Tetramers of two heavy and two light bosons

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Abstract

This article considers the bound states of two heavy and two light bosons, when a short-range force attracts the bosons of different mass, and a short-range force repel the light bosons. The existence of such four-body bound states results from the competition between these two forces. For a given strength of the attraction, the critical strength of the repulsion necessary to unbind the four particles is calculated. This study is motivated by the experimental realisation of impurity atoms immersed in an atomic Bose-Einstein condensate, and aims at determining in which regime only one boson contributes to binding two impurities.

1 Introduction

Since the observation of Efimov trimers in ultra-cold atomic gases [17, 6, 13, 19], there have been several theoretical [20, 27, 16, 24, 15, 9, 8, 10] and experimental [12, 21, 11] studies looking into the four-body bound states that exist around Efimov trimers. These tetramers are not “Efimov tetramers”, in the sense that they do not result from a four-body Efimov effect [7], yet they possess a universal character that originates, like the Efimov trimers, from the three-body Efimov effect. In particular, they follow the three-body Efimov scaling, such that each Efimov trimer is accompanied by one or several tetramer bound states or resonances.

The case of heteronuclear systems is particularly interesting, because the Efimov effect is enhanced when two heavy particles are attracted to a light particle. In this case, the light particle may be seen as a glue that binds the two heavy particles. This picture is clearly seen in the limit of large mass ratio between the heavy and light, where the Born-Oppenheimer approximation can be applied [19]. In this approximation, a light particle of mass $m$ creates an Efimov attraction potential $V(R) = -\frac{\hbar^2}{4\pi M^2} (|s_0|^2 - 1/4)$ between two heavy particles of mass $M$ separated by $R$, where

$$|s_0|^2 - 1/4 = \frac{M}{2m} (0.567143)^2,$$

resulting in a discrete-scale-invariant spectrum with a discrete scaling factor $e^{\pi/|s_0|}$. It turns out that a light particle can also glue three heavy particles together. The studies on the heteronuclear tetramers have so far focused on this situation when the three heavy particles are bosons [25, 6, 23, 22] or fermions [3, 4, 7, 2, 1].

Another interesting possibility is the case of two heavy particles and two light particles. In this case, in the large mass ratio limit, the two light particles are expected to provide twice the Efimov attraction of a single light particle, resulting in an Efimov series of tetramers that scale with a smaller scaling factor than that of the Efimov trimers. However, this is expected only when the interaction between the light particles may be neglected. If, on the other hand, the two light particles strongly repel each other, it might not be possible for the two light particles to bind to the two heavy particles; in other words, trimers are possible, while tetramers may not exist. The purpose of this article is to study how the spectrum changes between these two limiting cases, and determine the critical strength of repulsion required to unbind tetramers for a given attraction between the light and heavy particles.

This study is motivated by the question of heavy impurities immersed in a condensate of light bosons. The general treatment of this problem requires to include many excitations of the condensate created by the heavy impurities. However, when the light bosons repel each other sufficiently, a single excitation may be enough to capture the polaron physics of two impurities [18]. The present study aims at quantifying the strength of repulsion necessary to reach this regime. It should be noted that in an ultra-cold atomic experiment, the light bosons actually experience an attractive interatomic force. However, the scattering length of that interaction is positive, resulting in an effective repulsion at low energy that prevents the Bose-Einstein condensate from collapsing. One may therefore model the light boson interaction as a repulsive interaction, while bearing in mind that a realistic atomic interaction would in fact be attractive, and extra bound states would exist below the range of energies where the interaction has a repulsive effect, i.e. below the dimer energy of two light bosons.
2 System and method

We consider the following four-body Hamiltonian,

$$\hat{H} = \frac{\hbar^2}{M} (\hat{p}_1^2 + \hat{p}_2^2) + \frac{\hbar^2}{m} (\hat{p}_3^2 + \hat{p}_4^2) + \hat{V}_{13} + \hat{V}_{14} + \hat{V}_{23} + \hat{V}_{24} + \hat{U}_{34},$$

