Shallow Efimov tetramer as inelastic virtual state and resonant enhancement of the atom-trimer relaxation

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Abstract – We use exact four-bosons scattering equations in the momentum-space framework to study the universal properties of shallow Efimov tetramers and their dependence on the two-boson scattering length. We demonstrate that, in contrast to previous predictions, the shallow tetramer in a particular experimentally unexplored regime is not an unstable bound state but an inelastic virtual state. This leads to a resonant behaviour of the atom-trimer scattering length and thereby to a resonant enhancement of the trimer relaxation in ultracold atom-trimer mixtures.

Introduction. – The system of three identical bosons with short-range interactions in the unitary limit, i.e., when the two-particle scattering length $a$ is infinite and the dimer binding energy $b_d$ vanishes, was first studied by Efimov in 1970 [1]. He predicted an infinite number of zero-spin and positive-parity $(0^+)$ trimer states with geometric spectrum and accumulation point at the three-particle threshold, i.e., $b_n/b_{n-1} \approx 1/515$ for $n \to \infty$, where $b_n$ is the binding energy of the $n$-th Efimov trimer. The reason for this phenomenon, called the Efimov effect, is that a resonant two-particle interaction (large $|a|$) yields an effective long-range attraction in the systems with $N \geq 3$ particles [1]. The resulting few-body bound states (except, maybe, for few lowest of them) are of non-classical nature, i.e., their size is much larger than the range of the two-body interaction with the particles residing predominantly in an interaction-free region. As a consequence, the properties of such few-body systems are universal, i.e., independent of the details of the short-range interaction [2]. A characteristic feature in bosonic systems is a log-periodic $a$-dependence of few-body observables [2].

The experimental evidence for the Efimov physics was observed 35 years later in systems of ultracold atoms where the formation of the Efimov trimers led to a resonant enhancement or suppression of the recombination or relaxation processes [3–5]; large values of $a$ were achieved by variation of the external magnetic field in the vicinity of the Feshbach resonance. First steps in exploring the four-atom Efimov physics via ultracold atom experiments [6,7] have been made recently calling for accurate theoretical studies of the four-body systems with large $|a|$. Although there is no Efimov effect in the four-boson system, the three-boson Efimov effect has an impact on the atom-trimer scattering observables: scattering lengths, phase shifts, elastic and inelastic cross-sections are related to the corresponding trimer binding energies in a universal way [8]. Furthermore, it was predicted in refs. [9,10] that below each Efimov trimer two tetramers with spin/parity $0^+$ should exist. We label them by two integers $(n,k)$, where $n$ refers to the associated trimer and $k=1\,(2)$ for a more deeply (shallowly) bound tetramer. A schematic representation of the four-boson energy levels as functions of the two-boson scattering length $a$ is given in fig. 1. For a better visualization only two families of multimers are shown preserving only qualitative relations between them. The two lowest tetramers with $n=0$ are true bound states; all others lie above the lowest atom-trimer threshold (ATT) and therefore are unstable bound states (UBS) with finite width and lifetime that could not be calculated in refs. [9,10] using standard bound-state techniques. The widths of unstable tetramers in the unitary limit were determined using proper four-bosons scattering calculations [8]. Trimers and the associated tetramers exist also at large finite $|a|$ as predicted in refs. [9–11] and confirmed in experiments with ultracold atoms [6,7]. At specific large negative values of $a$ where the tetramers emerge at the four-free-atom threshold they lead to a resonant enhancement of the four-atom recombination process [6,10]. At

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scattering calculations in the momentum-space frame-
Efimov trimers. Our proof relies on rigorous four-boson
that would lead to a resonant enhancement of the trimer
(IVS); this scenario is schematically shown in fig. 1 for
the \( \text{d}+\text{d} \) and \( \text{d}+\text{a}+\text{a} \) thresholds.
However, in the present work we prove that this is not
true for the shallow tetramer in a particular experi-
mental not yet explored interval of positive \( a \) values
where it crosses the ATT and becomes an inelastic virtual state
(IVS); this scenario is schematically shown in fig. 1 for
the \( n \)-th (higher) multimer family. As a consequence,
the atom-trimer scattering length shows a resonant behaviour
that would lead to a resonant enhancement of the trimer
relaxation in an ultracold mixture of atoms and excited
Efimov trimers. Our proof relies on rigorous four-boson
scattering calculations in the momentum-space frame-
work. With some technical modifications [8] the method
follows the one of refs. [12–14] that has already been
applied successfully to the description of all four-nucleon
elastic and transfer reactions at low energies.

