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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 σ will present a sequence of zeros/minima at collision energies following closely the Efimov geometrical law. Our results, obtained with Faddeev calculations and supplemented by a Born-Oppenheimer analysis, 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.

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 ratio between the binding energies of the n and $n + 1$ levels is given by $B_3^{(n)}/B_3^{(n+1)} = \exp(2\pi/s_0)$, 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 a 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 discrete scaling has been studied with mass-imbalanced cold-atom mixtures with Caesium and Lithium, in experimental and theoretical works [3–5]. The ratio between the positions of two successive peaks in the three-body recombination rate, measured by varying the large negative scattering lengths (a_{HL}), was found in close agreement with the theory [3]. Complementary to this finding, what should be the fingerprint of the Efimov scaling in the s -wave ultra-cold atom-molecule cross-section, if one varies the incident momentum energy k instead of the scattering lengths? What to expect? Is it beyond the trimer crossing the corresponding continuum, which creates the resonant enhancement of the inelastic collisions of Caesium atoms with Caesium dimers as observed [6], or not?

Furthermore, there is an evident strong interest in ultra-cold heteronuclear atom-molecule collisions by experimental groups [7–10]. Trap setups with ultra-cold degenerated mixtures of alkali-metal-rare-earth molecules

with strong mass-imbalanced systems as Ytterbium and Lithium ($^{174,173}\text{Yb}-^6\text{Li}$) have also been reported in Refs. [11, 12]. We should mention that on the theory side [13], reactions at ultra-cold temperatures with three-body systems such as $^6\text{Li} + ^{174}\text{Yb}^6\text{Li}$ were also investigated. Therefore, the present possibilities to manipulate collisions with Lithium(Li)-Caesium(Cs) [14] and Ytterbium-Lithium [11, 12], as well as the molecules of LiCs and LiYb in ultra-cold experimental setups [15], open new opportunities to probe the discrete Efimov scaling with 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. We should add that in the present context it may be quite relevant to extend the experimental technique used in Ref. [16] (for mononuclear systems) to observe Efimov trimers close to the atom-dimer threshold to strongly mass imbalanced atomic mixtures.

Going back in time, what was known theoretically from the pioneer works for the tri-nucleon systems [17–20], was the existence of a pole in the spin doublet s -wave neutron-deuteron $k \cot \delta_0$, which was associated with a virtual state in the tri-nucleon system. Furthermore, such pole is also present in the neutron- ^{19}C scattering [21–23], with a corresponding pronounced minimum of the s -wave elastic cross-section. As it is well-known that the geometrical scaling factor can decrease considerably for systems with two heavy (H) and one light (L) particles, by extending the above investigation, our aim was to reply some relevant questions related to manifestation of Efimov physics at the scattering region, which can well be explored with the present experimental facilities. By considering collision of two condensates, the energy dependence of the three-body recombination rate was investigated in Ref. [24], with log-periodic oscilla-

tions been pointed out in the case of Cs-Cs-Li. Within our present approach, we are further investigating this property, by considering elastic scattering observables as cross-sections and scattering lengths, going to extreme limiting mass-imbalanced cases of H-(HL) atom-dimer collisions, where the dimer is weakly bound and the collision energy is also close to the threshold. By going to such limits, the expectation is to explore the singular behavior of $k \cot \delta$, which is associated to zeros of the corresponding cross-section due to the log-periodic oscillations of such observable.

As shown in the present work, considering the extreme mass imbalanced case for the $H - (HL)$ collision, a sequence of minima in the s -wave elastic cross-sections (poles in the $k \cot \delta_0$) was found, for large values of a_{HL} near the unitary limit. Further, this sequence is found to follow the same log-periodic behavior corresponding to the Efimov bound-state spectrum. This has not being pointed out before (as far we know) in the vast literature on the Efimov phenomena, because one should go to extreme HL mass ratios in order to confirm that the emergent scaling factor corresponds directly to the same bound-state three-body spectrum. As we are pointing out, one cannot verify more than one minima in the cross section if the mass ratio m_L/m_H is of the order or larger than 0.1, with a second minima emerging when this ratio is about 0.08. Therefore, our present results are quite consistent with the up to three log-periodic oscillations obtained for the $^{133}\text{Cs} + ^{133}\text{Cs} + ^7\text{Li}$ three-body recombination [24], as in such a case we have $m_L/m_H \sim 0.053$. This behavior can better be verified from the systematic study we have performed, where the emergent scaling factor obtained for scattering observables is confirmed to be close to the same one obtained in the corresponding Efimov spectrum. Physically, we can understand that from the characteristic log-periodic behavior carried out by the wave-function when the Efimov long-range potential is dominant, being reflected in the colliding energy ratios where we have the minima for the cross-section.