(2)

where $M$ is the mass of the two heavy particles, $m$ is the mass of the two light particles, $\hat{V}$ is the heavy-light attractive potential, and $\hat{U}$ is the light-light repulsive potential. The two heavy particles are identical bosons called $A$, and the two light particles are identical bosons called $B$. To simplify the resolution, both potentials are taken to be separable, i.e. of the forms

$$\hat{V} = \frac{4\pi\hbar^2}{2\mu} g|\phi\rangle\langle\phi|$$

(3)

$$\hat{U} = \frac{4\pi\hbar^2}{m} \xi|\chi\rangle\langle\chi|$$

(4)

where $\mu = (m^{-1} + M^{-1})^{-1}$ is the reduced mass, $g < 0$ is an attractive coupling strength and $\xi \geq 0$ is a repulsive coupling strength. After eliminating the centre of mass, the four-body Schrödinger equation resulting from the Hamiltonian Eq. (2) can be integrated as a set of integral equations on four-body components known as the Yakubovsky equations [26, 14, 20]. For the most general problem of four distinguishable particles, there are eighteen Yakubovsky components. In the present case, there are only four, which are denoted as $K_A$, $K_A'$, $H_A$, and $K_B$, and represented schematically in Fig. 1. These four components satisfy the four coupled integral equations:

$$K_A = \hat{G}_0 \hat{T}_{13} \hat{P}_{12} (K_A + K'_A + H_A)$$

(5)

$$K'_A = \hat{G}_0 \hat{T}_{13} \left[ \hat{P}_{34} (K_A + K'_A + H_A) + (1 + \hat{P}_{12}) K_B \right]$$

(6)

$$H_A = \hat{G}_0 \hat{T}_{13} \left[ \hat{P}_{12} \hat{P}_{34} (K_A + K'_A + H_A) \right]$$

(7)

$$K_B = \hat{G}_0 \hat{T}_{34} \left[ (1 + \hat{P}_{34}) (K_A + K'_A + H_A) \right]$$

(8)

where $\hat{G}_0$ denotes the four-body Green's function operator (without the centre of mass) at the four-body energy $E$, $\hat{P}_{ij}$ is the permutation operator for the coordinates of particles $i$ and $j$, and $\hat{T}_{ij}$ is the two-body $T$ matrix for the two-body interaction between particles $i$ and $j$. In momentum representation, we have:

$$\hat{G}_0 = \left( E - \frac{\hbar^2}{2\mu} p_{13}^2 - \frac{\hbar^2}{2\mu_{13,2}} p_{13,2}^2 - \frac{\hbar^2}{2\mu_{13,4}} p_{13,4}^2 \right)^{-1},$$

(9)

where the wave vectors $p_{13}$, $p_{13,2}$, and $p_{13,4}$ are the Fourier conjugates of the spatial vectors represented in the leftmost picture of Fig. 1. For the separable potentials Eqs. (3) and (4), we have:

$$\hat{T}_{13} = T_{13}(E_{13})|\phi\rangle_{13}\langle\phi|_{13} \quad \text{with} \quad T_{13}(E) = \frac{2\mu}{4\pi\hbar^2 g} + \int \frac{d^3p (\phi(p)|\phi(p)\rangle^2}{(2\pi)^3 \frac{\hbar^2}{2\mu} - E}$$

(10)

$$\hat{T}_{34} = T_{34}(E_{34})|\chi\rangle_{34}\langle\chi|_{34} \quad \text{with} \quad T_{34}(E) = \frac{m}{4\pi\hbar^2 \xi} + \int \frac{d^3p (\chi(p)|\chi(p)\rangle^2}{(2\pi)^3 \frac{\hbar^2}{m} - E}$$