**Atom-trimer scattering.** – We use exact four-
particle scattering equations that were introduced by
Alt, Grassberger, and Sandhas (AGS) [15,16]; they are
equivalent to the Faddeev-Yakubovsky formulation [17] of
the four-body problem. The AGS equations are integral
equations for the four-particle transition operators \( \mathcal{U}_{\alpha\beta} \);
in the case of identical particles they are given in refs. [8,12].
In the present work we are interested in the energy
regime where only the atom-trimer channels are open and
the AGS equations can formally be reduced to a single
integral equation

\[
\mathcal{U}_{11} = P_{34}(G_0 t G_0)^{-1} + U_2(1 + P_{34}) + P_{34} U_1 G_0 t G_0 \mathcal{U}_{11} + U_2 G_0 t G_0 (1 + P_{34}) U_1 G_0 t G_0 \mathcal{U}_{11}.
\]

(1)

The two-boson potential \( v \) enters the AGS equations
via the two-body transition matrix \( t = v + r G_0 t \) and the
symmetrized \( 1 + 3 (\alpha = 1) \) and \( 2 + 2 (\alpha = 2) \) subsystem
transition operators \( U_\alpha = P_\alpha G_0^{-1} + P_\alpha t G_0 U_\alpha \). All transition
operators acquire their dependence on the available
energy \( E \) via the free resolvent \( G_0 = (E + i 0 - H_0)^{-1} \)
with \( H_0 \) being the free Hamiltonian. The permutation
operators \( P_{ij} \) of particles \( (ij) \) and their combinations
\( P_1 = P_{12} P_{23} + P_{13} P_{23} \) and \( P_2 = P_{13} P_{24} \) ensure the desired
symmetry of the four-boson system. Thus, in a simplified
interpretation the integral equation (1) for the transition
operators \( \mathcal{U}_{\alpha\beta} \) can be viewed as a sum of the multiple
scattering series with all possible interactions in the four-
particle system up to infinite order. Introducing the transi-
tion operators \( t \) and \( U_\alpha \) at intermediate steps ensures that eq. (1) is mathematically well behaved and can be
solved numerically. Amplitudes for elastic and inelastic
atom-trimer scattering \( (f|T|g) = 3[\langle \phi | t G_0 \mathcal{U}_{11} | \phi \rangle ] \) are given by the
on-shell matrix elements of the transition operator (1)
between the Faddeev components \( |\phi_\alpha^n\rangle \) of the cor-
responding initial/final atom-trimer states.

We use the momentum-space partial-wave framework
[12,18] to solve the AGS equation (1) numerically.
The practical solution can be simplified significantly [8]
by using an \( S \)-wave separable two-boson potential
\( v = |g\rangle \lambda \langle g| \). To prove that the universal properties of the
four-boson system are independent of the short-range
interaction details, as in ref. [8] we performed calculations
with two choices of the momentum-space form factor

\[
\langle p|g \rangle = [1 + c_2 (p/\Lambda)^2] e^{- (p/\Lambda)^2},
\]

