Efimov states of heavy impurities in a Bose-Einstein condensate

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Abstract – We consider the problem of two heavy impurity particles embedded in a gas of weakly interacting light mass bosonic particles in the condensed state. Using the Bogoliubov approach to describe the bosonic gas and the Born-Oppenheimer approximation for the three-body dynamics, we calculate the modification to the heavy-heavy two-body potential due to the presence of the condensate. For the case of resonant interaction between the light bosons and the impurities, we present (semi)-analytical results for the potential in the limit of a large condensate coherence length. In particular, we find a formula for the modification of the Efimov scaling factor due to the presence of a degenerate bosonic gas background.

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Introduction. – The three-body spectrum for two heavy and one light particle with short-range resonant interactions between the heavy and light particles can be treated using the Born-Oppenheimer approximation. One decouples the slow degrees of freedom (relative motion of the two heavy particles) from the motion of the light particle to obtain an effective heavy-heavy potential. What is found is the famous Efimov spectrum of geometrically scaling three-body states where subsequent states differ by a simple factor of the form $e^{\pi/s_0}$, where $s_0$ is called the scaling parameter [1]. For equal mass particles, $e^{\pi/s_0} \sim 22.7$, which is a severe limiting factor in the quest for observing many states. However, in the heavy-heavy-light system the factor can be much smaller [2,3]. This has generated a lot of interest in studying three-body systems with mixed atomic species in the ultracold regime [4].

The ultracold gases used for three-body experiments are typically at very low densities. The three-body dynamics can thus be described by assuming that three-body states are essentially isolated entities in spite of the fact that there is always some finite density background present. However, experiments should be able to push into higher densities and thus be able to investigate the effects of the finite background on few-body properties. Some recent works have been devoted to the question of what happens when the particles are fermions that have to obey the Pauli principle [5–9]. Here we will address the related issue of what happens when there is a Bose gas background that is in the condensate phase. A few other papers have recently discussed this type of question from the many-body point of view [10,11]. Here we take a different point of view and consider the background condensate as a perturbation on the three-body state. For simplicity we will consider the case of two heavy impurity particles in a Bose gas of light bosons. For the two-body case the problem of an impurity in a condensate with strong interactions was revived recently [12–14], and likewise for the case of multiple such impurities [15,16]. The Bose-Fermi mixture in cold atomic gases was discussed in detail about a decade ago [17,18] and the later works address a particularly interesting regime with large imbalance in the populations. However, we are not aware of any works discussing the presence of an Efimov effect in a condensate background and the influence that the background can have on the universal three-body spectrum.

Our approach will be based on the Bogoliubov approximation for the condensate dynamics. We will work in the limit of a weakly coupled Bose gas with repulsive short-range interactions, i.e., small and positive scattering length, $a_B > 0$. The impurity-light boson interaction will be allowed to take on any value. The condensate coherence length, $\xi = 1/\sqrt{8\pi n_0 a_B}$ with $n_0$ the condensate gas density, will therefore be large and its inverse a useful expansion parameter. The problem we solve is very similar to the classical problem of the electron-electron interaction mediated by phonons; the impurities are the (heavy) electrons while the light bosons are the phonons. Of course, in the case of a Bose condensate of massive particle, the phonon dispersion is only linear for low momenta and eventually becomes quadratic. This will be properly taken
into account in our framework. The problem considered here is closely related to the bosonic Kondo problem with two impurities and a bosonic bath [19–24]. The study here should thus be of interest for both cold atomic gases and for condensed-matter physics.

**Theoretical model.**—We consider two heavy impurities of mass \( M \) and a gas of light bosonic particles of mass \( m \ll M \). The Hamiltonian is

\[
H = \sum_k \varepsilon_I(k) c_k^\dagger c_k + \sum_k \varepsilon_B(k) b_k^\dagger b_k + \sum_q n_B(q) n_B(-q) + U_{IB} \sum_q n_B(q) n_I(-q),
\]

where \( c_k \) are the impurity operators and \( b \) the boson operators. We use zero-range density-density impurity-boson and boson-boson interactions with \( n_I(q) = \sum_k c_k^\dagger c_k^\dagger q k \) and \( n_B(q) = \sum_k b_k^\dagger b_k^\dagger q k \). The dispersions are \( \varepsilon_I(k) = \hbar^2 k^2/2M \) and \( \varepsilon_B(k) = \hbar^2 k^2/2m \). In the weakly coupled limit we have \( U_{IB} = 4\pi \hbar^2 g_{AB}/m \). The parameter \( U_{IB} \) will be discussed later. We use Bogoliubov theory to describe the light bosonic particles [25]. We therefore transform to quasi-particles, \( \gamma_k \) and \( \gamma_k^\dagger \), in the standard way. Furthermore, we will assume that the condensate density is small so that the number of quasi-particles is also small. This allows us to neglect all terms except \( \gamma_k^\dagger \gamma_k \) in the transformed Hamiltonian. Dropping unimportant constant terms, the bosonic dispersion and the interaction term becomes

