Probing the Efimov discrete scaling in atom-molecule collision

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The discrete Efimov scaling behavior, well-known in the low-energy spectrum of three-body bound systems for large scattering lengths (unitary limit), is identified in the energy dependence of atom-molecule elastic cross-section in mass imbalanced systems. That happens in the collision of a heavy atom with mass $m_H$ with a weakly-bound dimer formed by the heavy atom and a lighter one with mass $m_L \ll m_H$. Approaching the heavy-light unitary limit the $s$-wave elastic cross-section $\sigma$ will present a sequence of zeros/minima at collision energies following closely the Efimov geometrical law. Our results open a new perspective to detect the discrete scaling behavior from low-energy scattering data, which is timely in view of the ongoing experiments with ultra-cold binary mixtures having strong mass asymmetries, such as Lithium and Caesium or Lithium and Ytterbium.

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The Efimov effect [1] refers to a discrete scaling symmetry, which emerges in the quantum three-body system at the unitary limit (when the two-body scattering lengths diverge). The optimal condition to observe this discrete scaling symmetry in cold atomic laboratories is now found for heteronuclear three-atom systems with large mass asymmetry and large interspecies scattering lengths. In the Efimov (unitary) limit, the shallow three-body levels are geometrically spaced, namely the energy ratio for three identical bosons is $\exp (2\pi/s_0)$, where $s_0$ is a universal constant, which depends only on the mass ratio and not on the details of the interaction. The energy ratio for three identical bosons is $\exp (2\pi/s_0) \approx 515$, decreasing for the case of two heavy particles and light one. When $m_L/m_H = 0.01$, for example, the value of this energy ratio goes to $\exp (2\pi/s_0) = 4.698$ [2].

The Efimov geometric scaling factor has been measured in a cold-atom experiment with mass-imbalanced mixtures of Caesium ($^{133}$Cs) and Lithium ($^6$Li) gases by different groups [3 [4]. The ratio between the positions of two successive peaks in the three-body recombination rate, obtained by varying the large negative scattering lengths ($a_{HL}$), was found in close agreement with the theory. Complementary to this finding, a fingerprint of the Efimov scaling can be found in the $s$-wave ultra-cold atom-molecule cross-section by varying the incident momentum energy $k$ instead of the scattering lengths. Natural, but not yet evidenced experimentally or theoretically. What we expect is beyond the trimer crossing the corresponding continuum, which creates the resonant enhancement of the inelastic collisions of Caesium atoms with Caesium dimers, as observed by Knoop et al. [5].

Furthermore, there is an evident strong interest in ultra-cold heteronuclear atom-molecule collisions by experimental groups [6][8]. Trap setups with ultra-cold degenerated mixtures of alkali-metal-rare-earth molecules with strong mass-imbalanced systems as Ytterbium and Lithium ($^{174,173}$Yb–$^6$Li) have also been reported in Refs. [9][10]. We should mention that on the theory side [11], reactions at ultra-cold temperatures with three-body systems such as $^6$Li + $^{174}$Yb$^6$Li were also investigated. Therefore, the present possibilities to manipulate collisions with Lithium(Li)-Caesium(Cs) [12] and Ytterbium-Lithium [9][10], as well as the molecules of LiCs and LiYb in ultra-cold experimental setups [13], open new opportunities to probe the discrete Efimov scaling with the large mass asymmetries. This can be achieved by using low-energy collisions of a heavy atom, such as Caesium or Ytterbium, in the weakly-bound molecules as LiCs or LiYb, with $m_L/m_H = 0.045$ and 0.034, respectively.

Going back in time, what was known theoretically from the pioneer works for the tri-nucleon systems [14][17], was the existence of a pole in the spin doublet $s$-wave neutron-deuteron $k \cot \delta_n$, which was associated with a virtual state in the tri-nucleon system. Furthermore, such pole is also present in the neutron-$^{19}$C scattering [18][20], with a corresponding pronounced minimum of the $s$-wave elastic cross-section. If the Efimov geometrical factor decreases, which is possible with atomic systems, our expectation for $H - (HL)$ collision is that several minima in the $s$-wave elastic cross-sections or poles in the $k \cot \delta_0$ would emerge from the characteristic log-periodic behavior carried by the wave-function in the region where the Efimov long-range potential is dominant and being reflected in a geometrical law for the spacing of the energies of cross-section minima corresponding to these poles.