(11)
where $E_{13} = E - \frac{\hbar^2}{2m_1} p_{13,2}^2 - \frac{\hbar^2}{2m_2} p_{13,3}^2$ and $E_{34} = E - \frac{\hbar^2}{2m_1} p_{34,1}^2 - \frac{\hbar^2}{2m_4} p_{34,12}^2$. The indices of $|\phi\rangle$ of $|\chi\rangle$ denote the relative coordinate of the pair on which they are acting. Thanks to the separable form of the $T$ matrices Eq. (10) and (11), the Yakubovsky equations can be written as:

\[
K_A = \tilde{G}_0|\phi\rangle_{13}K_A
\]

(12)

\[
K_A' = \tilde{G}_0|\phi\rangle_{13}K_A'
\]

(13)

\[
H_A = \tilde{G}_0|\phi\rangle_{13}H_A
\]

(14)

\[
K_B = \tilde{G}_0|\chi\rangle_{34}K_B
\]

(15)

where

\[
K_A = T_{13}(E_{13})|\phi\rangle_{13}P_{12}(K_A + K_A' + H_A)
\]

(16)

\[
K_A' = T_{13}(E_{13})|\phi\rangle_{13}\left[c_{13}^2(1 + 1)K_B \right]
\]

(17)

\[
H_A = T_{13}(E_{13})|\phi\rangle_{13}\left[c_{13}^2(1 + 1)K_B \right]
\]

(18)

\[
K_B = T_{34}(E_{34})|\chi\rangle_{34}\left[c_{13}^2(1 + 1)K_B \right]
\]

(19)

Inserting Eqs. (12-15) into Eqs. (16-19), one gets a closed set of integral equations on $K_A$, $K_A'$, $H_A$, and $K_B$. Using the linear relations between the various wave vectors of Fig. 1, one can write the final equations explicitly in momentum representation. Note that these equations are easier to solve than the original Yakubovsky equations because the number of (vector) arguments of $K_A$, $K_A'$, $H_A$, and $K_B$ is reduced by one from that of $K_A$, $K_A'$, $H_A$, and $K_B$, due to the integration over one vector argument implied by the action of $|\phi\rangle$ or $|\chi\rangle$ in Eqs. (16-19). This reduction of arguments is the usual simplification coming from the use of separable interactions. As a last simplification, we consider the solutions with zero total angular momentum, and omit the angular dependence of the vector arguments of $K_A$, $K_A'$, $H_A$, and $K_B$, which is known to be a very good approximation, since the decomposition of the four-body wave function in Yakubovsky components already captures most of its dependence on the particles’ angular momenta.

We are interested in expressing the results in terms of the scattering lengths $a$ and $a_B$ of the potentials $\hat{V}$ and $\hat{U}$. For this purpose, one can take $\hat{V}$ to the limit of a contact interaction of scattering length $a$, by setting $\phi(p) = 1$ up to some arbitrarily large cutoff $\Lambda$, and $\phi(p) = 0$ for $p > \Lambda$, expressing the equations in terms of the scattering length $a = (g^{-1} + \frac{3}{2}\Lambda)\^{-1}$ and taking the limit $\Lambda \rightarrow \infty$. Similarly, one can also set $\chi(p) = 1$ for $p < a_B$, and renormalise the result in terms of the scattering length $a_B = (\xi^{-1} + \frac{3}{2}\Lambda_B)\^{-1}$. However, the contact interaction limit $a_B \rightarrow \infty$ cannot be taken, because $\xi$ being positive, it can only result in $a_B \rightarrow 0$. This is the well-known fact that a repulsive contact interaction in three-dimensions does not scatter particles. On the opposite, one can take $\xi \rightarrow \infty$, i.e. the strongest possible repulsion, which results in $a_B = \frac{3}{2}\Lambda_B$. With these choices, $\hat{V}$ is only parameterised by $a$, and $\hat{U}$ is only parameterised by $a_B > 0$.

