantity

$$f(\mathbf{x})\int G_E(\sqrt{(\mathbf{x} - \mathbf{r}')^2 + y^2})d^3r' = f(\mathbf{x})e^{-\sqrt{-E}y}/4\pi y.$$

As y tends to zero we see that the terms proportional to $1/y$ in Eqs. (7) and (8) are equal and matching the next (regular) terms yields the equation for the function f:

$$(-R^*\nabla^2_{\mathbf{r}} + \hat{L}_E - a^{-1} + \sqrt{-E} - R^*E)f(\mathbf{r}) = F_0(\mathbf{r}), \quad (9)$$

where $F_0(\mathbf{r}) = 4\pi\Psi_0(\mathbf{r}, 0)$ and $\hat{L}_E$ is given by

$$\hat{L}_E f(\mathbf{r}) = 4\pi\int\{G_E(|\mathbf{r} - \mathbf{r}'|)[f(\mathbf{r}) - f(\mathbf{r}')] - 2G_E(\sqrt{r^2 + r'^2 + \mathbf{r}\mathbf{r}'})f(\mathbf{r}')\}d^3r'. \quad (10)$$

The operator on the left-hand side of Eq. (9) conserves angular momentum, and we can expand f in spherical harmonics to work only with a set of uncoupled equations for functions of a single variable r. In momentum space

$f(\mathbf{k}) = \int f(\mathbf{r}) \exp(i\mathbf{k}\mathbf{r}) d^3r$ and $\hat{L}_E$ is given by

$$\hat{L}_E f(\mathbf{k}) = (\sqrt{-E + k^2} - \sqrt{-E}) f(\mathbf{k}) - \frac{2}{\sqrt{3}\pi^2} \times \int \frac{f(\mathbf{q}) d^3q}{k^2 + q^2 + \mathbf{k}\mathbf{q} - 3E/4}. \quad (11)$$

Equation (9) was first obtained in Ref. [19] for $R^* = 0$. In that case its solution is not unique [20]—at small distances it behaves as $f \sim r^{-1} \sinlog(r/r_0)$ with arbitrary r_0. According to Eq. (6) the corresponding collision energy increases as $|E_c| \sim 1/r^2$ at small r, and for narrow resonances the two-body collisions would become off resonant at $r \sim R^*$. We show below that the solution in this case is smooth and unique. Equations (8) and (9) determine the three-body wave function and all low-energy properties of the system.

Consider the problem of an atom scattering by a weakly bound dimer ($a > 0$) at low collision energies when the scattering amplitude is dominated by the s-wave contribution. The corresponding scattering length, a_{ad}, is determined by the long-range asymptote of the atom-dimer wave function at zero collision energy. Namely, in the region $y \lesssim 1/\kappa \ll x$ the total three-body wave function factorizes into $\Psi(\mathbf{x}, \mathbf{y}) \approx \phi_b(y) \times (1 - 2a_{ad}/\sqrt{3}x)$. A comparison of this expression with Eqs. (3) and (5) gives $f(r) \propto 1 - 2a_{ad}/\sqrt{3}r$ at large r. Thus, we can find a_{ad} by solving Eq. (9) with $E = E_b$:

$$(-R^* \nabla^2_{\mathbf{r}} + \hat{L}_{E_b}) f(r) = 0. \quad (12)$$

To obtain Eq. (12) from Eq. (9) we note that $-a^{-1} + \sqrt{-E_b} - R^* E_b = 0$ and $\Psi_0 \equiv 0$ for $E < 0$.

