# Possible Efimov Trimer State in a Three-Hyperfine-Component Lithium-6 Mixture

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We consider the Efimov trimer theory as a possible framework to explain recently observed losses by inelastic three-body collisions in a three-hyperfine-component ultracold mixture of lithium 6. Within this framework, these losses would arise chiefly from the existence of an Efimov trimer bound state below the continuum of free triplets of atoms, and the loss maxima (at certain values of an applied magnetic field) would correspond to zero-energy resonances where the trimer dissociates into three free atoms. Our results show that such a trimer state is indeed possible given the two-body scattering lengths in the three-component lithium mixture and gives rise to two zero-energy resonances. The locations of these resonances appear to be consistent with observed losses.

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The experimental realization of ultracold Fermi gases has let us explore many fundamental aspects of few- and many-body physics. In particular, the study of mixtures of fermionic atoms in two different spin components has led to the observation of superfluid paired phases such as molecular Bose-Einstein condensates, Bardeen-Cooper-Schrieffer superfluids, and their crossover [1–5]. Recently, there has been some theoretical interest in Fermi systems with three different spin components [6–10], which can present analogies with color superfluidity in QCD [11]. Recent experiments [12,13] have been performed with ultracold mixtures of lithium-6 atoms prepared in the lowest three hyperfine states $|1\rangle$, $|2\rangle$, and $|3\rangle$. They indicated that, when an external magnetic field is applied, strong losses due to three-body inelastic collisions occur over a wide range of magnetic-field intensities. On the other hand, such losses are not observed when only two of the three hyperfine components are mixed. Therefore, the observed inelastic collisions are related to the specific scattering channel involving three atoms in the three different hyperfine components. The magnitude of the inelastic collisions is characterized by a loss rate coefficient $\mathcal{K}$, defined by the rate equation

$$\frac{dn_i}{dt} = -\mathcal{K} n_i n_j n_k, \quad \text{for } (i, j, k) = (1, 2, 3),$$

where $n_1$, $n_2$, and $n_3$ are the densities of each kind of atoms. The variation of the measured loss rate coefficient with respect to the intensity $B$ of the applied magnetic field is shown in the bottom panel of Fig. 1. It reveals a peak around $B = 130$ G which suggests an enhancement due to a resonance of three colliding atoms with a three-body bound state. We can envisage two kinds of resonance, depending on the origin of such a three-body bound state.

First, the three-body bound state may originate from another hyperfine channel and couple by hyperfine interaction to the three-body scattering continuum in the hyperfine channel $|1\rangle|2\rangle|3\rangle$. Since the bound state and scattering state belong to different hyperfine channels, they have different magnetic moments and become resonant only around a particular intensity of the magnetic field which brings them to the same energy. This situation would correspond to a "three-body Feshbach resonance" [14], a

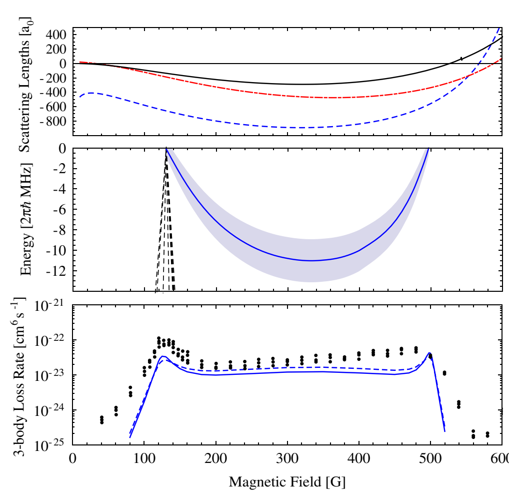


FIG. 1 (color online). Top panel: Variation of the two-body scattering lengths $a_{12}$, $a_{13}$, and $a_{23}$ for the lowest three hyperfine components of lithium 6 as a function of magnetic field. These curves were calculated by P. S. Julienne and taken from Ref. [12]. Middle panel: Energy of the Efimov trimer (solid curve) just below the three-body threshold as a function of magnetic field with $\Lambda_0 = (0.42a_0)^{-1}$. The shaded area corresponds to the width of the Efimov state, i.e., the imaginary part of its energy, for $\eta = 0.115$. The estimated energy of possible resonant trimers from all other spin channels with the same total projection $m_F = -3/2$ is indicated by dashed curves. Bottom panel: Experimental (dots, taken from Ref. [12]) and theoretical (curves) three-body inelastic collision loss rate coefficient as a function of magnetic field. The dashed curve is obtained by adjusting the short-range loss parameter $\eta$ to fit the experimental data ($\eta = 0.157$), and the solid curve by adjusting it to fit the shape of the left peak ($\eta = 0.115$).

