Universal Dimer in a Collisionally Opaque Medium: Experimental Observables and Efimov Resonances

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A universal dimer is subject to secondary collisions with atoms when formed in a cloud of ultracold atoms via three-body recombination. We show that in a collisionally opaque medium, the value of the scattering length that results in the maximum number of secondary collisions may not correspond to the Efimov resonance at the atom-dimer threshold and thus can not be automatically associated with it. This result explains a number of controversies in recent experimental results on universal three-body states and supports the emerging evidence for the significant finite range corrections to the first excited Efimov energy level.

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Few-body systems with a resonantly enhanced two-body scattering length \( a \) display universal properties in the sense that they are independent of the details of the short-range interaction potential [1]. In the two-body domain with repulsive interactions, the most weakly bound energy level of the universal dimer depends solely on \( a \), scaling as \( 1/a^2 \). The central paradigm in the three-body domain, predicted in the early 70s by V. Efimov [2], is associated with the infinite ladder of universal bound states with discrete scaling invariance. Beside \( a \), universal trimers depend on the three-body parameter, which accounts for all the short-range physics not already included in \( a \). In recent experiments with ultracold atoms many aspects of universality were verified mainly by localizing Efimov resonances which are associated with the crossing points of the trimers’ binding energy levels with either the three-atom (for \( a < 0 \)) or the atom-dimer (for \( a > 0 \)) continua (for a recent review see Ref. [3]). Surprisingly, positions of the lowest Efimov resonances for \( a < 0 \) were found to be universally related to the van der Waals lengths of the two-body interaction potentials in different atomic species [3, 4], indicating a universal three-body parameter. This remarkable experimental discovery has attracted intense theoretical attention which suggests a whole new understanding of Efimov physics in ultracold atoms [3, 11]. However, the situation with the Efimov resonances at the atom-dimer threshold (for \( a > 0 \)) remains unclear. It appears to significantly deviate from the universal picture in all species investigated to date [4, 6, 13, 17, 20]. Suggestions have been made that the finite range of interaction potentials might be responsible for these discrepancies. However, here we show that in some cases a different effect, directly related to the specifics of the experimental observables, can cause a significant shift in the resonances’ positions.

To show this effect we start by elaborating on two experimental strategies developed recently to localize an Efimov resonance at the atom-dimer threshold, denoted in the following as \( a_\ast \). Both are based on the theoretical prediction that resonant enhancements of the atom-dimer elastic (\( \sigma_e \)) and inelastic (\( \sigma_i \)) cross sections are expected in the vicinity of \( a_\ast \), according to the following analytical expressions [1, 21]:

\[
\sigma_e = \frac{84.9 \sin^2 [s_0 \ln(a/a_\ast) + 0.97] + \sinh^2 \eta a^2}{\sin^2 [s_0 \ln(a/a_\ast)] + \sinh^2 \eta a^2} \tag{1}
\]

\[
\sigma_i = \frac{20.3 \sin(2\eta a)}{3v \sin^2 [s_0 \ln(a/a_\ast)] + \sin^2 \eta a/m_A} \tag{2}
\]

where \( s_0 = 1.00624, \eta \) is the lifetime of the Efimov state, \( v \) is the velocity of the dimer and \( m_A \) is the mass of the atom [21]. In the first strategy, realized with ultracold Cs and \(^7\)Li, an atom-dimer mixture is initially prepared in a shallow optical trap and the decay rate of dimers is then monitored as a function of \( a \) [13, 17, 19]. Thus, this approach, the maximum of the enhancement in the atom-dimer inelastic collision rate is expected to coincide with \( a_\ast \). In the second strategy, pioneered with \(^3\)K [6] and then used with \(^7\)Li [3, 22], the three-body recombination induced loss rate of atoms is measured. In each recombination event a universal dimer is formed with initial kinetic energy equal to one third of its binding energy (\( E_\ast/3 \)), which is usually much higher than the shallow optical trap depth. Moreover, the dimer is formed with the largest probability at the trap center where the density is highest. Then, on its way out, it may undergo secondary collisions with atoms, eject them out of the trap and cause the number of lost atoms per recombination event to greatly exceed three. Therefore, in this approach, the position of the maximum of the atom-dimer elastic collision rate is anticipated to reveal \( a_\ast \).