We should remind that zeros or minima in scattering cross sections, actually can be considered as manifestations of the Ramsauer-Townsend effect [25]. This kind of effect was discovered by the occurrence of minima in the scattering cross-section of electrons from atoms of a noble gas at some small value of the electron energy [26]. On this regard, see Ref. [27], as well as reported experimental observations in Refs. [28, 29]. However, a quite different physical system is being explored in our approach, where the zeros (minima) in the cross-section of an atom-dimer system are associated to the log-periodic sequence of the corresponding three-body bound-state spectrum.

For the relation between the three-body bound-state spectrum with the minima in the s -wave elastic scattering cross section, another simple physical picture could emerge as related to the Levinson's theorem [30], when considering an effective two-body system. This theorem,

derived for the nonrelativistic quantum scattering theory, established a relation between the total number of bound states n with the energy-dependent scattering phase-shift $\delta(E)$ (at a given partial wave), such that for the s -wave we have $\delta_0(0) - \delta_0(\infty) = (n + 1/2)\pi$. Together with the fact that $\delta_0(\infty) = 0$, it is tempting to associate the number of zeros in the corresponding elastic cross-section to the number of bound states for the given effective potential of the atom-dimer scattering.

In our approach, we compute the s -wave phase-shifts by using the three-body Faddeev formalism with zero- and short-ranged interactions, as well as by considering the Born-Oppenheimer (BO) approximation [31]. The real part of the s -wave phase shift (δ_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. [31]. At short distances, the BO potential brings the details of the finite range pairwise potentials expressed as a boundary condition at $R_0 \ll |a_{HL}|$ 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 [31] to the scattering region, considering the collision of a heavy particle in the weakly-bound subsystem of the remaining ones. This approach (see also [32]) was used to interpret the results obtained with Faddeev calculations for the renormalized zero-range model [33], as well as for 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 $B_2 \rightarrow 0$ the three-body Efimov levels are given by $B_3^{(n)} \rightarrow e^{-(2n\pi/s_0)} B_3$, where $B_3 \equiv B_3^{(0)}$ 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 HHL system and E the colliding energy at the three-body center-of-mass, this function can be written as

$$\sigma B_3 = \mathcal{S}(E/B_3, B_2/B_3, A), \quad (1)$$

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 μ_{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 [22] and for the

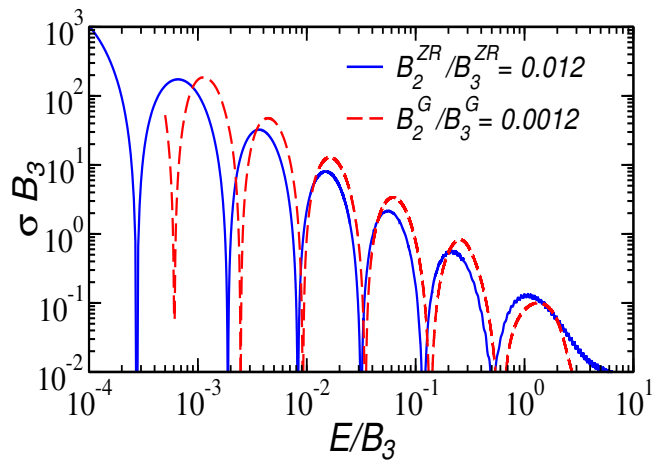


FIG. 1: The s -wave cross-section is shown as a function of the energy-collision E , for zero-ranged (ZR) (blue-solid lines) and finite-ranged Gaussian (G) (red-dashed lines) potentials, for fixed mass ratio $A = 0.01$ and given two-body energies (B_2^G is a factor smaller than B_2^{ZR} to keep both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

Gaussian potential model calculated with the method developed in Ref. [34], which was extended to energies above the breakup threshold in Ref. [35]. The Gaussian potential with r_0 being the interaction range is given by

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

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, at energy positions where $k \cot \delta_0$ has poles. We observe that positions of such poles tend to obey the Efimov law for $(ka_{HL})^{-1} \rightarrow 0$. 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 [36] for the Gaussian potential, excludes that. These results are also corroborating the conclusions of [21, 23] for the neutron- ^{19}C system, where no resonance is found when changing the neutron separation energy in ^{19}C .