 

generalization of the now well-known two-body Feshbach resonances which occur for two scattering atoms around certain magnetic-field values [15].

As a matter of fact, wide two-body Feshbach resonances are present in lithium 6 over the range of magnetic-field intensities where the three-body losses are observed. As a result, the two-body scattering lengths between two atoms in different states, namely, $|1\rangle|2\rangle$, $|1\rangle|3\rangle$, and $|2\rangle|3\rangle$, are modified by the applied magnetic field. The dependence of these three scattering lengths on the magnetic-field intensity is shown in the top panel of Fig. 1. Because of this dependence, the interactions among three atoms colliding in the hyperfine channel $|1\rangle|2\rangle|3\rangle$ are also modified by the magnetic field, and it may happen that a three-body bound state supported by these interactions within the same hyperfine channel is brought to the threshold of its three-body scattering continuum at a certain magnetic-field value, causing a "shape resonance." This constitutes the second possible kind of resonance.

Studying both kinds of resonance theoretically is involved and requires an extremely accurate knowledge of the interactions between atoms. However, in the case where the two-body scattering lengths are much larger than the range of the interatomic interactions, it is possible to predict the structure of the three-body bound states near threshold and their shape resonance simply in terms of the scattering lengths and a short-range three-body parameter. This was pointed out by Efimov [16], and the corresponding three-body bound states, known as "Efimov trimers," are purely quantum-mechanical states which enjoy special properties such as discrete scale invariance as the scattering lengths are varied. In particular, their energy spectrum forms an infinite series with a point of accumulation just below the continuum threshold when the scattering lengths become infinite. So far, signatures of Efimov trimers of identical bosons have been observed in helium 4 [17], cesium 133 [18,19], and potassium 39 [20] and have been assigned in the first two cases to the ground state of the Efimov series [21,22] and to the ground and first excited states in the case of potassium. Similar signatures of heteronuclear bosonic Efimov trimers of potassium and rubidium were recently reported in Ref. [23], while the evidence of fermionic Efimov trimers is yet to be found. It was suggested by the authors of Refs. [12,13] that their observations in three-component lithium 6 might be the manifestation of an Efimov trimer of distinguishable fermions. The purpose of this Letter is to test this hypothesis using the Efimov theory.

First, it should be noted that the two-body scattering lengths in the experimental conditions are indeed quite large, from about $-100$ to $-1000a_0$ (where $a_0 = 5.292 \times 10^{-11}$ m is the Bohr radius), but not always much larger than the range of the atomic interactions, typically given by the van der Waals length $\ell_{\mathrm{vdW}} = (mC_6/\hbar)^{1/4} \approx 60a_0$, where $C_6$ is the van der Waals dispersive coefficient, $m$ is the mass of lithium 6, and $\hbar$ is the reduced Planck's constant. Therefore, the applicability of Efimov theory is questionable, especially at low (around 100 G) and high (around 500 G) magnetic-field values where one or two of the scattering lengths become small. However, in the intermediate region, the necessary conditions for the existence of Efimov trimers are met.

The details of the Efimov theory can be found in Refs. [16,21]. It essentially treats the free three-body problem with boundary conditions at short distance imposing the known two-body scattering lengths between each pair of atoms. The three-body wave function $\Psi(R, \alpha, \theta)$ is expressed in terms of the hyperradius $R$ of the three-body system (a measure of the global distance among the three atoms) and the two angles $\alpha$ and $\theta$ describing the geometrical configuration of the atoms. More precisely, if we denote by $\vec{r}$ the relative vector between atoms 1 and 2 and by $\vec{\rho}$ the relative vector between atom 3 and the center of mass of atoms 1 and 2, then $R^2 = r^2 + \frac{4}{3}\rho^2$, $\theta$ is the angle between $\vec{r}$ and $\vec{\rho}$, and $\tan\alpha = \sqrt{3}r/(2\rho)$. By using the Faddeev decomposition [24] and restricting ourselves to the case of zero total angular momentum which is the most favorable for the Efimov effect to occur [16], the wave function can be written as