Because of the Efimov effect occurring for too heavy and one light bosons as well as one heavy and two light bosons, such three particles can experience an Efimov attraction from large distances to distances comparable to the range of $\hat{V}$. Since here the range of $\hat{V}$ is taken to zero by setting $\Lambda \rightarrow \infty$, nothing prevents the three particles from collapsing to a single point, which makes the problem ill-defined with no ground state. For such zero-range interactions, an extra three-body parameter must be introduced to cure this problem and set the energy of the trimers to a finite value. Here, it is implemented by imposing a finite cutoff $\Lambda_3$ on the wave vectors $p_{13,2}$, $p_{14,2}$, $p_{23,1}$ and $p_{34,12}$ between a heavy-light pair and a heavy particle, as well as the wave vectors $p_{31,4}$, $p_{32,4}$, $p_{41,3}$ and $p_{42,3}$ between a heavy-light pair and a light particle. In the end, the three parameters of the system are the two scattering lengths $a$ and $a_B$, and the length $\Lambda_3^{-1}$ which corresponds to the range of interactions, on the order of a few nanometres for atoms.

3 Results

In the following calculations, the range $\Lambda_3^{-1}$ is taken as the unit of length and $E_3 = \hbar^2 \Lambda_3^2 / (2\mu)$ as the unit of energy. One can then fix $a_B$ and vary $1/a$ from negative to positive values, corresponding to increasing attractive strength $g$ between heavy and light particles. The point $1/a = 0$ corresponds to the unitary point at which a heavy-light $AB$ dimer is formed, and around which the Efimov effect occurs for $AAB$ and $ABB$ systems.

3.1 Equal-mass case

Let us first consider the case of equal masses $M = m$. In this case, the Efimov attraction is weak, with a scaling factor $e^{-\pi / |a|} \approx 1986$ between consecutive trimer states [19]. In the energy spectrum as function of $1/a$ shown in
Fig. 2: Energy spectrum (rescaled as a binding wave number \( k = -\sqrt{2m|E|/\hbar} \)) for a system of two identical bosons \( A \) and two identical bosons \( B \) of equal mass, as a function of the inverse scattering length \( 1/a \) between the two kinds of bosons. Each panel corresponds to a different value of the scattering length \( a_B \) between two bosons \( B \), as indicated at the top of each panel. The black dotted lines represent the energies of one and two \( AB \) dimers. The red dashed curve represents the energy of the \( AAB \) ground trimer. These curves correspond to the thresholds of scattering continua indicated by shaded areas. The green solid curves represent the \( AABB \) tetramer bound states.

Fig. 3: Same as figure 2 for a system of two heavy bosons \( A \) and two light bosons \( B \), with mass ratio 19. Each panel corresponds to a different value of the scattering length \( a_B \) between the light bosons \( B \).
Fig. 2: Only the ground-state AAB trimer (degenerate with the ground-state ABB trimer) can be seen, the other trimer states being too weakly bound to be seen. For $a_B = 0$, corresponding to no interaction between the $B$ particles, one finds at least three Borromean $AABB$ tetramer states below the ground-state trimer (there might be more weakly bound tetramers that are not resolved in the present numerical calculation). The tetramers are here significantly more bound than the trimers: at unitarity ($1/a = 0$), the ground-state tetramer binding energy $0.016E_3$ is 400 times larger than the ground-state trimer binding energy $0.00037E_3$.

As the value of $a_B$ is increased, the tetramers are weakened and gradually pushed to the $AAB + B$ threshold, as seen in Fig. 2. Although they are significantly weakened, it is not possible to fully unbind all the tetramers, even for $a_B$ as large as $10\Lambda_3^{-1}$. For larger values of $a_B$, the tetramers become more strongly bound again, and in the limit $a_B \to \infty$, one retrieves the original spectrum obtained for $a_B = 0$. This is because the repulsive effect of the boson interaction becomes more and more diluted over large distances as $a_B$ is increased. In the limit of large $a_B$, only the weak tetramers with a size on the order of $a_B$ are significantly affected by the light boson repulsion. This situation qualitatively reproduces what would happen with an attractive $BB$ interaction with large positive scattering length $a_B$: only the tetramers with an energy above the $BB$ dimer energy $-\hbar^2/(ma_B^2)$ would be pushed up, while the tetramers below that energy would be pushed down, due to the avoided crossing with the $BB$ dimer. However, the results are not expected to be quantitative for such large values of $a_B$, so we shall disregard this regime and focus on $a_B \lesssim \Lambda_3$.