In this letter, we show that the $s$-wave elastic cross-section for the $H - (HL)$ collision has minima at geometrically spaced incident energies, for large values of $a_{HL}$ near the unitary limit. We compute the $s$-wave phase-
shift using the three-body Faddeev formalism with zero- and short-ranged interactions, as well as by considering the Born-Oppenheimer (BO) approximation [21]. The real part of the $s$–wave phase shift ($\delta_0$) shows zeros and $k \cot \delta_0$ has a sequence of poles at colliding energies which tend to follow the Efimov geometric scaling.

The BO approximation applied to the $H$–($HL$) system provides a universal long-range attractive $1/R^2$ effective potential ($R$ is the relative $H$ – $H$ distance) close to the unitary limit, which acts up to distances $\sim |a_{HL}|$, as shown in Ref. [21]. At short distances, the BO potential brings the details of the finite range pairwise potentials expressed as a boundary condition at $R_0 << |a_{HL}|$ that determines the reference energy $B_3$. The eigenstates of the $H$ – $H$ effective hamiltonian has the characteristic log-periodic solutions for $R_0 \lesssim R \lesssim |a_{HL}|$, which leads to the geometrical ratio between the binding energies and also to the log-periodic properties of $s$–wave scattering observables. We extend the procedure used in [21] to the scattering region, considering the collision of a heavy particle in the weakly-bound subsystem of the remaining ones. This approach was used to interpret the results obtained with the renormalized zero-range model [22], as well as with the Gaussian finite-range interactions.

To simplify our study, we assume no interaction between the heavy particles and that the heavy-light molecule ($HL$) has a weakly-bound energy $B_2$. When $B_2 \to 0$ the three-body Efimov levels are given by $B_3^{(n)}/B_3^{(0)} \sim (2n+3/2)$, where $B_3^{(0)} = E^{(0)}$ is the ground state binding energy of the models we use in our approaches to obtain the $s$–wave cross-sections.

We start our analysis by introducing a scaling function for the dimensionless product of the $s$–wave cross-section and energy. With $B_3$ and $B_2$ as the scales of the $HHHL$ system and $E$ the colliding energy at the three-body center-of-mass, this function can be written as

$$\sigma B_3 = S(E/B_3, B_2/B_3, A),$$

where $A \equiv m_L/m_H$. This is strictly valid at the zero-range limit where $B_2 = 1/(2\mu_{HL} a_{HL}^2)$, with $\mu_{HL}$ being the reduced mass for the $HL$ subsystem. Here and in the next, the units are such that $\hbar = 1$ and $m_L = 1$.

The scaling function for $A = 0.01$ is shown in Fig. 1 for the renormalized zero-range model [19] and for the Gaussian potential model calculated with the method developed in Ref. [23], which was extended to energies above the breakup threshold in Ref. [24]. The Gaussian potential with $r_0$ being the interaction range is given by

$$V(r) = V_0 e^{-r^2/r_0^2},$$

where we have used $a_{HL}/r_0 = 50$ and $B_2/B_3 = 0.0012$.

Noticeable, are the minima of the $s$–wave cross-section, where $k \cot \delta_0$ has poles. We observe that positions of such poles tend to obey the Efimov law for $(k a_{HL})^{-1} \to 0$. Between the zeros, there is a sequence of maxima for the cross-section where the phase-shift passes through $(2n + 1)\pi/2$, as seen in Fig. 1. It is tempting to associate the maxima obtained for the cross-section with resonances; however, a calculation by using the complex scaling method [25] for the Gaussian potential, excludes that. These results are also corroborating the conclusions of [18] for the neutron$^{19}$C system, where no resonance is found when changing the neutron separation energy in $^{19}$C.

FIG. 1: The $s$–wave cross-section is shown as a function of the energy-collision $E$, for zero-ranged (ZR) (blue-solid lines) and finite-ranged Gaussian (G) (red-dashed lines) potentials, for fixed mass ratio $A = 0.01$ and given two-body energies ($B_2^R$ is a factor smaller than $B_2^ZR$ to keep both results close to the unitary limit). Results are in units of $B_3$.