$$\Psi(R, \alpha, \theta) = \frac{2}{R^2}\left(\frac{\tilde{\chi}^{(1)}(R, \alpha_+)}{\sin 2\alpha_+} + \frac{\tilde{\chi}^{(2)}(R, \alpha_-)}{\sin 2\alpha_-} + \frac{\tilde{\chi}^{(3)}(R, \alpha)}{\sin 2\alpha}\right),$$

where $\sin 2\alpha_\pm = \{1 - [\frac{1}{2}\cos\alpha \pm (\sqrt{3}/2)\sin\alpha\cos\theta]^2\}^{1/2}$.

Note that the functions $\tilde{\chi}^{(i)}$ depend on only one hyperangle, because we assumed that the total angular momentum is zero. They satisfy the free Schrödinger equations

$$\left(\frac{\partial^2}{\partial R^2} + \frac{1}{R}\frac{\partial}{\partial R} + \frac{1}{R^2}\frac{\partial^2}{\partial \alpha^2} + \frac{mE}{\hbar^2}\right)\tilde{\chi}^{(i)}(R, \alpha) = 0 \tag{1}$$

for a given energy $E$, with the boundary conditions

$$\frac{\partial \tilde{\chi}^{(i)}}{\partial \alpha}(R, 0) + \frac{4}{\sqrt{3}}\left[\tilde{\chi}^{(j)}\left(R, \frac{\pi}{3}\right) + \tilde{\chi}^{(k)}\left(R, \frac{\pi}{3}\right)\right] = -\frac{R}{a_{jk}}\tilde{\chi}^{(i)}(R, 0), \tag{2}$$

$$\tilde{\chi}^{(i)}\left(R, \frac{\pi}{2}\right) = 0 \tag{3}$$

for any $R > R_0$ and

$$\frac{\partial \ln \tilde{\chi}^{(i)}}{\partial R}(R_0, \alpha) = \Lambda(R_0), \quad \text{for any } \alpha \in \left[0, \frac{\pi}{2}\right], \tag{4}$$

where $i, j, k$ is any permutation of 1, 2, 3.

The first boundary condition (2) imposes the form of the wave function in the two-body sectors consistent with the known two-body scattering lengths $a_{12}$, $a_{13}$, and $a_{23}$ among the three kinds of atoms. The last boundary condition (4) fixes the logarithmic derivative of the wave function at short hyperradius $R_0 \ll a_{ij}$ to some value $\Lambda(R_0)$ independent of the energy $E$. In this region, the last term of Eq. (2) is negligible, and one can show that the solution of

Eqs. (1) takes the separable form $\tilde{\chi}^{(i)}(R, \alpha) \approx \sin[|s_0| \ln(KR) + \Delta] \sin[s_0(\pi/2 - \alpha)]$, where $K = \sqrt{mE}/\hbar$, $\Delta$ is a phase shift, and $s_0 \approx 1.006\,24i$ is the imaginary solution of the equation $-s_0 \cos(s_0\pi/2) + 8/\sqrt{3} \sin(s_0\pi/6) = 0$, which follows from applying the boundary condition Eq. (2). In order for $\Lambda$ to be energy independent, the phase shift $\Delta$ must be of the form $-|s_0| \ln(K/\Lambda_0)$, where $\Lambda_0$ is some fixed wave number. This sets

$$\Lambda(R_0) = \frac{|s_0|}{R_0} \cot[|s_0| \log(R_0\Lambda_0)].$$

This way, the choice of $R_0$ is arbitrary. The only requirement is that $R_0$ should be much smaller than the scattering lengths. In our calculation, we fixed $R_0$ to $1a_0$. Thus, the only free parameter of the theory is $\Lambda_0$. It captures the effects of the unknown short-range three-body physics on the wave function at larger hyperradii.