At distances $r \ll 1/\kappa$ we can approximate the Green function in Eq. (10) by $G_{E_b}(X) \approx 1/4\pi^3 X^4 = G_0(X)$. This gives $\hat{L}_{E_b} \approx \hat{L}_0$. The operator $\hat{L}_0$ has the property that $\hat{L}_0 r^\nu = \lambda(\nu) r^{\nu-1}$ for $-3 < \mathrm{Re}(\nu) < 1$. The function $\lambda(\nu)$ has two roots, $\nu_\pm = -1 \pm i s_0$, where $s_0 \approx 1.006\,24$. Thus, the solution of Eq. (12) for $R^* = 0$ and $r \ll 1/\kappa$ is

$$f(r) \propto r^{-1} \sin[s_0 \ln(r/r_0)]. \quad (13)$$

In the regime of small detuning Eq. (13) remains valid at distances $R^* \ll r \ll a$, where the Laplacian in Eq. (12) can be neglected. However, for $r \ll R^*$ the differential operator is dominant and f should tend to a finite value [21]. Then, the integral operator acts as a Coulomb potential $\hat{L}_0 \approx \lambda(0)/r$, where $\lambda(0) = -4/\sqrt{3}$. Note that the two-body collision energy $|E_c| \lesssim 1/R^* R_e \ll D$, which justifies the use of the zero-range method.

Expression (13) and scaling properties of Eq. (12) at small distances show that the long-range asymptote of f does not change if R^* is multiplied or divided by $\exp(\pi/s_0) \approx 22.7$, provided that R^* remains much smaller than a. Obviously, the atom-dimer scattering length has the same property. Numerical integration of Eq. (12) in the limit $R^* \ll a$ yields $r_0 \approx 0.5R^*$.

In the regime of intermediate detuning the integral operator $\hat{L}_{E_b}$ in Eq. (12) is a perturbation to the differential one with the small parameter $1/(R^*\kappa) \approx \sqrt{a/R^*}$. In the zeroth order $f = \mathrm{const}$, i.e., there is no scattering. The first two corrections yield

$$a_{ad}/a \approx -8/3[1 + (11/6)\sqrt{a/R^*}]. \quad (14)$$

In Fig. 1 we plot a_{ad}/a as a function of R^*/a calculated numerically from Eq. (12). The resonances in a_{ad} occur when there is a Efimov state of zero-energy relative to the atom-molecule continuum. We find that the first Efimov state arises at $R^*/a \approx 2.2$, the second—at $R^*/a \approx 0.07$. With high accuracy a_{ad}/a is periodic on a logarithmic scale as we further decrease R^*/a. At large R^*/a we recover the analytic result (14).

We now turn to the problem of three-body recombination to a weakly bound level. This process occurs when three atoms approach each other to distances of the order of $1/\kappa$. Therefore, at energies $E \ll |E_b|$ the recombination probability is energy independent and we can consider the zero-energy limit of Eq. (9). Let the function Ψ_0 describe three noncondensed ideal bosons in a unit volume. Then in the region important for the recombination $\Psi_0 \approx 1/\sqrt{6}$ and Eq. (9) acquires the form

$$(-R^* \nabla^2_{\mathbf{r}} + \hat{L}_0 - a^{-1}) f(r) = 4\pi/\sqrt{6}. \quad (15)$$

The solution of Eq. (15) at large r contains a term $A \exp(i\kappa r)/r$. By virtue of Eqs. (3) and (5) the corresponding part of the three-body wave function is $\Psi(\mathbf{x}, \mathbf{y}) \approx A\sqrt{(1 + 2\kappa R^*)/8\pi\kappa}\,\phi_b(y) \exp(i\kappa x)/x$ and describes an atom and a dimer flying apart. Given the factor A, the derivation of the rate constant of three-body recombination α_{rec} is straightforward. We solve Eq. (15) in momentum representation and determine A by the residue of the function $f(k)$ at the pole $k = \kappa$.