By considering different mass-ratios, with $A = m_L/m_H$ varying from 0.01 till 0.08, our results for the cross-sections σ (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 σ as a function of E/B_3 . From these panels, one can notice a sequence of zeros (or minima) appearing for σ as we decrease the mass ratio A , for a fixed interval of the colliding energy, such that $E/B_3 < 1$. Within the intervals for A shown in Fig. 2, by examining the case with $B_2/B_3 = 0.01$, one should noticed that, for the less-pronounced mass-imbalance case, $A = 0.08$,

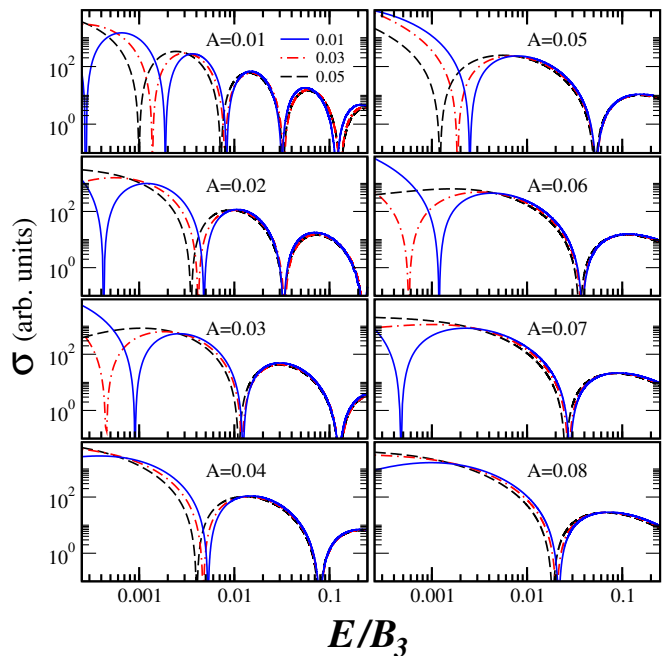


FIG. 2: The zero-ranged results for σ (in arbitrary units) as functions of E/B_3 are given in eight panels, with mass-ratios $A \equiv m_L/m_H$ as shown inside the frames. In all the panels the two-body energies are fixed such that $B_2/B_3 = 0.01$ (solid-blue lines), 0.03 (dot-dashed-red lines) and 0.05 (dashed-black lines).

we have the occurrence of only one zero for σ within the given energy range, whereas for $A = 0.01$ it is possible to verify the existence of up to five zeros. (In more detail, this number goes to seven, when considering the energy interval shown in Fig. 1). Also, as indicated by the curvature behavior, we noticed that a second minimum should appear in $A \approx 0.08$ for an energy much close to zero, as well as a third minimum in case of A close to 0.04 .

Therefore, the large mass asymmetry ($A \ll 1$) is more favorable for the occurrence of several zeros/minima in σ . 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 σ for a collision energies much larger than the breakup threshold. As we can observe, in this case, the value of the minimum in σ is affected by absorption, an expected behavior for energies above the break-up threshold. Therefore, σ 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 $E \gg B_2$ 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. Semiclassically, 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 imbalanced 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. [35]). 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 [37].

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 $B_2/B_3 \rightarrow 0$, 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 σ . Within

a convention that $E_{n+1} > E_n$, this function is given by

$$E_{n+1}/E_n = \mathcal{R} \left(1/(E_{n+1}^{1/2} a_{HL}), A \right), \quad (3)$$

where $\mathcal{R}(0, A) = e^{2\pi/s_0}$ is the unitary limit.