We solve these equations by discretizing the arguments $(R, \alpha)$ of the functions $\tilde{\chi}^{(i)}$ on a two-dimensional grid, evaluating the derivatives by finite differences, and diagonalizing the resulting matrix. The maximal value of $R$ is set to $50\,000a_0$, which is on the order of the particle spacing in the experiments. At each value of the magnetic field, the three scattering lengths $a_{12}$, $a_{13}$, and $a_{23}$ are obtained from the top panel of Fig. 1. The only unknown quantity is $\Lambda_0$. First, we make the assumption that it does not depend on the magnetic field. In reality, it may actually depend on it, but, provided that no accidental resonance occurs, it is reasonable to assume that its variations are less pronounced than that of the scattering lengths. Second, we make the fundamental assumption that the observed three-body losses are due to a shape resonance with an Efimov trimer. The measured three-body loss rate coefficient as a function of the magnetic field shows a distinctive peak around $B = 130$ G—see the bottom panel of Fig. 1. Assuming that this is the point where an Efimov state reaches the continuum threshold, we find that we should adjust $\Lambda_0$ to about $(0.42a_0)^{-1}$. Once $\Lambda_0$ is fixed, we can obtain the eigenstates and their energy around the threshold.

In the middle panel of Fig. 1, we plotted the energy of the Efimov trimer just below threshold as a function of magnetic field. By construction, the trimer appears at $B = 130$ G. Interestingly, its binding energy increases until $B = 350$ G and then decreases until the trimer reaches the continuum again, causing a second zero-energy resonance around $B = 500$ G. This simply results from the magnetic-field dependence of the scattering lengths.

Since the two-body scattering lengths are all negative in this range of magnetic field, there are no two-body bound states just below the two-body continuum. As a result, when inelastic three-body collisions occur, two of the three atoms have to form a deeply bound dimer. A direct calculation of the rate for such processes would require a detailed analysis of the deeply bound dimers. However, we can easily calculate its enhancement by the Efimov resonance. Indeed, by assigning a complex value $|\Lambda_0|e^{i\eta}$ to the three-body parameter $\Lambda_0$, and therefore a complex value to the logarithmic derivative $\Lambda$, one can impose a probability loss at short hyperradius ($R = R_0$) in order to model the overall effect of losses by recombination to deeply bound dimers [21]. This makes any scattering state $\Psi$ quasistationary, and, by calculating the time variation of the total probability $\int |\Psi|^2 d^3\vec{R} d^3\vec{r}$, one can derive the following three-body loss rate coefficient:

$$\mathcal{K} = \frac{2\hbar}{m} |\mathrm{Im}\Lambda| \rho(R_0). \tag{5}$$

As one would expect, this coefficient is proportional to the imposed velocity $\mathcal{V} = \frac{2\hbar}{m}|\mathrm{Im}\Lambda|$ at $R = R_0$ and the probability density $\rho(R_0)$ of finding three atoms at that hyperradius, defined by the hyperangular average

$$\rho(R) = 3^{3/2}\pi^2 R^5 \int_0^{\pi/2} (\sin 2\alpha)^2 d\alpha \int_0^{\pi} \sin\theta d\theta |\Psi(R, \alpha, \theta)|^2, \tag{6}$$

where $\Psi$ is normalized to be asymptotically equal to the noninteracting limit $8J_2(KR)/(KR)^2$, $J_2$ being the Bessel function. This probability density, and thus the inelastic processes, is strongly increased at short distance by the presence of an Efimov trimer just below threshold. Physically, this is due to the fact that the three atoms almost bind during their collision and therefore spend more time together. One can see in Fig. 2 that, while $\rho(R)$ is unaffected at a large distance, it changes significantly at a short distance when the magnetic field is varied around the zero-energy resonance.

The calculated loss rate coefficient of Eq. (5) is plotted in the bottom panel of Fig. 1. We obtain a profile delimited by two peaks. In between the two peaks, we observe a plateau due to the presence of the Efimov state below threshold. Outside, the probability becomes very low, due to the absence of a near-threshold Efimov trimer. From the