(2)
namely, with \( c_2 = 0 \) and \( c_2 = -0.17 \), that yield very different
off-shell behaviour of the resulting potential whose
strength \( \lambda \) is adjusted to reproduce the given value of
\( a \). Further technical details on our four-boson scattering
calculations can be found in refs. [8,12,18]. In the case of
the true bound state \( (n = 0) \) we solve Faddeev-
Yakubovsky equations [17] in the version of ref. [19].
Extraction of tetramer properties. – For the classification of the states we follow ref. [20]. A true four-boson bound state corresponds to a simple pole of the transition operators \( U_{\beta\alpha} \) in the physical sheet of the complex energy plane. In contrast, an UBS corresponds to the pole of \( U_{\beta\alpha} \) in one of the unphysical sheets adjacent to the physical sheet and therefore may lead to a resonance-like behaviour of the scattering observables. Let \( E_{n,k} = -B_{n,k} - i\Gamma_{n,k}/2 \) be the complex energy of the \((n,k)\)-th unstable tetramer, where \(-B_{n,k}\) is the position relative to the four-free-particle threshold and \(\Gamma_{n,k}\) is the width of the state. The energy dependence of \( U_{\beta\alpha} \) in the physical region close to \(E \approx -B_{n,k}\) can be given by
\[
U_{\beta\alpha} = \sum_{m=1}^{\infty} U_{\beta\alpha}^{(n,k,m)}(E - E_{n,k})^m, \tag{3}
\]
where only the first few terms yield non-negligible contributions. This allows to extract the values of \(-B_{n,k}\) and \(\Gamma_{n,k}\) from the calculated atom-trimer scattering amplitudes or observables. Since the shallow tetramer \((k = 2)\) is very close to the ATT, \(B_{n,2}\) and \(\Gamma_{n,2}\) alternatively can be obtained from the atom-trimer scattering length \(A_n\) and effective range \(r_n\) [20,21]. The elastic S-wave scattering amplitude as a function of the on-shell momentum \(k_o\) is given by
\[
T^S_n(k_o) = -[\pi\mu_1(k_o \cot \delta^S_n - i k_o)]^{-1}, \tag{4}
\]
where \(\mu_1\) is the reduced atom-trimer mass. The complex phase shift \(\delta^S_n\) at small momenta \(k_o\) can be expanded as \(k_o \cot \delta^S_n = -1/A_n + r_n k_o^2/2 + O(k_o^4)\). Thus, the approximate value of the complex binding momentum \(K_n\), corresponding to the pole of the amplitude, can be obtained from the equation
\[
r_n K_n^2/2 - i K_n - 1/A_n = 0. \tag{5}
\]
The root \(K_n\) that is closer to the threshold, i.e., smaller in the absolute value, relates to the tetramer position and width as
\[
-B_{n,2} - i\Gamma_{n,2}/2 = -b_n + K_n^2/2\mu_1. \tag{6}
\]
For the UBS \(\Re K_n < 0\), \(\Im K_n > 0\), and \(\Gamma_{n,2} > 0\) [20], while for the true bound state \(\Re K_n = 0\), \(\Im K_n > 0\), and \(\Gamma_{n,2} = 0\). The method based on the effective range expansion (5), although slightly less precise than the one of eq. (3), has an advantage of being applicable also for the IVS in the S-wave that does not lead to a resonant behaviour of the scattering observables around \(E \approx -B_{n,2}\). IVS corresponds to the pole of the amplitude (4) with \(\Re K_n < 0\), \(\Im K_n < 0\) and \(\Gamma_{n,2} < 0\) in the sheet of the complex energy plane more distant from the physical one [20]. A particular case of the S-wave IVS when there is no lower threshold is a virtual (unbound) state with \(\Re K_n = 0\), \(\Im K_n < 0\), and \(\Gamma_{n,2} = 0\). In contrast, the near-threshold unbound states with non-zero angular momentum have different properties and are called the Breit-Wigner resonances [20]; a universal four-boson system does not support such states [8].