FIG. 2: The zero-ranged results for $\sigma$ (in arbitrary units) as functions of $E/B_3$ are given in eight panels, with mass-ratios $A$ as shown inside the frames. In all the panels the two-body energies are fixed such that $B_2/B_3 = 0.01$ (solid-blue lines), 0.03 (dot-dashed-red lines) and 0.05 (dashed-black lines).
By considering different mass-ratios $A$, varying from 0.01 till 0.08, our results for the cross-sections $\sigma$ (in arbitrary units) are presented in Fig. 2 for three fixed weakly-bound two-body energies $B_2/B_3 = 0.01, 0.03$ and 0.05. In the given eight panels we are presenting $\sigma$ as a function of $E/B_3$. From these panels, one can notice a sequence of zeros (or minima) which can appear for $\sigma$ as we decrease the mass ratio, by considering a fixed interval for the collision energy, such that $E/B_3 < 1$. Within this interval, when the mass-imbalance is less pronounced, e.g. for $A = 0.08$, we can verify the occurrence of only one zero for $\sigma$ within the given energy range, whereas for $A = 0.01$ it is possible to verify the existence of up to six zeros. Therefore, the large mass asymmetry ($A << 1$) is more favorable for the occurrence of several zeros/minima in $\sigma$. In order to verify the emergence of a possible scaling factor between the position of successive zeros/minima in the $s$-wave cross-section, in correspondence with the Efimov bound-state spectrum, one should be able to extrapolate the two-body bound-state energies to the unitary limit (i.e., to $B_2 = 0$).

Corresponding to the upper-left panel of Fig. 2 when $B_2/B_3 = 0.01$ and $A=0.01$, we also have Fig. 1 where $E/B_3$ was extended up to 1, which showed that it is possible to observe another minimum in $\sigma$ for a collision energies much larger than the breakup threshold. As we can observe, in this case, the value of the minimum in $\sigma$ is affected by absorption, an expected behavior for energies above the break-up threshold. Therefore, $\sigma$ is not being reduced to zero, but have just a minimum, with the value of the energy $E$ also being deviated slightly to the right as $B_2$ is increased in Fig. 2. The ratio between the energy position of the successive zeros is about the Efimov geometric factor as one can easily check (we will explore such feature in a systematic way later on), and as one could expect it should be distorted by absorption effects, but far away from the breakup threshold.

It is noticeable to find minima of the cross-section for $E >> B_2$ and quite deeply immersed in the three-body continuum, where still the $s$-wave inelasticity parameter is very close to unity. This astonishing suppression of the breakup channel for energies of about two orders of magnitude the two-body binding is a manifestation of the long-range coherence between the heavy and light particles and the associated diluteness of the target, making it hard to destroy the system, where the light particle binds with any one of the heavy particles and the dynamics is dominated only by the exchange of the light particle between the two heavy ones. The $HL$ molecule becomes invisible to the collision of the heavy one. Semi-classically, the possibility of the destructive interference between the direct trajectory and the one from the exchange process gives the zeros of the phase-shift.

The fact that the breakup channel is suppressed is closely related to the non-existence of resonances. In the adiabatic hyper-spherical representation of this mass im-balanced three-body system, it happens that the coupling between the lowest adiabatic channel, which asymptotically goes to the atom-dimer channel, with the breakup channels is weak (see e.g. 24). In addition, asymptotically the lowest adiabatic hyper-spherical potential is attractive, while the breakup channels have a barrier around $\rho \sim |a_{HL}|$. Indeed, in the case of Borromean systems, such barrier makes the Efimov turn to a continuum resonance when $|a_{HL}|$ is decreased 26.

We summarize the findings presented in figures 1 and 2 as: (i) the number of minima of the $s$-wave cross-section decreases significantly when $A$ and the Efimov ratio increases, and (ii) more minima are seen when $B_2/B_3$ decreases. Particularly, with respect to the second point, we found that the zeros of the cross-section are coming out from the scattering threshold and the $H-(HL)$ scattering length passes through zero values when $B_2/B_3$ is driven towards the more favorable condition for the Efimov effect. That is the counterpart of the unitary limit where virtual states come from the second energy sheet to become bound states. In the continuum region, zeros and maxima of the cross-section come one by one as $B_2/B_3 \to 0$, which completes the final picture of the Efimov limit including the scattering region.