\[
\sum_{k \neq 0} E(k) \gamma_{k}^\dagger \gamma_k + U_{IB} \sum_{q k k'} c_{-k-q}^\dagger c_k^\dagger q k' \gamma_{k'}^\dagger \gamma_{k'},
\]

where \( E(k) = \sqrt{U_B n_B \hbar^2 k^2/2m_B + (\hbar^2 k^2/2m_B)^2} \). This corresponds to impurity particles with dispersion \( \varepsilon_I(k) \) interacting with Bose gas particles with dispersion \( E(k) \) through a contact interaction with strength \( U_{IB} \). In the case where \( E(k) \) is linear in \( k \), this corresponds to a system of (heavy) electrons interacting with phonons through a non-dispersive zero-range interaction.

We now proceed to solve the three-body problem of two heavy impurities and one light bosonic quasi-particle. Note that these states should be considered resonances similar to the three-boson case in recent experiments [4]. The absolute ground state should be a bound state containing both impurities and all the bosons which is not experimentally realized in these dilute atomic gases. We also note that there can be two light bosons and one impurity three-body bound states in the system. However, this configuration of masses strongly disfavors the Efimov effect (\( e^{\gamma_{k}} \) is very large [2,3]) and will not be discussed here.

**Born-Oppenheimer approximation.**—As we have just argued, we can model the interaction of the impurities and the bosons via a zero-range interaction, and we thus write \( V(r) = U_{IB} [\delta(r - R/2) + \delta(r + R/2)] \), where we assume that the two heavy impurities are located at \( \pm R/2 \). This potential needs to be regularized since as it stands it leads to an ultraviolet divergence. We return to this point below. The essence of the Born-Oppenheimer approximation is that we first solve for the dynamics of the light bosonic particles while assuming that \( R \) is fixed, and then proceed to consider the Schrödinger equation for the two heavy particles as a function of \( R \). The relative distance of the heavy particles, \( R \), is our adiabatic variable which we assume changes on a much slower time scale than the positions of the bosonic particles.

Now we consider the Schrödinger equation for the particle of mass \( m \) in this potential \( H \phi = E_R \phi \), where \( E_R \) is the energy and \( \phi \) the wave function of a light bosonic (quasi-)particle. Since \( V(r) \) contains delta-functions, it is convenient to work in momentum-space. The Schrödinger equation in momentum-space can then be written as

\[
E(k) \phi(k) + \frac{1}{(2\pi)^3} \int dk' \phi(k') V(k - k') = E_R \phi(k),
\]

where \( V(q) = 2U_{IB} \cos(q R/2) \). Integration over \( k \) on both sides, assuming that \( \phi \) is an even function of \( k \) (s-wave solutions), and elementary trigonometric manipulations reduce the equation to the form

\[
1 - \frac{U_{IB}}{(2\pi)^3} \int dk k^3 E(k) - E_R = \frac{U_{IB}}{(2\pi)^3} \int dk \cos(k \cdot R) \frac{E(k) - E_R}{E(k)},
\]

We now relate \( U_{IB} \) and the scattering length of the interaction between the impurity and the bosonic particles, \( a \). While this can be done most elegantly by using Tan’s pseudopotential [26,27], we use a traditional approach that is very easy in the Born-Oppenheimer limit. From the Lippmann-Schwinger equation for the impurity-boson scattering we have

\[
\frac{1}{(2\pi)^3} \int dk \frac{1}{k^2} = \frac{\mu}{2\pi a^2} - \frac{1}{(2\pi)^3} \int \frac{d^3k}{k^2},
\]

where \( \mu = mM/(m + M) \) and \( c_k^\dagger c_k = \hbar^2 k^2/2m \) are reduced mass and energy. Since we assume \( m \ll M \), we can safely use \( \mu = m \) and \( c_k^\dagger c_k = c_k \). Note that we do use the bare dispersion of the bosons, \( \hbar^2 k^2/2m \), and not \( E(k) \). This is necessary since the heavy-light scattering length, \( a \), is defined in vacuum and the Lippmann-Schwinger problem must therefore also be solved in vacuum. Inserting the relation between \( U_{IB} \) and \( a \) we arrive at our central equation