In this Letter we consider the problem of secondary collisions of dimers with atoms and develop a model to calculate their mean number as a function of \( a \). Our central message is that the elastic and the inelastic processes are intimately interrelated and can not be considered independently. According to Eqs. (1) and (2), \( \sigma_i \) and \( \sigma_e \) are both enhanced when \( a = a_\ast \), however variations in \( \sigma_e \) may exceed those of \( \sigma_i \) by orders of magnitude which impacts the experimental observables in a
nontrivial way. Applying this model to the experimental results of Refs. [23], we show that main controversies in the second experimental approach can be resolved when these processes are correctly included. We clarify the Efimov resonance’ positions in $^7$Li and $^{39}$K and support the emerging evidence for significant finite range corrections to the first excited Efimov energy level in both systems [23].

In the following we assume that the number of dimers is always very small compared to the number of trapped atoms and thus we neglect collisions between them. This situation is correct for all the experimental realizations considered here. We start with presenting two possible scenarios (Sc) that a dimer can undergo on its way out of the trap:

Sc1: The dimer collides elastically with $k$ atoms and leaves the trap due to a high enough kinetic energy.

Sc2: After $k$ elastic collisions, the dimer undergoes one inelastic collision, decays to a deeper bound state and leaves the trap without any further scattering events because $\sigma_i$ and $\sigma_e$ are enhanced only for the weakly bound universal dimers.

To evaluate the probabilities of each Sc, we divide the total length $l$ of the dimers’ journey through the atomic cloud into $N$ segments of infinitesimally small length $\delta l$. Then, most generally, the probability to have an elastic/inelastic collision in the length segment $\delta l$ is: $p_{e/i} = \sigma_{e/i} \pi \delta l$, where $\pi$ is the mean density of atoms [28]. Consequently, the probability to have no events in the same segment is: $p_{none} = 1 - p_e - p_i$.

According to Eq. (2), $\sigma_i$ depends on velocity and thus changes at each elastic collision because the dimer transfers a part of its initial kinetic energy to an atom. However, it is instructive to start with the assumption that $\sigma_i$ remains constant independent of energy which makes the model clearer and analytically more tractable. Moreover, this simplification is reasonable in the limit of few collisional events and high initial energies of the dimer. Experimentally it is realized in the region of relatively small scattering lengths and moderate atom densities which corresponds to some of the experimental conditions considered later on.

Energy independent (analytical) model.

Sc1: The probability for $k$ elastic events to occur can be expressed by the choice of $k$ segments out of total $N$, \( \binom{N}{k} \), in which the elastic scattering occurs with the probability $p_e^k$ and multiplying it by the probability $p_{none}^{N-k}$ that in the remaining $(N-k)$ segments no events happen. This probability is given by:

$$p_{k,0} = \binom{N}{k} p_e^k p_{none}^{N-k} \to P(k; \sigma_e \pi l) \exp (-\sigma_i \pi l). \quad (3)$$

where $P(k; x)$ is the Poisson distribution. Note that although an inelastic event is not involved in Sc1, the probability $p_{k,0}$ does depend on $\sigma_i$. This is because the probability of no inelastic event has to be included as a factor.

Sc2: The inelastic event, which happens after $k$ elastic collisions, has to occur at any of the $N-k$ last segments with the probability $p_i$. First, we fix the inelastic event at the $m-th$ place where $m \in [k+1, N]$. Then, the procedure is similar to that of Sc1. The probability for $k$ elastic collisions to occur is expressed by the choice of $k$ segments out of total $m-1$, \( \binom{m-1}{k} \), with the probability $p_e^k$ multiplied by the probability $p_{none}^{m-1-k}$ that in the remaining $m-1-k$ segments no scattering events occur. Thus, the total probability for Sc2 is just the sum over all possible locations of $m$:

$$p_{k,1} = \sum_{m=k+1}^{N} \binom{m-1}{k} p_e^k p_{none}^{m-1-k} p_i \to \int_{\delta l \to 0} d\delta l \frac{(\sigma_e \pi l)^k}{k!} \exp (-\sigma_e + \sigma_i \pi l) \sigma_i \pi l \, dl. \quad (4)$$

The mean number of scattering events in each Sc is then evaluated as the sum of weighted probabilities [29]:

$$\bar{N}_{e,0} = \sum_{k=1}^{\infty} k p_{k,0} = \sigma_e \pi l \exp (-\sigma_i \pi l), \quad (5)$$

$$\bar{N}_{e,i} = \sum_{k=0}^{\infty} (k+1) p_{k,1} = (1 - \exp (-\sigma_i \pi l)) + \frac{\sigma_e}{\sigma_i} (1 - \exp (-\sigma_i \pi l) (1 + \sigma_i \pi l)). \quad (6)$$

Finally, the total mean number of events is then: $N = \bar{N}_{e,0} + \bar{N}_{e,i}$. The central result of the paper is already seen in Eqs. (3,6): both of them include the interplay between elastic and inelastic cross sections which strongly affects the experimental observables.