The manifestation of the Efimov discrete scaling in the atom-molecule collision can be systematically studied by the ratio between the energies of successive zeros/minima as a function of the mass ratio and a dimensionless ratio between two and three-body scales as follows. For that, a scaling function is introduced relating the energies of two adjacent minima obtained for the cross-section $\sigma$. Within a convention that $E_{n+1} > E_n$, this function is given by

$$E_{n+1}/E_n = R \left(1/(E_{n+1}^{1/2} a_{HL}), A\right),$$

where $R(0,A) = e^{2\pi/s}$ is the unitary limit.

The universal scaling function (3) is shown in Fig. 3 for the extreme case $A = 0.01$, calculated with the Gaussian and zero range potentials. The curious behavior of the scaling function around the Efimov ratio, indicated by the horizontal dashed line, by departing from the unitary limit decreases, has a minimum and then increases, namely the zeros more distant. Note that we have plotted results for the renormalized zero-range potential with different $B_2$ and scattering lengths, ranging from 0.001 $\leq B_2/B_3 \leq 0.05$. With the Gaussian potentials, within our numerical accuracy, we were able to approach more closely the Efimov limit. However, when going to smaller values of $1/(E_{n+1}^{1/2} a_{HL})$, we stand above the breakup threshold and evidently the coupling to the breakup channel affects the ratio, as the figure suggests.

The curious behavior of the ratio, namely when starting from smaller to larger collision energies it is first above the Efimov geometrical factor then it decreases and increases again towards it, can be qualitatively understood by considering the collision within the BO ap-
The wave number is related to the collision energy. For larger collisions, we can obtain exact solutions by considering a mass-imbalanced system. As shown by [21], the Born-Oppenheimer (B-O) results (connected by a dashed-blue line in Fig. 3) come from the Coulomb-like correction. As shown by using different values for the position of the hard wall at short distances, there are no significative range corrections. Therefore, we note that the first two terms of the BO potential are quite relevant to provide a qualitative description of the scaling function. This approximation is working surprisingly well in particular for large values of $E_{n+1}^{1/2} a_{HL}$, when approaching the Efimov limit monotonically from above when decreasing $1/(E_{n+1}^{1/2} a_{HL})$. The minimum observed in the BO results (dashed-blue curve in Fig. 3) comes from the Coulomb-like correction. As shown by considering a mass-imbalanced system $A \ll 1$ with no interaction between the two-heavy particles and with the heavy-light sub-system bound with energy close to zero (near unitary limit). This is shown by considering a mass-imbalanced system $A \ll 1$ with no interaction between the two-heavy particles and with the heavy-light sub-system bound with energy close to zero (near unitary limit).

Practical implications. The poles of $k \cot \delta_0$, which correspond to the zeros/minima of the $s$-wave cross section, are directly connected with the Efimov spectrum of the heavy-heavy-light (HHL) system near the unitary limit. This is shown by considering a mass-imbalanced system $A \ll 1$ with no interaction between the two-heavy particles and with the heavy-light sub-system bound with energy close to zero (near unitary limit).

By considering the mass ratio between Li and Yb, $A = 0.034$, the cross-section for the Yb + LiYb collision can in principle present a couple of zeros. We can imagine a situation where $a_{Yb-Li}$ is adjusted at some large position, with the colliding energy being varied slowly. In this case, $\sigma$ should present minima at some specific colliding energies, whose positions are approximately geometrically spaced. In conclusion, we suggest as the best approximation in this case we consider the leading term $1/R^2$ for the interaction. In the present extension to scattering energies, we can also verify analytical solutions for the Eq. (4), which are given by Whittaker functions. This eigenvalue equation has no lower bound energy, namely, the Thomas collapse is present, which requires a short-range scale imposed by a boundary condition at $R = R_0 \ll a_{HL}$. In what follows, a hard wall will be used, and from the boundary condition at $R = a_{HL}$ the phase-shift is finally obtained. In this way, the log-periodicity of the $s$-wave phase-shift with the energy is only deformed by the presence of the $1/R$ contribution.

As a result, if the BO potential in Eq. (4) is given only by the Efimov term, the ratio (not plotted in Fig. 3) would approach the Efimov limit monotonically from above when decreasing $1/(E_{n+1}^{1/2} a_{HL})$. The minimum observed in the BO results (dashed-blue curve in Fig. 3) comes from the Efimov limit. As shown by considering a mass-imbalanced system $A \ll 1$ with no interaction between the two-heavy particles and with the heavy-light sub-system bound with energy close to zero (near unitary limit).

The effective two-body equation for the collision of the heavy-heavy-light ($HHL$) system near the unitary limit.

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