In Fig. 2 we plot $\alpha_{\mathrm{rec}}/a^4$ as a function of R^*/a calculated numerically from Eq. (15). In the regime of small

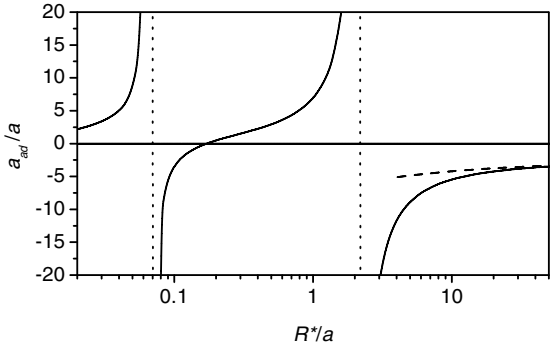

FIG. 1. The ratio a_{ad}/a versus R^*/a. The dashed curve is given by Eq. (14) and corresponds to the limit $a \ll R^*$. Dotted lines indicate the points $R^*/a \approx 2.2$ and $R^*/a \approx 0.07$, where the first and the second Efimov states emerge.

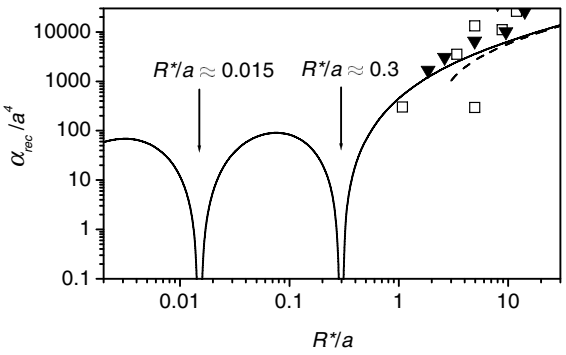

FIG. 2. The ratio $\alpha_{\rm rec}/a^4$ versus R^*/a. The dashed curve is given by Eq. (16). Arrows indicate values of R^*/a at which $\alpha_{\rm rec}$ vanishes. Scatter points correspond to experimental data taken near the 907 G Feshbach resonance in Na at MIT [1].

detuning our approach leads to the periodic dependence of $\alpha_{\rm rec}/a^4$ on $\log(a)$ with the maximum value ≈ 68 consistent with Refs. [7,8]. In fact, our results for a_{ad} and for $\alpha_{\rm rec}$ in this limit coincide with those obtained by using the effective field theory [8,9]. The three-body parameter, Λ_*, introduced there is related to R^* by $\Lambda_* \approx 6.6/R^*$.

In the regime of intermediate detuning the operator $R^*\nabla_{\mathbf{r}}^2$ in Eq. (15) dominates and we calculate $\alpha_{\rm rec}$ perturbatively. Expanding in $\sqrt{a/R^*}$, the first two terms are

$$\alpha_{rec} \approx 192\sqrt{3}\pi^2\sqrt{a^7R^*}\left[1-\left(\frac{4\pi}{3\sqrt{3}}-1\right)\sqrt{\frac{a}{R^*}}\right]. \quad (16)$$

Our results agree with measurements at MIT [1]. In particular, $\alpha_{\rm rec}/a^4 \gg 68$ in this regime.

Finally, we point out that on the magnetic field axis the region of intermediate detuning is a factor of R^*/R_e wider than the region of small detuning and is, therefore, more accessible. Note, that in both MIT [1] and MPIQ [15] experiments on narrow resonances $a \lesssim R^*$.

The method presented here can be generalized to describe fermions and fermion-boson mixtures with different masses. The significant dependence of two- and three-body observables on R^* suggests that properties of a many-body system should also depend on R^*.

The atom-dimer scattering can be probed by a direct collision of atomic and molecular clouds. It is remarkable that near the wide resonance associated with the first Efimov state ($a \approx 0.45R^*$) the atom-dimer scattering length can be tuned to be an order of magnitude larger than a. In a degenerate atom-molecule mixture one has either a phase separation or a collapse depending on the sign of a_{ad}. We may also consider the formation of trimers by adiabatic sweep across this resonance. Their detection can be based on the Stern-Gerlach technique [3–5] as atoms, dimers, and trimers all have different magnetic moments. The vanishing of the recombination to the weakly bound level at $a \approx 3.3R^*$ can be used to produce a long-lived strongly interacting atomic gas.

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