Triatomic continuum resonances for large negative scattering lengths

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We study triatomic systems in the regime of large negative scattering lengths which may be more favorable for the formation of condensed trimers in trapped ultracold monoatomic gases as the competition with the weakly bound dimers is absent. The manipulation of the scattering length can turn an excited weakly bound Efimov trimer into a continuum resonance. Its energy and width are described by universal scaling functions written in terms of the scattering length and the binding energy $B_3$, of the shallowest triatomic molecule. For $a^{-1} < -0.0297 \sqrt{m B_3/\hbar^2}$ the excited Efimov state turns into a continuum resonance.

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It is by now well established that shallow dimers are formed in trapped ultracold or condensed monoatomic gases, as it has been reported for $^{23}$Na \cite{1}, $^{87}$Rb \cite{2}, and $^{85}$Rb \cite{3}. In the experiment in Ref. \cite{3}, an atom-molecule coherence in the Bose-Einstein condensate was also observed. The measured oscillation frequency of the quantum superposition of $^{85}$Rb dimers and atoms in the condensate was in agreement with the shallow $^{85}$Rb\_2 binding energy over a wide range of values near a Feshbach resonance. However, the formation of triatomic molecules has not yet been observed.

Recently, the energy of the shallowest bound triatomic molecule in trapped ultracold and condensed monoatomic gases was predicted using the value of the measured recombination rate into a shallow dimer; the energies ranged from 7.75 mK down to 0.24 nK near a Feshbach resonance \cite{4}. Condensed triatomic molecules coexisting with dimers and atoms near a Feshbach resonance would present an oscillatory dependence of observables on the trimer binding energy \cite{4}. For negative scattering lengths and zero energy, the recombination rate into deep diatomic molecular states shows a resonant peak at values of $a$ for which the trimer Efimov state \cite{6} hits the three-body continuum threshold \cite{6}. If the magnitude of the large negative scattering length is decreased after an Efimov state hits the continuum, it turns into a three-body resonance, as we will show. Therefore, at non zero energies, or temperatures, the resonant peak of the recombination rate would in principle appears when the resonance energy matches the energy of the continuum triatomic system.

Furthermore, the manipulation of the scattering length in monoatomic condensates in the regime of large and negative values offers an interesting possibility. No shallow dimers can exist in this case. Then, the formation of triatomic molecules may be more favorable as the main competitors are absent. If a coherent quantum superposition of atoms and trimers or resonances appears, it will present an oscillatory frequency corresponding only to the shallow three-body bound or resonant state. As we will show, this frequency scales with the scattering length and with a triatomic physical scale in the form of a universal function. Here, the binding energy of the shallowest trimer state is chosen as the three-body physical scale.

In 1970, Efimov predicted that infinitely many weakly bound three-boson states appear when the $s$–wave two-boson scattering lengths, $a$, goes to the limit of $a \to \pm \infty$ \cite{8}. For large scattering lengths, an attractive long-ranged effective interaction binds the three-particle system in a range of about $|a|$ (See also \cite{8}). A new bound state appears for every increase of $|a|$ to $\sim 23|a|$. For positive $a$, at the threshold of the new state, the trimer binding energy is $6.9B_2$ \cite{23} \cite{8} \cite{11} \cite{11} ($B_2$ is the dimer binding energy). For $a < 0$, a new state becomes bound when the trimer has an energy of $\sim 1100B_2$ \cite{23}, where now $B_2$ is the energy of the virtual dimer state. Due to the large size of the system, the threshold conditions for the existence of excited Efimov trimers are universal \cite{23} \cite{12}, i.e., independent of the detailed potential shape, and exhibit a scaling form for large values of $a/r_0$ \cite{23} \cite{4} \cite{11} \cite{11} (the interaction range is $r_0$). The three-body system heals through regions that are outside the potential action, where the wave function is essentially a solution of the free Schrödinger equation, and therefore the properties of the system are defined by few physical scales.

The dimer and trimer binding energies are the only physical scales that survive in the limit of $(a/r_0) \to \pm \infty$ (scaling limit), which essentially relates the Thomas collapse of the trimer state for $r_0 \to 0$ \cite{13} to the Efimov effect $(|a| \to \infty)$ \cite{13}. In the scaling limit, the three-boson observables are functions of the shallowest trimer binding energy (reference three-body energy) and $B_2$. These functions approach universal curves \cite{23} \cite{4}. The collapse of the three-boson system in the limit of a zero-range force makes the trimer energy the three-body scale of the system beyond the two-body energy \cite{13}.

For large scattering lengths, an excited Efimov state turns into a virtual state when $a > 0$ is decreased \cite{14}. The threshold moves faster than the energy of the excited state. Therefore, with the increase of $a > 0$, states pump out from the second sheet of energy to become bound
states. If \( a < 0 \) is decreased in magnitude, the trimer bound states dive into the continuum. It is our aim here to evaluate the scaling properties of the energy and width (for the decay into the three-body continuum) of the resonance born from an Efimov state, when a large \( a < 0 \) is varied.