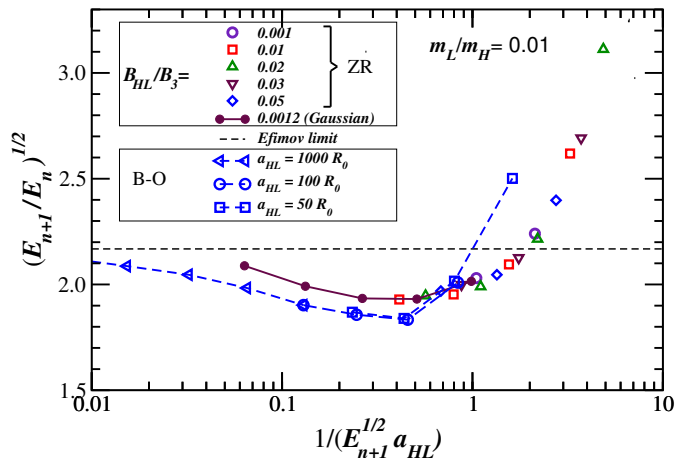


FIG. 3: Ratio between the energy positions of the successive zeros $(n+1, n)$ of the cross-section σ plotted versus $1/(E_{n+1}^{1/2} a_{HL})$ for mass-ratio $A = 0.01$. The results obtained from Faddeev calculations with renormalized zero-range (ZR) model, for given two-body energies, are indicated inside the frame. The straight dashed line indicates the Efimov limit for $A = 0.01$. The solid-line with dots shows the results obtained from Faddeev calculations with the Gaussian potential (2). The Born-Oppenheimer (B-O) results (connected by a dashed-blue line) are shown for three boundary conditions.

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 approximation. In this case, the effective $H-H$ long-range potential is supplemented by a boundary condition at some short distance R , with the continuity of the logarithmic derivative of the wave-function $u(R)$ imposed

at $R = a_{HL}$. In our illustration, the elastic scattering S -matrix is found from the boundary condition at $R = a_{HL}$. To make our point clear, we assume no two-body $H-H$ potential; and, we expand the effective BO potential [31], where the leading-order term is $\sim 1/R^2$, and we also consider the effect of the next order term, implying in the inclusion of a Coulomb-like $1/R$ interaction. Therefore, as one can extract from the expansion of the potential presented in [31], we have the following effective two-body equation for the collision of the heavy particle H with relative momentum k with respect to the HL dimer:

$$\left[-\frac{d^2}{dR^2} - \frac{s_0^2 + \frac{1}{4}}{R^2} g\left(\frac{R}{a_{HL}}\right) \right] u(R) = k^2 u(R), \quad (4)$$

where $g(y) \equiv 1 + 2y + 2.07y^2$, such that the leading term in the interaction, $-(s_0^2 + 1/4)/R^2$, provides the Efimov limit. The wave number is related to the collision energy by $k = \sqrt{2\mu_{H,HL}E}$, where $\mu_{H,HL} \equiv m_H(1+A)/(2+A)$. The expansion for $g(y)$ is found by requiring an approximation of the BO potential valid not only for $R \ll a_{HL}$, but also for $R/a_{HL} \sim 1$. With this approximation, the Coulomb-like correction $-2(s_0^2 + 1/4)/(a_{HL}R)$ is added to the Efimov term, as well as a constant which is negligible for larger scattering lengths. As shown by [31], in case of negative-energies we can obtain exact solutions for the Eq. (4), given by Bessel functions in 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 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, considering that in this limit the coupling to the breakup channel (which is not being taken into account) is expected to be relevant. For smaller values of $E_{n+1}^{1/2} a_{HL}$ the expansion

of the BO potential starts to breakdown due to its poor efficacy when decreasing the collision energy, with the wavelength being of the order of the scattering length.

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). In view of the consistency of the results obtained in the present work with a picture based on the Levinson's theorem, which relates the number of zeros in the s -wave scattering length with the number of bound states, for a given effective two-body potential, an interesting perspective to be worked out is to further explore analytically this theorem in the context of atom-dimer systems. Other aspects of interest to be more deeply investigated, which could impact in the accuracy of the predicted minima, are related to higher partial-wave contributions to the cross-sections, as well as possible effects due to existence of deeply molecular bound-states.

With respect to actual experimental realizations in ultracold atomic gases, to observe effects of the zeros (or minima) in the cross-sections a possibility is to study the two-condensate collision, as following a suggestion given in Ref. [24]. In the present case, the colliding condensate is formed by the single heavy particle, whereas the target is the heavy-light dimer condensate.

As we have pointed out, the observation of a sequence of zeros in the cross section can only be verified for quite large mass ratios, such that the main focus for recent ultracold atomic experiments are binary condensed systems combining atomic species such as Li, Yb or Rb. 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 positive values, with the colliding energy being varied slowly. In this case, σ should present minima at some specific colliding energies, whose positions are approximately geometrically spaced. In conclusion, we suggest as the best possible situation to probe the Efimov discrete scaling in the continuum to consider the atom-molecule scattering with large mass asymmetry through cold collisions, which are now feasible [14]. The challenge in these experiments would be to control the scattering length towards the large values and then observe the cross-section minima at geometrically spaced colliding energies.

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