Efimov states in asymmetric systems

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Abstract. – The conditions for occurrence of the Efimov effect is briefly described using hyperspherical coordinates. The strength of the effective hyperradial $\rho^{-2}$ potential appearing for two or three large scattering lengths is computed and discussed as function of two independent mass ratios of the three constituent particles. The effect is by far most pronounced for asymmetric systems with three very different masses. One Efimov state may by chance appear in nuclei. Many states could be present for systems with one electron and two neutral atoms or molecules. Estimates of the number of states and their sizes and energies are given.

Introduction. – More than 30 years ago Efimov realized that a three-body system could have a large number of bound states when two or three of the two-body subsystems simultaneously have (virtual or bound) s-states sufficiently close to zero energy \[1\]. This effect has been discussed in a number of subsequent publications \[2,3,4,5\]. External fields can be used to tune the effective two-body interaction aiming at approaching the zero energy condition \[6,7,8\].

The picture describing the Efimov effect is that one particle effectively has large-distance interaction simultaneously with both the other two particles building up a coherent wave function fully exploiting the interactions. When only one scattering length is large the effect does not occur since the effective large-distance interactions only involve two of the particles while the third can avoid contributing by being far away without interacting.

The atomic helium trimer system is usually considered to be the most promising candidate for naturally occurring Efimov states \[9,10\]. It has so far escaped direct experimental detection \[11\]. Other systems may however be much better candidates possibly with many Efimov states. The purpose of this letter is to pin-point both the class of best suited candidates and the crucial properties optimizing the occurrence conditions.

Basic properties. – The hyperspheric adiabatic expansion combined with the Faddeev decomposition of the wave function has proven very efficient for investigations of weakly bound and spatially extended three-body systems \[3\]. Efimov states can then be computed and without loss of generality even with the simplifying restriction that the potentials act only on s-waves which are the only contributors at the asymptotic large distances \[4\].

The hyperradius $\rho$ defined by

$$m_\rho^2 \equiv \frac{1}{M} \sum_{i<k} m_i m_k (r_i - r_k)^2,$$

(1)
where \( m_i \) is the mass, \( \mathbf{r}_i \) the coordinate of particle \( i \in \{1, 2, 3\} \) and \( m \) is an arbitrary normalization mass. Thus \( \rho \) is a measure of the average size of the system. After solving the eigenvalue problem for the remaining (angular) coordinates the method provides a hyperradial equation with mass \( m \) and an effective potential \( U(\rho) \), which for intermediate distances of \( \rho \) has the simple form

\[
U(\rho) = -\frac{\hbar^2}{2m} \left( \frac{\xi^2 + 1/4}{\rho^2} \right), \quad R_e \leq \rho \leq a_{av},
\]

(2)

where \( \xi^2 \) is a positive or negative constant depending on the interactions and the average effective range \( R_e \) and average scattering length \( a_{av} \) will be defined later. This potential has the generic form for the Efimov states.

At distances smaller or comparable with the interaction ranges \( U(\rho) \) is more complicated and generally without divergence as \( \rho^{-2} \). This small distance region provides the scale for the energies of the possible Efimov states and is otherwise completely unimportant for spatially extended states. At distances larger than the scattering lengths the potential has the form [4]

\[
U(\rho) = -\frac{\hbar^2}{2mp^2} \frac{16}{\pi} \sum_{i<k} \sqrt{\mu_{ik} a_{ik}} \rho \sqrt{m} \equiv \frac{\hbar^2}{2mp^2} \frac{48}{\pi \sqrt{2}} a_{av} \rho,
\]

(3)

where the reduced mass is \( \mu_{ik} = m_i m_k / (m_i + m_k) \), the s-wave scattering length is \( a_{ik} \) for system \( ik \), and the average scattering length is defined as

\[
a_{av} \sqrt{m} \equiv \frac{\sqrt{2}}{3} \sum_{i<k} \sqrt{\mu_{ik} a_{ik}}.
\]

(4)

When all three particles are identical the expression for \( a_{av} \) reduces to the common value of \( a_{ik} \).