The \(^4\)He excited trimer state calculated also with realistic models offers a good example of an Efimov state and its universal scaling properties with the shallow dimer and trimer binding energies. These molecules are special due to the large spatial size which spreads out much beyond the range of the potential. The \(^4\)He-\(^\text{He}_3\) root-mean-square distance in \(^4\)He\(^3\) for the ground and excited states are of the order of 5 to 10 Å and of about 50 to 90 Å, respectively. The product of the mean-square interatom distance with the separation energy of one atom from the trimer in units of \( \hbar = m = 1 \) (\( m \) is the atom mass) is about 1 in the ground and the excited states, while the ratio of the binding energies \( B_3^{(0)}/B_3^{(1)} \approx 500 \) \( B_3^{(N)} \) is the binding energy of the \( N^{\text{th}} \) trimer state).

In the present work we calculate the three-boson resonance energy and width for the decay into continuum states for large and negative scattering lengths. In this case it is justifiable to use a Dirac-\( \delta \) potential. We solve subtracted homogeneous equations defined within a renormalization scheme applied to a three-body system interacting with \( s \)-wave zero-range pairwise potentials. We present the results for the energies and widths in the form of a universal scaling function, which gives the trajectory of the three-body energy in the complex plane as a function of the shallow two-body virtual state energy. We show that a resonance becomes an excited trimer Efimov state when the large \( a < 0 \) is decreased. We go beyond Ref. 10, where it was found the dependence of the virtual three-body state energy with \( a > 0 \) born from an Efimov state which entered in the second energy sheet.

One can fix the energy of one three-body bound-state (the three-body physical scale), and the two-body scattering length, and get other observables. All the detailed information about the short-range force, beyond the low-energy two-body observables, is retained in only one three-body physical information in the limit of zero-range interaction. The existence of a three-body scale implies in the low energy universality found in three-body systems, or correlations between three-body observables. In the scaling limit one has

\[
O(E, B_3, B_2)(B_3)^{−n} = \mathcal{F} \left( \sqrt{E/B_3}, \pm \sqrt{B_2/B_3} \right), \tag{1}
\]

where \( O \) is a general observable of the three-body system at an energy \( E \), with dimension of energy to the power \( n \). This equation means that any observable of the system can be represented by a function that depends only on one three- and one two-body scales. The three-body scale is brought by the reference energy \( B_3 \) (binding energy) of the shallowest trimer state. The \( \pm \) sign denotes positive or negative scattering lengths. In the case of the energies of a resonance, of an excited or virtual trimer states, instead of Eq. \( \tag{1} \), the scaling function is written as:

\[
E_3 = B_3 \mathcal{E} \left( \pm \sqrt{B_2/B_3} \right). \tag{2}
\]

(Throughout this paper, we use units such that \( \hbar = m = 1 \), where \( m \) is the mass of the atom.)

After partial wave projection, the \( s \)-wave subtracted integral equation for three identical bosons is given by

\[
\chi(q) = 4\pi \tau(q) \int_0^{\infty} dq' q'^2 \int_1^{\infty} dy \chi(q') \times \frac{1}{E_3 - q^2-q'^2 - q q' y} - \frac{1}{-\mu^2 - q^2-q'^2 - q q' y},
\]

where \( \xi = E_3 - \frac{3}{4} q^2 \), \( \mu \) is the subtraction point and \( \tau \) is given by

\[
\tau^{-1}(\xi) = -2\pi^2 \sqrt{B_2} - 4\pi \xi \int_0^{\infty} dp \frac{dp}{\xi - p^2}, \tag{4}
\]

here \( B_2 \) is the dimer virtual state energy. (For positive values of the real part of \( E_3 \), Eqs. \( \tag{3} \) and \( \tag{4} \) are analytically extended to the second energy sheet, as we discuss below.)

Throughout this work we perform calculations only considering \( a < 0 \) for a virtual dimer state. We use a contour deformation method to calculate the resonance energy and width. The homogeneous equation, is analytically continued to the second sheet of energy, by making \( q' \rightarrow q e^{-\alpha \theta} (q'e^{-\alpha \theta}) \) with \( 0 < \theta < \pi/4 \). For large enough \( \theta \), the solution of Eq. \( \tag{3} \) in the complex energy plane is found for \( \tan(2\theta) > -1m(E_3)/Re(E_3) \).

In the limit of a virtual dimer energy tending to zero an infinite number of Efimov states appears from the solution of Eq. \( \tag{3} \) for negative \( E_3 = -B_3 \). The \( N^{\text{th}} \) Efimov state has binding energy given by \( B_3^{(N)} \) with \( N = 0 \) indicating the ground state obtained from Eq. \( \tag{3} \). When the \( N^{\text{th}} \) Efimov state turns into a resonance its complex energy is denoted by \( E_3^{(N)} \). In figure, it is shown the real part of the complex energies, in units of \( \mu = 1 \), for the first three states obtained by solving numerically Eq. \( \tag{3} \). In the figure, the values of \( |Re(E_3)|^{1/2} \) for the first three resonances are described by the positive part of the plot.

