Finite-range effects in energies and recombination rates of three identical bosons

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Abstract
We investigate finite-range effects in systems with three identical bosons. We calculate recombination rates and bound state spectra using two different finite-range models that have been used recently to describe the physics of cold atomic gases near Feshbach resonances where the scattering length is large. The models are built on contact potentials which take into account finite-range effects; one is a two-channel model and the other is an effective range expansion model implemented through the boundary condition on the three-body wavefunction when two of the particles are at the same point in space. We compare the results with the results of the ubiquitous single-parameter zero-range model where only the scattering length is taken into account. Both finite-range models predict variations of the well-known geometric scaling factor 22.7 that arises in Efimov physics. The threshold value at negative scattering length for creation of a bound trimer moves to higher or lower values depending on the sign of the effective range compared to the location of the threshold for the single-parameter zero-range model. Large effective ranges, corresponding to narrow resonances, are needed for the reduction to have any noticeable effect.

(Some figures may appear in colour only in the online journal)

1. Introduction

Low-energy quantum mechanical bound states present a number of surprising results when the state contains three or more particles. The most famous case is the Efimov effect that occurs when a three-body system has two-body subsystems that have a two-body bound state with zero energy. In this situation one can mathematically prove that an infinite number of three-body states appear when the particles are bosons [1]. More generally, the effect can also take place for two-component fermionic systems whenever the mass ratios are large enough [2–4]. In recent years, it has become clear that few-body effects such as this can be studied in great detail in experiments with ultracold atomic gases via tunable Feshbach resonances [5, 6]. Producing a two-body bound state at zero energy is thus routinely done and signatures of three- and even four-body resonances have been observed [7–17].

The few-body features that are studied in ultracold atom experiments are often identified through the rate at which atoms are lost from the experimental trapping potential. In fact, the densities and lifetimes of typical Bose–Einstein condensates (BEC) are limited by loss effects, primarily due to three-body recombination, a process where three particles interact and create a bound system of two particles (dimer) and the third particle carries away excess energy and momentum, generally resulting in a loss of all three particles from the confining trap. The loss rate is given by \( \dot{n} = -\alpha n^3 \) where \( n \) is the particle density and the recombination coefficient is \( \alpha = C(a)\hbar a^4/m \) with \( C(a) \) a log-periodic function of the two-body scattering length \( a \) with period 22.7 [2]. A strongly interacting BEC can be created by use of Feshbach resonances where the scattering length can be tuned using an external magnetic field [6].

The \( a^4 \) scaling of the recombination coefficient is valid when the scattering length is much larger than the range...
of the inter-atomic potential. Here we use different models to estimate the effect of the finite range of the interactions. All the models we use are based on contact interactions, but in contrast to the typical one-parameter implementation, we also incorporate a non-zero effective range. This is done by either modifying the Bethe–Peierls boundary condition using the effective range expansion or by using a two-channel model which not only has an inherent effective range but also qualitatively describes the physics of Feshbach resonances.

The hyperspherical adiabatic approach is used to handle the three-particle problem. This method works equally well for the three scattering models we consider (zero-range contact interaction, effective range expansion and two-channel contact interaction). In order to calculate the recombination rate, we use the WKB method with hidden crossings [18], which takes the three-body system from the initial incoming scattering channel into the atom plus dimer channel of lower energy via an excursion into the complex plane. Since this approach depends critically on the presence of a bound dimer, it is only applicable to the positive $a$ side of a Feshbach resonance and we only consider recombination rates for $a > 0$. Along the way, we discuss the hyperspherical potentials for the different models, and also the scaling properties of consecutive Efimov resonances when effective range corrections are included.

In order to also address the negative $a$ side of the resonance, we calculate the spectrum of bound low-energy trimers within different models and study their dependence on the effective range corrections. Recent experiments have shown that the lowest three-body Efimov state has a breakup threshold at the three-atom continuum on the $a < 0$ side of the resonance that seems to be uniquely determined by the background van der Waals parameter of the atomic system under study [15]. In fact, the threshold, $a(-)$, is experimentally found to fulfil $a(-) \sim -9.8 r_{vdW}$, where $r_{vdW}$ is the two-body van der Waals length scale [15]. This finding has induced a number of theoretical studies that aim to explain the proportionality and calculate the constant factor from basic knowledge about the two-body atomic potentials [19–24]. It can be most easily understood as a consequence of the hard-core repulsion of the atom–atom interaction (typically $r_{vdW}$ is $\sim -9.8 r_{vdW}$). This fact induces a hard-core repulsion in the three-body potential around $r_{vdW}$ as shown numerically in [21] and soon after by analytical means in [23]. Here we calculate the three-body spectrum for different scattering models and study the influence of effective range corrections on the threshold and the scaling properties of the states. Finite-range corrections beyond the scattering length approximation have been considered before within various approaches [25–35]. However, to the best of our knowledge, systematic studies using simple zero-range models have not been presented. Since zero-range models are extremely convenient in both few- and many-body studies, it is important to gauge their applicability which is one goal of the current study.