\[
\frac{R}{a^2} = \frac{1}{\pi} \int_0^\infty dx \frac{x^2}{|x^4 + A^2x^2 + 1|^{1/2} + 1},
\]

where we have defined \( a^2 = -2mE_R/\hbar^2 \) and \( A = 1/(\alpha\xi) \). In the case where the bosons are non-interacting, i.e. \( a_B \to 0 \), we have \( \xi \to \infty \) and thus \( A \to 0 \). In this limit the integrals can be performed analytically and we arrive at the well-known formula

\[
\alpha R = \frac{R}{a} + e^{-\alpha R}.
\]
In the case of resonant interactions, $|a| = \infty$, the equation has the solution $\alpha R = x_0 \sim 0.567$. To lowest order in $R/a$ (i.e., for large $|a|$ and/or small radii), we find

$$E_R = -\frac{\hbar^2 x_0^2}{2mR^2} \left[ 1 + \frac{1}{x_0^2(1 + e^{x_0})} \frac{R}{a} \right].$$ \hfill (8)

Another interesting limit, is $R \gg a$. In that case we can neglect the exponential term in eq. (7), and we find a well-known result $E_R = -\frac{\hbar^2}{2mR^2}$. Notice that this only works for $a > 0$, since the $a < 0$ case has no solution. This energy is the usual energy of a particle of mass $m$ in the delta-function potential of a much heavier particle of mass $M \gg m$ (i.e., a fixed potential center). The physical interpretation is that the small mass particle forms a bound state with one of the heavy particles.

**Heavy-light two-body states.** – We first consider a single impurity. This problem can be handled in the same manner as the discussion above. The only difference is that in eq. (6) the integral with the sine term is absent. The first integral in eq. (6) is analytically tractable but the expression is long and cumbersome and does not really yield any insights. However, since we are concerned with the large $\xi$ limit we can make an expansion in $A$ inside the integral. This requires the stronger condition of $a\xi$ large, which must be checked after doing the integral. After expansion one has

$$\int_0^\infty dx \left[ \frac{x^2}{x^2 + A^2/2 + 1} - 1 \right],$$ \hfill (9)

and using this we arrive at $\frac{1}{\alpha} = \alpha + \frac{1}{4a\xi^2}$ which is a hidden second-degree equation in $\alpha$ with one positive root

$$\alpha = \frac{1}{2a} \left[ 1 + \sqrt{1 - \frac{a^2}{\xi^2}} \right],$$ \hfill (10)

which requires $\xi/a \geq 1$.

In fig. 1 we show the two-body binding energies of the heavy-light system with and without the presence of a condensate. We see a clear tendency of the condensate to push the threshold away from unitarity and into the regime of small positive $\alpha$, i.e., one needs stronger attraction to bind the light-heavy system in the presence of a condensate. A shift of the two-body threshold is found due to the condensate background. For $\frac{\xi}{a} \gg 1$, the condensate and vacuum solutions become indistinguishable. The dotted (red) curve is obtained from eq. (10). The atom-dimer continuum is on the right side of the curves, while we expect universal three-body states to appear on the left. A clear change of threshold at small binding energy is found due to the condensate background.

**Surface moves closer to zero momentum as the mass of the fermions increase. This implies that there is a strong similarity of an impurity interacting with a Fermi sea of heavy fermions and an impurity interacting with a condensate of light bosons. Whether this holds as a general mapping between the two situations also away from the extreme light/heavy mass regions cannot be addressed within the Born-Oppenheimer approximation. This is an interesting question for future studies.**

**Two impurities in a condensate.** – We now proceed to consider the effect of a condensate of light particles on two impurities. The solution for the potential of the two heavy impurities, given implicitly through $\alpha$, is found by solving eq. (6). While the first integral in eq. (6) is exactly solvable, the second term is very difficult to handle both analytically and numerically. We have solved it using various approximation schemes and present the results in fig. 2. The lines termed “full” are an expansion of eq. (6) to the 2nd and 4th order in $A$. The full solution to second order yields the equation

$$\alpha R + \frac{1}{4} \alpha R A^2 = \exp \left( -\alpha R - \frac{1}{4} \alpha R A^2 \right),$$ \hfill (11)

from which the “lowest Taylor” is obtained by second-order expansion around $R/\xi = 0$. In the absence of the condensate, the solution is given by the first term in eq. (8) which can be written $\alpha R = x_0$. We thus see that the effect of the condensate and the corresponding change in the dispersion of the light particle is to suppress the attraction between the impurities. The scale of this suppression is

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which is always negative. This indicates that $E_R$ does indeed change sign as $R \sim \xi$. However, taking the limit of $R \to \xi$ in this result yields $-\frac{1}{2}$ and $A^2$ is now of order one which is in conflict with the limit we used to derive the expression. However, it strongly suggests that $E_R$ will go to zero for some values of $R/\xi$.