Table 1: Positions and widths of shallow tetramers in the unitary limit.

| \(n\) | \((B_{n,2}/b_n - 1) \times 10^4\) | \((\Gamma_{n,2}/2b_n) \times 10^4\) |
|-----|-----------------|-----------------|
| 0   | 41.9            |                 |
| 1   | 1.06            | 3.82            |
| 2   | 2.17            | 2.14            |
| 3   | 2.27            | 2.36            |
| 4   | 2.28            | 2.38            |
| 5   | 2.28            | 2.38            |

Results. – We present our results in a universal form such that they do not depend on the values of the particle mass or the cutoff parameter \(\Lambda\). The binding energy of the \(n\)-th excited trimer \(b_n\) and the associated length scale \(L_n = (2\mu_1 b_n)^{-1/2}\) (in our convention \(\hbar = 1\)) will often be used to build dimensionless ratios, in particular, \(B_{n,k}/b_n\) and \(\Gamma_{n,2}/2b_n\) that are expected to be universal numbers. To achieve the universal limit we have to consider reactions with highly excited Efimov trimers that are of large size such that the short-range details become negligible. This is a serious challenge in the numerical calculations since the binding energies of the involved trimers differ by many orders of magnitude and therefore the momentum grids of correspondingly broad range must be used. In this work we consider reactions with up to six open atom-trimer channels and show that this is fully sufficient to obtain universal results. The predictions for the positions and widths of shallow tetramers in the unitary limit are collected in table 1. The agreement between the two methods based on eqs. (3) and (5), (6) is better than 0.5% for \(n > 0\). For highly excited tetramers, \(n \geq 3\), the results approach the universal values for both choices of the form factor (2). In contrast, large deviations can be seen for lower tetramers where the finite-range corrections become important.

In the following we do not demonstrate explicitly the convergence of our results, however, they are checked to be independent of \(c_2\) and \(n\) for \(n \geq 3\) with good accuracy. The energy dependence of the elastic and inelastic cross-sections for the atom scattering from the highest available trimer \((m = n - 1)\) in the vicinity of the \((n,2)\)-th tetramer, i.e., at \(E \approx -B_{n,2}\), is shown in fig. 2. Since the tetramer is UBS in the unitary limit, both cross-sections exhibit a resonant behaviour. However, they deviate slightly from the exact Breit-Wigner shape due to non-negligible contributions of non-resonant (background) terms corresponding to \(m \geq 0\) in eq. (3).

We consider next the shallow tetramer in the interval of positive two-boson scattering length \(a\) between the unitary limit \(a \rightarrow \infty\) and the intersection of the
atom-trimer and dimer-dimer thresholds $a = a_{n,2}^{dd}$ where $b_n = 2b_d$. The evolution of the binding momentum $K_n$ with $a$ is shown in fig. 3; we use the dimensionless ratio $a_{n,1}^{dd}/a$. While $\text{Re} K_n L_n$ remains negative and varies very slowly, $\text{Im} K_n$ changes two times such that $\text{Im} K_n < 0$ for $a \in (a_n^{v,1}, a_n^{v,2})$ and $\text{Im} K_n > 0$ elsewhere. These critical values are

$$a_{n,1}^{dd}/a_n^{v,1} \approx 0.0729, \quad (7)$$

$$a_{n,2}^{dd}/a_n^{v,2} \approx 0.99836. \quad (8)$$

Thus, the shallow tetramer is an IVS for $a \in (a_n^{v,2}, a_n^{v,1})$ but an UBS elsewhere. The evolution of the tetramer properties is displayed in fig. 4. Solid parts of the curves correspond to UBS, while the dash-dotted ones to IVS. Starting at the unitary limit and increasing $a_{n,1}^{dd}/a$ the tetramer UBS moves towards the ATT while its width decreases. $\Gamma_{n,2}$ passes through zero at $a = a_n^{v,1}$ where the tetramer becomes an IVS. By further increase of $a_{n,1}^{dd}/a$ the tetramer IVS moves away from the ATT but turns around at $a \approx 0.65 a_{n,2}^{dd}$ and at $a = a_n^{v,2}$ where $\Gamma_{n,2} = 0$ becomes an UBS again. Note that in very narrow intervals close to $a = a_n^{v,j}$ the tetramer (in both UBS and IVS cases) is slightly above the ATT, i.e., $B_{n,2} < b_n$. This is evident from eq. (6) with $\text{Im} K_n = 0$ and can be seen in the top inset of fig. 4.