It should be noted that if the boson-boson interaction were modelled by a hard-core repulsion, all tetramers would of course unbind for $a_B \gtrsim 10\Lambda_3$, although this would not be a physically correct description of atoms with large scattering length.

3.2 Large mass imbalance $M/m = 19$

For larger mass imbalance, the Efimov attraction mediated by a particle $B$ is stronger and the $AAB$ trimers are more strongly bound, whereas the Efimov attraction mediated by a particle $A$ is weaker and the $ABB$ trimers are more weakly bound. We consider the mass ratio $M/m = 19$ corresponding to a mixture of two cesium-133 and two lithium-7 atoms. In the energy spectrum shown in Fig. 3, the lowest three $AAB$ trimers can be seen, while the $ABB$ trimers are too weak to be seen. The ground-state $AAB$ trimer is now bound with a binding energy of $0.053E_3$ at unitarity. For $1/a < 0$ and around unitarity, one finds only one Borromean $AABB$ tetramer state for $a_B = 0$. Its binding energy at unitarity is $0.092E_3$. While both the trimers and tetramers are more strongly bound with respect to the equal-mass case, their relative separation is reduced. As a result, it is easier to push the tetramer to the $AAB + B$ threshold. Fig. 3 shows that the tetramer nearly reaches the $AAB + B$ threshold for $a_B \gtrsim 1.5\Lambda_3^{-1}$. However, as in the equal-mass case, it is not possible to fully unbind the tetramer, and for larger values of $a_B$ the tetramer gradually recovers its original binding energy.

3.3 Very large mass imbalance $M/m = 1000$

Although the mass ratio $M/m = 19$ may be considered as large, only one tetramer bound state is found near unitarity. As mentioned in the introduction, at large mass ratio, the two heavy particles are expected to undergo twice the Efimov attraction $V(R) = -|s_0|^2 + 1/4)/R^2$ mediated by each of the two light bosons, resulting in
an infinite Efimov series of $AABB$ tetramers. The scaling factor of this Efimov series is therefore
\[
\lambda = e^{\pi/s_0'}, \quad \text{with } s_0' = \sqrt{2|s_0|^2 + 1/4},
\]
where $|s_0|$ is given by Eq. (1).

It is however not easy to observe these tetramers at mass ratio 19, because they are hidden as resonant states in the $AAB + B$ scattering continuum, which are difficult to extract within the present calculations. Nevertheless, by further increasing the mass ratio, one can observe more tetramer bound states emerging from the $AAB + B$ threshold, as shown in Fig. 4 for the mass ratio $M/m = 1000$. Figure 5 shows that these tetramers form indeed a discrete scale invariant spectrum with the scaling factor $\lambda$ given in Eq. (20). Although they are expected to persists inside the $AAB + B$ scattering continuum as universal four-body resonances, their Efimov spectrum may be significantly altered by its multiple crossings with the excited trimer+particle thresholds.

Finally, it can be checked again that the ground-state tetramer can be pushed near dissociation into a $AAB$ trimer and $B$ particle for a moderately repulsive interaction between the light bosons $B$. Such a situation is shown in the right panel of Fig. 4 for $a_B = 1.5\Lambda_3^{-1}$.

4 Conclusion

In a system of two heavy bosons and two light bosons, a near-resonant ($a \gg \Lambda_3^{-1}$) attractive force between the heavy and light bosons is required to overcome quantum fluctuations and bind the system into tetramers. On the other hand, a relatively weak non-resonant ($a_B \sim \Lambda_3^{-1}$) repulsion between the light bosons can nearly unbind the tetramers. This suggests that in the polaron problem of heavy bosonic impurities immersed in a Bose-Einstein condensate of light bosons, the attraction between two impurities mediated by the condensate is carried mostly by a single light boson (or single excitation) for a relatively moderate repulsion between the light bosons.

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