Energy dependent model. Now we revamp the model taking into account the energy dependence of $\sigma_i$. When
a dimer is created via a three-body recombination, its energy is significantly larger than the kinetic energy of atoms. The mean energy of the dimer is reduced by a factor of $1/\alpha^2 = 5/9$ per elastic collision with a nearly stationary atom [24]. As before, we calculate the probabilities and the mean number of events for each $\text{Sc}$. 

**Sc1:** Let us consider $k$ elastic events. Then the first one can occur only at any of the first $N - (k - 1)$ segments with the probability $p_e$. We fix its location at the segment $j_1$ leaving the remaining $j_1 - 1$ segments to have no scattering events with the probability $(1 - p_e \alpha^0 - p_e) j_1^{-1}$. Next, we fix the second scattering position $j_2$ which then can only occur between segments $j_1 + 1$ and $N - (k - 2)$ with the probability $p_e$. In the remaining $(j_2 - j_1)$ segments no events happen with the probability $(1 - p_e \alpha^1 - p_e) j_2 - j_1^{-1}$ and so on until the location $j_k$ is fixed. Finally, the total probability of $k$ elastic events is evaluated by the sum of all these cases:

$$
p_{k,0} = p_e^k \sum_{j_1=1}^{N-k+1} \sum_{j_2=j_1+1}^{N-k+2} \cdots \sum_{j_k=j_{k-1}+1}^{N} \prod_{m=1}^{k} (1 - p_e \alpha^{m-1} - p_e) j_m - j_{m-1}^{-1} (1 - p_e \alpha^k - p_e) N-k, \text{ where } j_0 = 0. \quad (7)
$$

**Sc2:** Here the probability is constructed almost identically to that of $\text{Sc1}$ but with one variation. Before counting the elastic events we fix the segment where a single inelastic event occurs at the $m$-th position where $j_0 = 0$. In the limit of $\delta l \to 0$, eqs. (7,8) take the form:

$$
p_{k,0} = \left( \frac{\sigma_e}{\sigma_i} \right)^k \sum_{j=0}^{k} \frac{\exp (- (\sigma_e \alpha^j + \sigma_i) \overline{nl})}{\prod_{m=0, m \neq j}^{k} (\alpha^m - \alpha^j)}, \quad (9)
$$

$$
p_{k,1} = \left( \frac{\sigma_e}{\sigma_i} \right)^k \sum_{j=0}^{k} \frac{\exp (- (\sigma_e + \sigma_i) \overline{nl})}{\prod_{m=0, m \neq j}^{k} (\alpha^m - \alpha^j)}, \quad (10)
$$

which reduce to eqs. (7,8) as $\alpha \to 1$. The mean number of events $\overline{N}(a)$ can now be evaluated numerically based on the sum of weighted probabilities (see Eqs. (7,8)). We now turn to apply the model to the recent experimental results which use the second experimental strategy.

**2Li:** Ref. [3] reports $a_s = 608a_0$, which should be corrected to $a_s \sim 410a_0$ due to the shift in position of the Feshbach resonance [3, 22]. However, recent measurement of Machtey et. al. (MSGK) [23], based on the same experimental technique reveals $a_s = 196(4)a_0$ which is away from the Rice result by many times the experimental uncertainty. There is, however, a major difference in the experimental conditions used by the two groups: while MSGK work with a low density thermal gas [3, 23], the Rice experiment is performed on a Bose-Einstein condensate (BEC). According to Ref. [3], the mean density of atoms in the BEC is $\overline{n} \approx 5 \times 10^{12}$ cm$^{-3}$ and half of the geometrical mean of the Thomas-Fermi radius is $l \approx 160 \mu$m. In the MSGK case, for a typical temperature of $T = 1.4$ µK, radial and longitudinal trap frequencies of $\omega_r = 2\pi \times 1.3$ kHz and $\omega_z = 2\pi \times 190$ Hz and $\sim 3.5 \times 10^4$ atoms, the mean atom density is $\overline{n} \approx 1 \times 10^{12}$ cm$^{-3}$. The geometrical mean size of the atomic cloud is $l = 9.5 \mu$m (one standard deviation of the Gaussian distribution). Therefore the column density $\overline{nl}$ in the Rice experiment is larger by a factor of $\sim 80$.