The Efimov states are found at intermediate distances as solutions corresponding to the potential \( U(\rho) \) in eq.(2). The wave function is \( K_{\xi}(\kappa \rho) \), where \( K \) is the modified Bessel function with an imaginary index and the binding energy is \( B = \hbar^2 \kappa^2 / (2m) \). By expansion of \( K \) for small and large values of \( \rho \) the radial wave function \( f_n \) is

\[
f_n \propto \sqrt{\rho} \sin \left( \xi \ln \left( \frac{\rho}{R_e} \right) \right) \quad \text{for} \quad \kappa \rho < 1,
\]

(5)

\[
f_n \propto \exp(-\kappa \rho) \quad \text{for} \quad \kappa \rho > 1,
\]

(6)

where the zero point for the first oscillation in \( \rho \) is assumed to be \( R_e \), which in analogy to eq.(4) roughly could be defined as

\[
R_e \sqrt{m} \equiv \frac{\sqrt{2}}{3} \sum_{i<k} \sqrt{\mu_{ik} R_{ik}}.
\]

(7)

reducing to the common two-body effective radius \( R_{ik} \) when all particles are identical. The form of the wave function in eq.(5) is easily found by confirming that \( f_n(\rho) \propto \sqrt{\rho} \rho^{(\pm \xi)} \) is a solution to the Schrödinger equation with the potential in eq.(2) valid at intermediate distances where the energy term can be neglected. The exponential decrease at large distance occurs for all bound states for distances \( \kappa \rho \) larger than 1, where the effective radial potential falls off at least as fast as \( \rho^{-3} \).
Thus \( f_n \) oscillates periodically as \( \sin(\xi \ln \rho) \). The number of Efimov states \( N_E \) corresponds then to the number of oscillations between the average interaction range \( R_e \) and \( 48a_{av}/(\pi \sqrt{2}) \approx 11a_{av}, \) i.e.

\[
N_E \approx \frac{\xi}{\pi} \ln \left( \frac{11a_{av}}{R_{eff}} \right) . 
\]  

(8)

The energies and sizes of these states are related by

\[
\frac{E_n}{E_{n+1}} = \frac{(\rho^2)_{n+1}}{(\rho^2)_n} = e^{2\pi n/\xi}, 
\]  

(9)

which reveals the exponential increase of sizes towards infinity and decrease of energies towards zero, respectively. This behavior originates from the generic \( 1/\rho^2 \) potential in eq. (2).

**Strength of the potential.** The all decisive parameter \( \xi \) must now be determined for systems where Efimov states may occur. At least two of the three scattering lengths must be large. The formal analysis in [4] leads to transcendental equations for \( \xi \). For identical bosons we obtain the usual Efimov equation rewritten with real quantities, i.e.

\[
8 \sinh(\xi \pi/6) = \xi \sqrt{3} \cosh(\xi \pi/2) 
\]  

(10)

with the solution \( \xi \approx 1.0063 \). The result is independent of the mass of the particles.

For non-identical bosons, still when all three scattering lengths are large, we find instead

\[
\left( \frac{\xi \cosh(\xi \pi/2)}{2F} \right)^3 - \frac{\xi \cosh(\xi \pi/2)}{2F} \left( f_1^2 + f_2^2 + f_3^2 \right) F^2 = 2 = 0 , 
\]  

(11)

where \( F = (f_1 f_2 f_3)^{1/3} \) and

\[
f_k = \frac{\sinh(\xi (\pi/2 - \varphi_k))}{\sin(2\varphi_k)} , 
\]  

(12)

\[
\varphi_k \equiv \arctan \left( \frac{\sqrt{m_k (m_1 + m_2 + m_3)}}{m_i m_j} \right) . 
\]  

(13)

In general the solution \( \xi \) then depends on two ratios of masses, e.g. \( m_2/m_1 \) and \( m_3/m_1 \). When all masses are equal (\( \varphi_k = \pi/3, f_i = F = 2 \sinh(\xi \pi/6)/\sqrt{3} \)) eq. (11) reduces to three simpler equations

\[
\frac{\xi \sqrt{3} \cosh(\xi \pi/2)}{4 \sinh(\xi \pi/6)} = \left\{ \begin{array}{c} 2 \\ \pm 1 \end{array} \right\} , 
\]  

(14)

where 2 on the right hand side produce eq. (10) while \( \xi = 0 \) is the only real solution for \( \pm 1 \).

When only the two scattering lengths \( a_{jk} \) and \( a_{ik} \) (not \( a_{ij} \)) are large the Efimov equation for \( \xi \) becomes

\[
\xi \cosh(\xi \pi/2) \sin(2\varphi_k) = 2 \sinh(\xi (\pi/2 - \varphi_k)) , 
\]  

(15)

where the solution now only depends on the angle \( \varphi_k \) varying between 0 and \( \pi/2 \). Still \( \varphi_k \) in eq. (13) in turn depends on the above two mass ratios.