The curves represent \( E_3^{(0)} \) (solid line), \( E_3^{(1)} \) (dashed line) and \( E_3^{(2)} \) (dotted line), i.e., the complex energies of the first three states of Eq. \( \tag{3} \). Note that the subtraction present in Eq. \( \tag{3} \) regularizes it, and the Thomas collapse is avoided. When \( B_2 \) is decreased the resonance turns into a bound state and the negative part of the plot give the energies of the ground \( (B_3^{(1)}) \), first \( (B_3^{(1)}) \) and second \( (B_3^{(2)}) \) bound trimer states. One realizes that the form of the curves are very similar which indicates that the function \( \mathcal{E} \) of Eq. \( \tag{2} \) does not depend on the state, which will be confirmed later on, in the scaling plot of figure.
The values of $\sqrt{B_2}$ in units of $\mu = 1$ at which the Efimov-state becomes unbound are 0.066, 0.0028 and 0.00013 for the ground, first and second states, respectively. The ratios $(0.066/0.0028)^2 \approx (0.0028/0.00013)^2 \sim 500$ are practically independent of the state, in agreement with the scaling limit implied by Eq. (2). It is curious that the real part of the resonance energy tends to zero for $B_2$ large enough, while the width is nonzero.

In figure 2, the results for the imaginary part of the resonance complex energy are shown as a function of $B_2$ in units of $\mu = 1$. The solid, dashed and dotted lines are, respectively, the correspondent imaginary part of $E_3^{(0)}$, $E_3^{(1)}$ and $E_3^{(2)}$. The threshold values of $B_2$ for which the resonant state becomes bound are clearly seen in the figure and the resonance width, $\Gamma_3^{(N)} = 2|Im[E_3^{(N)}]|$, increases with the virtual dimer energy. The results shown in figures 1 and 2 give the complete trajectory of a three-body bound Efimov state when the two-atom interaction with $a < 0$ is changed, as can be done for trapped atoms near a Feshbach resonance. These results extend the findings of Ref. [10]. Now, we can give a complete picture of the route of an Efimov state when $a$ is varied passing through a Feshbach resonance. If one begins with positive $a$ and increases it, a virtual trimer state becomes bound, then crossing a Feshbach resonance and decreasing the magnitude of the large negative value of $a$, the trimer bound state becomes unbound and turns into a resonance. The results for the trimer bound state or resonance energies can be expressed in the form of a universal scaling function, Eq. (2), that depends only on the ratio of the two- and the reference three-body energies. From the calculations given in figures 1 and 2, we construct the scaling plots of figures 3 and 4, respectively. For this purpose, we use the first and second Efimov states (bound or resonant) and we numerically obtain

$$E_3^{(N)} = B_3^{(N-1)} \mathcal{E} \left( -\sqrt{B_2/B_3^{(N-1)}} \right),$$

using $N$ equal to 1 and 2. (In Eq. (3) the states are in fact indexed, which was not explicitly shown in Eq. (2)).
We show the results for the real and imaginary part of the resonance energy in a form of scaling plots in figures 3 and 4, respectively. In these figures the solid line corresponds to $N = 1$ and the dotted line to $N = 2$. In figure 3, the negative values of $|Re(E_3)/B_3|^{1/2}$ give the trimer bound state results, while the positive values come from the resonant state. It is clear that a universal curve for the scaling function $E(\sqrt{B_2/B_3})$ (bound dimer states) obtained previously in [9] and [10] to negative values of the argument and for the trimer resonance region.

In conclusion, we have obtained the trajectory of an Efimov state when the two-atom interaction crosses a Feshbach resonance, in a form of a scaling function. The value of the resonance energy and width depends only on the dimer bound or virtual energy and the shallowest trimer binding energy. The route of an Efimov state when $\alpha$ is varied passing through a Feshbach resonance can be summarized as follows: beginning from a large positive $\alpha$ and increasing it further, a virtual trimer state becomes bound and then after crossing a Feshbach resonance and decreasing the magnitude of the large negative value of $\alpha$, the trimer bound state becomes unbound and turns into a resonance, for $\alpha^{-1} < -0.0297(\sqrt{m B_3/h^2}$, where $B_3$ is the binding energy of the shallowest trimer state. In this respect, the study of trapped Bose-Einstein condensates near a Feshbach resonance can be fruitful not only to reveal the properties of an interacting coherent quantum state under extreme conditions, but could also give new insights in the few-body physics underlying the curious phenomenon of Efimov resonant states.

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\[\text{FIG. 4: Ratio of the imaginary part of } E_3^{(N)} \text{ and } B_3^{(N-1)} \text{ as a function of } B_2/B_3^{(N-1)}. \text{ Curves labelled as in fig.3.}\]

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