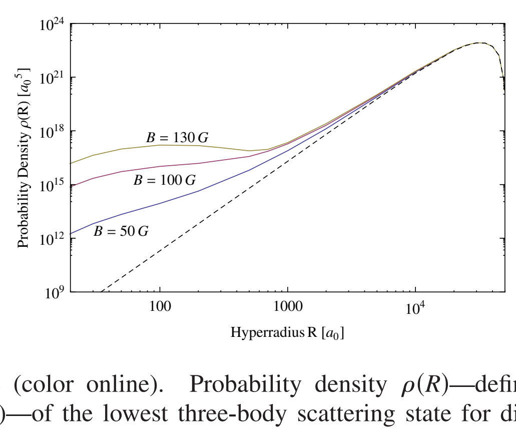


FIG. 2 (color online). Probability density $\rho(R)$—defined by Eq. (6)—of the lowest three-body scattering state for different values of the magnetic field. In all cases, the wave function $\Psi$ is normalized to be asymptotically equal to the noninteracting limit $8J_2(KR)/(KR)^2$, where $J_2$ is the Bessel function and $K$ is the wave number. This limit is indicated by the dashed curve. Here $K$ is set by the size of the numerical grid.

energy spectrum, it is clear that the second peak around 500 G is related to the second zero-energy resonance with the Efimov state. We can then adjust the value of $\eta$ to fit the experimental data. It should be noted that $\eta$ has two effects: It sets the overall magnitude of the loss rate coefficient, as can be seen from (5), and it also smooths the peaks (because they are naturally broadened by the losses). It turns out that there exists a range of values for $\eta$ which can approximately fit both the overall magnitude of the rate coefficient and its shape. Using a least-square minimization method, we found that the best fit to the experimental data is obtained for $\eta = 0.157$, while fitting only the first peak gives $\eta = 0.115$.

The behavior of the calculated three-body decay rate coefficient is very reminiscent of the measured one, which has a similar profile between 130 and 500 G. This suggests that the local maximum near $B = 500$ G found in the experiment is caused by a second resonance. The agreement with the observations is only approximate, however, as the experimental data show a much more diffuse local maximum. As we noted earlier, the Efimov theory is not strictly applicable to the present system, and it is expected that short-range corrections are needed for a better agreement. A magnetic-field dependence of $\Lambda_0$ might also play a role. These effects may very well explain the remaining discrepancies. Yet, it is quite remarkable that the Efimov theory already provides a basic description which qualitatively explains the experimental observations. In this interpretation, a relatively "pure" Efimov trimer state is expected around 300 G (where the scattering lengths are largest) and connects continuously to trimer states which are partly affected by short-range physics ("impure" Efimov trimer) and eventually dissociate in the continuum at both resonances. We find that the pure Efimov trimer at $B = 300$ G has a binding energy of about $2\pi\hbar \times 10$ MHz and a width (imaginary part of the energy) of about $2\pi\hbar \times 3$ MHz, corresponding to a lifetime of about 50 ns. However, these values result from an adjustment near $B = 130$ G, where the Efimov theory may need corrections. Thus, the actual values might be slightly different.

The present interpretation may be confirmed or refuted by further experimental investigation, in particular, direct observation of the trimers below threshold—for example, by radio frequency spectroscopy. For comparison with the first interpretation discussed in the introduction, we calculated the expected energy of possible resonant trimers coming from other channels, assuming that their magnetic moment is simply the sum of the magnetic moments of the three separated atoms. Since the interaction conserves the projection of the total spin, we considered only the channels with the same projection $m_F = -3/2$ as the incoming channel $|1\rangle|2\rangle|3\rangle$ and shifted the energy of the possible resonant trimers such that it crosses the three-body threshold of the incoming channel at $B = 130$ G. The resulting energies as a function of magnetic field are plotted in Fig. 1 as dashed curves. One can see that they have a monotonic behavior and depart steeply from the continuum threshold. On the other hand, if the Efimov interpretation is correct, the trimer is expected to follow a different and rather unusual behavior: It connects to the continuum via two zero-energy resonances, resulting in an energy minimum as a function of magnetic field. Thus we have provided a significant difference between the two scenarios, which may serve as a test in future experiments.

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*Note added.*—Upon finishing this Letter, we became aware of the work by Braaten *et al.* [25], which uses the Skorniakov–Ter-Martirosian equations to directly calculate the loss rate. After this Letter was submitted, similar results were reported in Ref. [26], using a different model involving the formation of a trimer. Both of these works yield results consistent with the loss rate coefficient given in Fig. 1.

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