The conclusion is that the strength of the potential has to be found by solving eq. (11) when all scattering lengths are large and eq. (15) when only two scattering lengths are large. The Efimov effect does not occur when only one scattering length is large. Eq. (10) is the limit of eq. (11) when all masses are equal. The parameters are the three angles \( \varphi_k \), which through eq. (13) are functions of two independent mass ratios.
We show in fig. 1 the 3d plot of $\xi$ as function of these independent parameters. The smallest values slightly above 1 are found in a valley passing the symmetric point of three equal masses and extending towards one very large mass and one moderate mass ratio around unity. This case with two light masses and one heavy mass corresponds to the smallest $\xi$ where the Efimov effect is least pronounced.

On the other hand large values of $\xi$ extending to infinity are obtained for two heavy and one light mass. This is seen in fig. 1 when both coordinates are large ($m_2 \ll m_1 \ll m_3$, $m_2 \sim m_3$), and along both axes when the other coordinate is very small ($m_2 \ll m_1 \ll m_3$ and $m_3 \ll m_1 \ll m_2$). Thus moderate values of $\xi$ arise for symmetric systems while exceedingly large strengths are possible for asymmetric systems. In all cases the assumption is that all three two-body subsystems simultaneously have an $s$-state close to the threshold of binding. This is most likely for a symmetric system of identical bosons where only one interaction is involved.

For non-identical particles two tuned subsystems is the least demanding to exhibit the Efimov effect. If furthermore two of the clusters are identical particles only one independent requirement of an $s$-state close to zero is left. In this case where only two subsystems contribute (two large scattering lengths) the strength $\xi$ is found from eq. 15 as function of the angle $\varphi_k$ corresponding to the subsystem with the small third scattering length. The result displayed in fig. 2 show the divergence as $1/\varphi_k$ for $\varphi_k \rightarrow 0$ and the linear convergence to zero as $4(\pi/2 - \varphi_k)/(\pi\sqrt{3})$ for $\varphi_k \rightarrow \pi/2$. When all masses are equal $\varphi_k = \pi/3$ and eq. 15 reduces to eq. 10 with the left hand side divided by two. The resulting solution $\xi = 0.499$ is roughly two times smaller than 1.0063 obtained when all three subsystems contribute.

The angle $\varphi_k$ is a function of two mass ratios. When $m_k$ is much smaller than both the other masses $\varphi_k$ approaches zero and $\xi$ is very large. When $m_k$ is much larger than at least one of the other masses $\varphi_k$ approaches $\pi/2$ and $\xi$ is very small. Thus extremely large $\xi$ is only possible for two contributing subsystems when the particle $k$ related to both these subsystems has a comparatively small mass. The Efimov effect occurs in all cases but is only pronounced for large $\xi$.

In fig. 3 we show solutions to eq. 11 corresponding to three very large scattering lengths for a series of different mass ratios. The striking features are as described in connection with the 3d plot in fig. 1.
Fig. 2 – The strength parameter $\xi$ obtained from eq. (15) as function of the angle $\varphi_k$.

with fig. 3 that $\xi$ is very small for one heavy and two light particles, relatively small for similar masses and huge for one light and two heavy particles. Comparing figs. 2 and 3 we conclude that the mass ratios determine the order of magnitude of the strength $\xi$ whereas the contribution from the third subsystem is marginal.

Possible examples. – Large values of $\xi$ favor occurrence of (many) Efimov states, see eq. (8). It should be emphasized that at least two scattering lengths must be sufficiently large to allow the effect in the first place. An interaction in one two-body subsystem of longer range than the generic $\rho^{-2}$ potential prohibits occurrence. For nuclei this leaves only two neutrons combined with a charged ordinary nucleus \[5\]. There might be a chance to produce one Efimov state but the second would not appear as illustrated by $^{11}$Li ($^{9}$Li+n+n) where $\xi \approx 0.074$ according to eq. (9) corresponds to an increase of the radius by a factor of $3 \cdot 10^{18}$.

In atomic and molecular physics the possibilities are much better. For identical particles $\xi$ is mass independent. The molecular prototype is the atomic helium trimer $^{4}$He$_3$ with an excited Efimov state of binding energy 0.18 $\mu$eV and radius about 50 Å. Correspondingly $\xi \approx 1.0063$ and the radius increase between neighboring Efimov states is a factor of 22. Equal masses and only two contributing subsystems change this factor to about 542 implying that the radius of the second Efimov state then would exceed 1 $\mu$m. By far the most favorable case is one light and two heavy identical particles. One small step in this direction is the asymmetric helium trimer $^{3}$He$^{4}$He$_2$ with one bound (pronounced halo) state of binding around 1 $\mu$eV and radius about 13 Å \[9, 12\].