Our results for the potential between the two heavy impurities, $E_R$, are plotted in fig. 3. We see that the presence of the condensate tends to make the potential go to zero faster than $R^{-2}$ as $R$ increases. An effective repulsive effect is thus seen to originate from the many-body background in the light-particle component. The Efimov effect depends on the $R^{-2}$ functional form of the potential, and of course on the fact that it is attractive [2,3]. Our results imply that the condensate coherence length, $\xi$, must be considered when estimating the Efimov effect in a degenerate Bose gas setting. Moreover, the length scale of the modification is $\xi$ to within a factor of order one.

We therefore conclude that at unitarity, the number of universal three-body bound state can be estimated by analogy with Efimov’s original formula [1] and becomes

$$N_B \approx \frac{s_0}{\pi} \log \left( \frac{\xi}{R_0} \right),$$

where $s_0$ is the scale factor and $R_0$ is a short-distance cutoff [1]. More generally, we expect that whichever is smaller of $|\alpha|$ and $\xi$ will cut off the number of states allowed in the spectrum.

We note that our findings do not indicate any modification of the potential for small distances. This can be understood from the dispersion relation of the light particles which become quadratic at high momenta corresponding to short distance. Condensates modify the behavior at long range (where low-energy universal three-body states may reside), the short distance is left more or less undisturbed. This means that the short-distance cut-off that is

Fig. 2: (Colour on-line) $aR$ as a function of $R/\xi$. A full solution could only be found for $R/\xi < x_0$. The full (blue) line is the full solution to 2nd order in $A$, while the dashed (red) line shows the full solution to 4th order. For comparison, the dotted (black) line shows the second-order expansion around zero. The thin dotted lines guide the eye to the positions beyond which no full solutions were found.

Fig. 3: (Colour on-line) Effective potential for the two heavy impurities, $E_R$, as a function of their relative distance $R$. The solid (blue) curve shows the result from a second-order expansion of eq. (6) with respect to $(\alpha \xi)^{-1}$, while the dashed (black) curve gives the results with no condensate background ($-\frac{\pi^2}{4\hbar^2}$). The end point of the solid curve is at $R/\xi = x_0$ where the second-order solution ceases to exist. However, our results generally indicate that the potential $E_L$ goes to zero faster than $R^{-2}$ for large $R/\xi$.
necessary to bound the attractive $R^{-2}$ and avoid collapse is provided by short-distance physics ($R_0$ in eq. (14), often called the three-body parameter). However, recent studies have found a strong connection between $R_0$ and the two-body physics of the systems as given by the van der Waals length, $r_{vdW}$ [28–34]. In the case studied here where the impurity is much heavier than the light constituent, $R_0$ is given simply by the details of the heavy-heavy system as is seen from the derivation of $E_{R}$ above (and from the numerical results of ref. [35]). We therefore expect that $R_0 \sim r_{vdW}$ to within factors of order unity (between $\sqrt{2}$ [33] and 2 [32]). Note that we are assuming that there are no resonances in the heavy-heavy system. This should always be closely investigated in realistic setups where interactions are typically controlled by external fields [36] that affect both heavy-light and heavy-heavy systems.

**Experimental considerations.** – We now discuss some systems of experimental relevance to the physics studied above. Light alkali atoms that have been condensed are $^7$Li and $^{23}$Na, although the latter is not really light when taking ratios with other interesting systems. However, recent advances in studies of metastable helium, $^4$He$^*$ [37,38] and the potential of those experiments to make mixtures of $^4$He$^*$ and $^{87}$Rb makes that a very interesting system [39]. Likewise, the mixture of $^7$Li and $^{133}$Cs [40] or $^7$Li and $^{87}$Rb [41] would be favourable, and also potential mixtures of ytterbium isotopes (mass numbers 168–176) [42,43] and $^7$Li or $^4$He.