We do not show the evolution of the tetramer properties for $a_{n,2}^{dd}/a > 1$ where our preliminary results are in qualitative agreement with ref. [11]: the (n,2)-th tetramer is an UBS with $B_{n,2} > 2b_d$ and finite width until it intersects the dimer-dimer threshold at $a = a_{n,2}^{dd} < a_n^{dd}$.

The tetramer IVS resides on a sheet of the complex energy plane that is not adjacent to the physical one. It therefore affects the atom-trimer scattering observables in a completely different way as compared to UBS: the cross-sections around $E \approx -B_{n,2}$ do not exhibit the resonance-like behaviour seen in fig. 2 but may have a cusp at the ATT ($E = -b_n$) if the IVS pole is very close to it. This is illustrated in fig. 5 where the atom-trimer inelastic ($n - 1 \rightarrow n - 2$) cross-section is shown for two cases. At $a_n^{dd}/a \approx 0.0820$ the tetramer IVS with $(b_n - B_{n,2} - i\Gamma_{n,2}/2)/b_n \approx (-1.93 + i2.44) \times 10^{-5}$ is very close to the ATT while it is more distant at $a_n^{dd}/a \approx 0.1682$ with $(b_n - B_{n,2} - i\Gamma_{n,2}/2)/b_n \approx (-2.04 + i0.22) \times 10^{-3}$. As a consequence, the cusp at the ATT is clearly pronounced in the first case but hardly visible in the second. We emphasize that such behaviour is characteristic to S-waves only as the unbound states with non-zero angular momentum close to the threshold are the Breit-Wigner resonances.

The resonant peak for the UBS and the cusp for the IVS can be understood given the pole factor in the amplitude (4) that is common for all elastic and inelastic
channels. For simplicity we consider the case $|k_n|, |K_n| \ll 1/|r_n|$, i.e., when the available scattering energy and the UBS/IVS poles are very close to the $n$-th ATT. Then the energy dependence of the cross-sections (up to channel-dependent factors) is approximately given by
\begin{align*}
\sigma & \sim |K_n - k_n|^{-2} \\
&= \frac{1}{b_n} \left[ (\text{Re} K_n)^2 + (\text{Im} K_n - \sqrt{2\mu_1 |b_n + E|})^2 \right]^{-1} \\
&\quad \times \Theta(-b_n - E) \\
&\quad + \left[ (\text{Im} K_n)^2 + (\text{Re} K_n - \sqrt{2\mu_1 |b_n + E|})^2 \right]^{-1} \\
&\quad \times \Theta(b_n + E).
\end{align*}
(9)

Here $\Theta(x)$ is the Heaviside step function with values 1 and 0 for $x > 0$ and $x < 0$, respectively. Given $\text{Re} K_n < 0$ it is easy to see that a resonant peak only takes place for $\text{Im} K_n > 0$ at $E < -b_n$, i.e., for the UBS below the $n$-th ATT. In contrast, for $\text{Im} K_n < 0$ the cross-sections reach maximum value at $E = -b_n$ that corresponds to the IVS cusp at the ATT.

The two intersections of the ATT with the tetramer at $a = a_n^{n-1}$ lead to a resonant behaviour of the atom-trimer scattering length $A_n$ as demonstrated in fig. 6. The positive (negative) peaks of $\text{Re} A_n$ correspond to tetramer UBS (IVS) with $B_{n,2} = b_n$ while $A_n = 0$ and negative peaks of $\text{Im} A_n$ correspond to $\Gamma_{n,2} = 0$. No experiments have been performed so far in this regime but the UBS-IVS conversion could be observed by creating an ultracold mixture of atoms and excited Efimov trimers in a trap and measuring the trimer relaxation as a function of $a$. According to ref. [8], the zero-temperature limit of the trimer relaxation rate constant is $\beta_n^n = (4\pi/\mu_1) \text{Im} A_n$. Thus, a resonant enhancement of the trimer relaxation process takes place at $a = a_n^{n-1}$ that should be visible at sufficiently low temperature, possibly partially smeared out due to the thermal averaging. On the other hand, in the real experiments deviations of $\alpha_n^{n-1}$ from the universal values (7), (8) can be expected due to finite-range effects and/or presence of deeply bound dimers.