Substituting one helium atom by an alkali atom reduces the two-body binding energy \[13\] and produce spatially extended three-body systems like $^{7}$Li$^{4}$He$^{3}$He and $^{23}$Na$^{3}$He$_2$ with $\xi \approx 0.255, 0.085$ \[12\]. In $^{6}$Li$^{4}$He$^{3}$He we anticipate an Efimov state with a size larger than the 50 Å expected in $^{4}$He$_3$. Other combinations with one helium and two alkali atoms are easily conjectured from the results in \[13\]. For example $^{4}$He$^{23}$Na$_2$ and $^{3}$He$^{133}$Cs$_2$ give $\xi \approx 1.22, 2.75$ implying that the second Efimov state only is 13, 3.1 times larger than the first.

Another type of combinations are even more favorable. One charge is allowed, since the destructive Coulomb-like long-range interaction still is not present. One electron and
two identical atoms (or molecules) then maximize the $\xi$-value. It is sufficient with a large scattering length for the two electron-atom (molecule) systems and if also the atom-atom (molecule-molecule) contributes the effect could be even larger. Then $\xi$ could be as large as 100 (electron-atom (or molecule) mass ratio $\leq 10^{-5}$) and the radius increase per state from eq. (9) could be less than 5%. The number of Efimov states within practical reach would increase dramatically while they still remain relatively stable [14].

However, this scenario requires a large electron-atom scattering length or equivalently an $s$-state energy very close to zero. Since the scattering length $a$ at least should be larger than $5-10\ \text{Å}$ the electron binding $\frac{\hbar^2}{2ma^2}$ should at least be smaller than 0.1 eV. This is an established fact for the bound negative ions Ca, Ti and Sr and furthermore a number of atoms (He, Be, N, Ne, Mg, Ar, Mn, Zn, Kr, Cd, Xe, Hg, Rn) cannot bind an electron although the distance from the threshold in general is unknown [15].

The three-body system should now consist of the electron plus a pair of the above atoms chosen as close as possible to the threshold of $s$-state binding. Here $^4\text{He}+e+^4\text{He}$ is the obvious combination but unbound with respect to $^4\text{He}_2$ leaving the possible Efimov states as excited states with a large decay probability. Substituting $^6\text{Li}$ for one of the helium atoms reduces the atomic binding and $^4\text{He}+e+^6\text{Li}$ is then a promising candidate. Other examples like Mg+$e$+Mg, Mg+$e$+Ne, Mg+$e$+Ar, Mg+$e$+Kr and Mg+$e$+Xe were investigated in [16]. Adding an electron to the weakly bound two-body systems Ar-Ar, Cd-Cd, Cl-Xe, Cs-Hg, He-Hg, Hg-Hg [17], also present Efimov candidates, but pairs like H-H, Ca-Ca, Li-Li, Na-Na could be more suitable.

Instead of atoms we could try to use molecules with very small electron binding, combining them pairwise and adding an electron, see [17,18] for candidates. If this should create Efimov states the internal structure of the molecules is not allowed to change within the pair. This might be possible but requires a separate investigation.

The Efimov conditions of two zero energy subsystems can be fulfilled without lower lying bound two-body states, but it is much more probable to encounter systems where the state

![Graph](image-url)
of zero energy is an excited two-body state. The resulting Efimov states are clearly more unstable and their structure more difficult to study directly. However, signals should show up in scattering experiments \cite{10, 19, 20}. The properties of the Efimov states are in any case determined by the scattering lengths and the size of $\xi$ as discussed above.

**Conclusion. –** The strength of the attraction in the effective hyperradial $\rho^{-2}$ potential for three particles is for large scattering lengths determined by simple equations depending only on two independent mass ratios. We survey this mass dependence and provide information about favorable mass combinations. The larger the strength the more pronounced is the Efimov effect. The density of Efimov states increases with the square root of the strength which for existing mass combinations can vary by several orders of magnitude. Two contributing subsystems for one light and two heavy particles is much more favorable than three contributing subsystems with similar masses. Careful choices of the three particles can then simultaneously optimize the Efimov conditions of large strength and large scattering lengths. This may allow detection of several or many members in a series of Efimov states or alternatively allow detection of the first Efimov state in cases when the conditions are less well fulfilled. We suggest a number of possible combinations of an electron and two neutral atoms or molecules, or alternatively one light atom and two heavy atoms or molecules.

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