The results we have presented here show that the Efimov spectrum can be modified at large distances by the presence of a condensate background, and also that there is no effect at short distance from the condensate. If we insert the definition of $\xi$ into eq. (14), we find the following formula for the expected number of three-body Efimov states at unitarity (which effectively assumes that $|\alpha| \gg \xi$) for our setup

$$N_B = \frac{s_0}{2\pi} \ln \left[ 2.7 \cdot 10^{10} \frac{a_0}{a_B} \left( \frac{a_0}{r_{vdW}} \right)^2 \frac{10^{13} \text{cm}^{-3}}{n_0} \right],$$

(15)

where $n_0$ is the condensate density, $a_B$ is the scattering length of the condensed bosons, and $r_{vdW}$ is the two-body van der Waals length associated with the interatomic potential of the two heavy impurities. The unit $a_0$ is the Bohr radius. If we consider the $^4$He-$^{87}$Rb or $^7$Li-$^{133}$Cs cases, the mass ratios are roughly the same and we have $s_0 = 1.98$. For the $^4$He$^*$-$^{87}$Rb case, $a_B \sim 142a_0$ [37,39] and $r_{vdW}(^{87}\text{Rb}) \sim 83a_0$ [36], and we obtain $N_B \sim 3.2$ at $n_0 = 10^{13} \text{cm}^{-3}$. One-order-of-magnitude increase in $n_0$ or $a_B$ brings this down to $N_B \sim 2.5$, so we see a sizable effect. Of course we are assuming that there are non-overlapping resonances in $^4$He-$^{87}$Rb and $^{87}$Rb-$^{87}$Rb which is currently unknown. The example of $^7$Li-$^{133}$Cs is slightly more complicated since $^7$Li has attractive interactions at zero magnetic fields [36]. However, let us for the moment assume that we can tune the scattering length away from the attractive region and also find a good resonance in the Li-Cs system (as recently done for the closely related case of $^6$Li-$^{133}$Cs [44,45]). If we assume that $a_B \sim 100a_0$ and use $r_{vdW} \sim 101a_0$ [36], we find more or less exactly the same scenario as in the $^4$He-$^{87}$Rb case. We thus see that the effect of condensation of light particles in heavy-heavy-light three-body systems should be accessible in current experiments.

Other mixtures are being pursued at the moment that are relevant for our purposes since they contain Bose components that can be condensed, but for which the mass ratios are too large for the Born-Oppenheimer approximation to be fully justified. Examples are $^{23}$Na mixed with $^{40}$K [46] and $^{87}$Rb with $^{133}$Cs [47]. For the latter system the experiments that are probably most interesting for our purposes are those with a few heavy impurities in a condensate of the lighter species by the Widera group [48,49]. While the approximations used here are not expected to be accurate in relation to these less mass imbalanced mixtures, we do expect that similar signatures should occur, and that the Efimov effect, if present, will be modified by a condensate background when $\xi$ is sufficiently small.

**Discussion.** – We have considered the influence of a condensate background on three-body bound-state physics in the case of two heavy impurity atoms embedded in a condensate of light particles and assuming that the light-heavy interaction is short-ranged. Using the Born-Oppenheimer approximation we calculate the modification of the heavy-heavy interatomic potential when the light-particle dynamics is integrated out. Our results demonstrate that this potential is strongly modified at length scale corresponding to the condensate coherence length, and eventually turns from attractive inverse square (necessary for the Efimov effect), through zero, and then most likely into a repulsive potential at very large distance. These findings indicate that the coherence length must be considered as a length scale when estimating the potential for such systems to form universal three-body bound states. In the case where the heavy-light interaction is resonant (infinite scattering length), the coherence length replaces the scattering length in the famous Efimov formula, eq. (14). We have estimated the effects of our findings on experimental mixtures of current interest and find that by tuning the interaction strengths and condensate density, it should be possible to manipulate the number of universal three-body states.

In future studies it is necessary to go beyond the Born-Oppenheimer approximation in order not to rely on large mass imbalance. Furthermore, two or three of the constituents may be condensed and it would be interesting to study the effects that this will have on the three-body spectrum. From the current study we would expect that some combination of coherence lengths and scattering lengths would decide the number of bound states. It would also be interesting to study the addition of degenerate Fermi components. Here the coherence length is replaced by the Fermi momentum $[6,7]$. 

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Another important way in which to improve the current study is in the description of the Bose condensate through the Bogoliubov formalism. If we have a strongly interacting condensate one needs to consider modifications here. Also the neglect of states with quasi-particles (phonons) may not be justified and then we need to consider instead a starting point in line with the Fröhlich polaron system [50]. However, we do expect to see qualitatively the same physics, i.e. that the presence of backgrounds will modify the universal three-body spectrum and in many cases suppress the bound-state formation.

The essential assumption used here was that the light particle had a linear dispersion at low energy. This is reminiscent of the low-energy dispersion of a system like graphene [51] or the surface of a topological insulator [52] where it is electrons that have linear dispersion at low-energy. Adding impurities to such systems and studying bound states induced by the electronic surroundings with linear dispersion is an interesting prospect.

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