**Comparison with previous works.** – Finally, we would like to discuss the differences between our results and those of ref. [10]. At the unitary limit ref. [10] predicts $(B_{n,2}/b_n - 1) \approx 0.01$ to be more than 4 times larger than our universal result 0.00228 presented in table 1. The results of ref. [10] were obtained using the hyperspherical framework in coordinate space and neglecting the finite width of the tetramer. In addition, for the $(n, 2)$-th tetramer they were limited to $n \leq 1 \ (n = 0 \ \text{with strong repulsive three-body force})$ and by far have not reached the level of convergence comparable to ours. For example, our five best-converged results for $(B_{n,2}/b_n - 1)$ are 0.00228 within 0.5% accuracy while the three best-converged results of ref. [10] are 0.006, 0.03, and 0.001. On the other hand, our $n \leq 1$ results given in table 1 that receive non-negligible finite-range corrections show deviations from the universal limit comparable to those of ref. [10]. In the presence of finite-range effects we found that increasing $(B_{n,2}/b_n - 1)$ at $a \to \infty$ shifts $\alpha_n^{dd}/\alpha_n^{1}$ to larger values thereby shrinking the IVS region. Thus, when the tetramer at $a \to \infty$ is sufficiently far from the ATT, it may even remain UBS (true bound state if $n = 0$) in the whole regime $a_n^{dd}/a_n^{1} \leq 1$. Such a situation takes place also for the non-universal $(0, 2)$-th tetramer of the present work. However, by choosing $c_2 > 1$ in eq. (2) we obtain the $(0, 2)$-th tetramer that mimics the universal behaviour, i.e., makes transition into a virtual state. This proves again that low $n$ states are sensitive to the short-range details and may explain why the tetramer IVS could not be predicted in ref. [10].

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Fig. 5: (Colour on-line) Cross-section for the inelastic atom-trimer $(m = (n - 1)$-th state) scattering leading to the $(n - 1)$-th trimer state in the vicinity of the $n$-th ATT. Two cases differing in the complex energy of the $(n, 2)$-th tetramer IVS are shown.

Fig. 6: (Colour on-line) Atom-trimer scattering length $A_n$ as a function of the two-boson scattering length $a$. 

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In the case of the deeper \((k = 1)\) tetramer there is a reasonable agreement between our value \(B_{n,1}/b_n = 4.611(1)\) obtained in ref. [8] and the one of ref. [10], 4.58, the latter having about 1% uncertainty.

**Summary.** – We studied the universal properties of the shallow Efimov tetramer. Since this four-boson state lies in the continuum, we solved exact AGS four-particle equations for the atom-trimer scattering. The momentum-space partial-wave framework was employed. The universal limit of the results is achieved accurately in reactions with highly excited trimers (up to 5th excited state). Positions and widths of shallow tetramers were calculated as functions of the two-boson scattering length. We demonstrated that, in contrast to previous predictions by other authors [6,10] obtained with some limitations, the universal shallow tetramer intersects the ATT twice and in a regime between these intersections \(a \in (a_{1}^{0}, a_{1}^{1})\) it is an inelastic virtual state. The tetramer is an unstable bound state outside the above interval of \(a\), in qualitative agreement with the results of refs. [10,11]. We studied how the atom-trimer scattering observables are affected by these changes of the tetramer properties. In particular, we demonstrated a resonant behaviour of the atom-trimer scattering length that could be observed as a resonant enhancement of the trimer relaxation in the ultracold mixture of atoms and excited trimers.

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