For the second strategy, all $\text{Sc}$’s contribute to the experimental observable and so we show $\overline{N}(a)$ in Fig. 1 for both experiments. We used the energy dependent model with $a_s = 196a_0$. The solid red (dashed-dotted blue) line corresponds to the MSGK (Rice) experimental conditions. In the MSGK case, the maximum in $\overline{N}$ nearly perfectly coincides with the position of $a_s$, which indicates that the experimental observable indeed reveals the position of the Efimov resonance. However, for the Rice experimental parameters, the maximum of $\overline{N}$ is not...
at $a_*$ but rather appears at $\sim 375a_0$, in very good agreement with the reported result [3]. A simple intuitive understanding of this difference can be obtained when the limit of $\sigma_M \ll 1 \gg 1$, roughly matching MSGK (Rice) experimental conditions, is taken in Eqs. (5,6). Then in the MSGK case, $\overline{N} \approx \sigma_M$, which corresponds to the mean number of the elastic collisions and peaks at the maximum of $\sigma_e$, i.e., at $a = a_*$. However, for the Rice case, $\overline{N} \approx 1 + \sigma_e/\sigma_t$, which is maximized at a different position, namely when $s_0 \ln(a/a_*) + 0.97 = \pi/2$ (see Eqs. (11,12), 30). This corresponds to $a/a_* \approx 1.8$ in agreement with the energy dependent model and the Rice result.

Note that the model predicts a larger width of the $\overline{N}(a)$ maximum for the Rice experimental conditions, qualitatively well identified in the experimental results [4,23] and, thus, further strengthening our model. However, quantitative comparison requires inclusion of additional conditions such as reduction of the dimer energy below the trap depth after a certain number of elastic collisions. Here we only associate the maximum in the three-body recombination loss rate with the maximum in the mean number of secondary collisions. In the region of large $a$ not all of them, if any, lead to atom loss, which cuts down the long tail of $\overline{N}(a)$. This is, however, beyond the scope of the present discussion.

$^{39}$K: In Ref. 4 two Efimov resonances at the atom-dimer threshold are reported at $a_{1,2} = 30.4a_0$ and $a_{3,4} = 930a_0$. We shall concentrate our analysis on the second resonance as the first one is deeply inside the nonuniversal region where $a_{1,2} < r_0$ with $r_0 = 64.5a_0$ being the van der Waals length of $^{39}$K. The experiment is also performed in a BEC with $\sigma_0 \approx 6.5 \times 10^{12} \text{ cm}^{-3}$ and half of the geometrical mean of the Thomas-Fermi radius is $l \approx 7 \mu \text{m}$. As before our model predicts a significant shift in the real position of the resonance as compared to the reported one. To agree with the experimental value of $\sim 930a_0$ we need to take $a_*=515a_0$, which reflects the same numerical factor of 1.8 as before. $\overline{N}(a)$ is shown in Fig. 2. In the inset we represent the second peak located at $\sim 23a_0$ and calculated with the slightly different experimental parameters in accordance to Ref. 33 with the same $a_*$. Although it is close to the measured value it might be merely a coincidence. Note also the difference in widths of the two features which again qualitatively agrees with the experiment.

We can now compare the newly extracted positions of the Efimov resonances at the atom-dimer threshold for both species with the values predicted by universal theory (see Table I). In both cases $a_*$ is notably shifted to lower values. MSGK associate this shift with the manifestation of finite range corrections [23,24]. For $^7$Li the shift is smaller than for $^{39}$K. In both cases the Feshbach resonances are of intermediate character between being closed and open channel dominated, but $r_0$ of $^7$Li is about half that of $^{39}$K. It is interesting to note that in Cs the shift is even larger despite the open channel dominated character of the Feshbach resonance (see Table I, 4,17,18). However, the $r_0$ of Cs is the largest among the other species and we can then conclude that the recent experimental results support a scaling of the finite range corrections in $r_0$. Finally, we note that experiments provide growing evidence for a good agreement of the position of the lowest minimum in the three-body recombination spectrum with universal theory despite the fact that it is measured at even lower scattering lengths than $a_*$ [1,4], which still remains a puzzling question.

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[27] We use the correct sign before 0.97 in Eq. (1) as it appears in Ref. [21] as opposed to Ref. [1].
[28] For the sake of simplicity we consider column density as the mean density \( \langle n \rangle \) multiplied by the mean path-length of the dimer through the atom cloud \( l \) instead of the mean column density \( n l \) [26]. The difference between the two is a constant of order 1 and will have negligible effect on the results presented here.
[29] Note that the sum of all probabilities is exactly 1.
[30] This simple condition is only obtained when \( v \propto 1/a \) reflecting the situation when the dimer is produced via three-body recombination with the initial kinetic energy proportional to \( E_d \).