The paper is organized as follows: in section 2 we first present the hyperspherical adiabatic method which constitutes our theoretical framework and discuss the differences in the solutions to the hyperspherical three-body potential within the different two-body interaction models that we employ. Section 3 discusses the recombination rate within the different models using the hidden crossing technique. In section 4, we discuss the spectrum of three-body bound states with the various models and map out the dependence on the effective range. Section 5 contains a short summary along with conclusions and outlook.

2. Formalism

We consider a system of three identical bosons of mass $m$ using hyperspherical coordinates defined from the Cartesian coordinates $r_i, r_j, r_k$ of particles $i, j, k$ as $x_i = \frac{r_j - r_k}{\sqrt{2}}, \quad y_i = \sqrt{\frac{2}{3}} \left( r_i - \frac{r_j + r_k}{2} \right)$, $\rho^2 = |x_i|^2 + |y_i|^2, \quad \tan \alpha_i = \frac{|x_i|}{|y_i|}$, where $|i, j, k|$ are cyclic permutations of $\{1, 2, 3\}$, $\rho$ is the hyperradius and $\alpha_i$ is a hyperangle [2]. The directions of $x_i$ and $y_i$ comprise four additional hyperangles which, along with $\alpha_i$, are denoted collectively as $\Omega$. The hyperradius $\rho$ is independent of the choice of $|i, j, k|$.

The wavefunction is expanded on adiabatic basis states $\Phi_i(\rho, \Omega)$. In the hyperspherical adiabatic approximation only the first term in this expansion is kept; this has been proven to be a good approximation when dealing with Efimov three-body states (trimers) [2]. The wavefunction is then

$$\Psi(\rho, \Omega) = \rho^{-5/2} f_0(\rho) \Phi_0(\rho, \Omega),$$

where $\Phi_0(\rho, \Omega)$ is the solution to the hyperangular equation

$$\left( \Lambda + \frac{2m\rho^2}{\hbar^2} V \right) \Phi_0(\rho, \Omega) = \lambda_0(\rho) \Phi_0(\rho, \Omega),$$

where $\Lambda$ is the grand angular momentum operator in hyperradial coordinates (see [2]) and $\lambda_0$ is the corresponding eigenvalue. The hyperradial function $f_0(\rho)$ is a solution to the hyperradial equation

$$\left( -\frac{d^2}{d\rho^2} + \frac{\lambda_0(\rho) + 15/4}{\rho^2} - Q_{\rho0}(\rho) - \frac{2mE}{\hbar^2} \right) f_0(\rho) = 0,$$

with

$$Q_{\rho0} = \left( \Phi_0 \left[ \frac{\partial^2}{\partial \rho^2} \Phi_0 \right] \right) \Omega,$$

where brackets indicate integration over all hyperangles. Numerically, $Q_{\rho0}$ is found to be extremely small compared to other terms and we will not include it in further calculations. In the following we will suppress the subscript 0.

2.1. Two-body potential models

Our main concern is the introduction of finite-range effects beyond the single-parameter zero-range approximation (where only the scattering length is included) but still using only contact interactions. There are different ways to do this. Here we use a boundary condition model (or range expansion model) and a two-channel model, and compare to the usual
zero-range approximation with only the scattering length. To make our discussion self-contained and well defined, we now proceed to introduce first the zero-range model with only the scattering length and then the two effective range models.

2.1.1. Zero-range model. The so-called zero-range models generally use a contact interaction potential which is defined by a boundary condition on the logarithmic derivative of the wavefunction at zero separation. In hyperspherical coordinates this boundary condition becomes

\[ \frac{\partial (\alpha_i \Phi)}{\partial a_i} \bigg|_{a_i=0} = -\sqrt{2} \rho \frac{1}{a_i} \alpha_i \Phi \bigg|_{a_i=0}, \tag{7} \]

where \( a_i \) is the scattering length between particles \( j \) and \( k \). Since all particles are equal we will suppress indices on scattering variables such as \( a \). Using the Faddeev decomposition of the angular wavefunction with \( s \)-states only,

\[ \Phi = \phi_1 + \phi_2 + \phi_3, \tag{8} \]

where

\[ \phi_1 = N(\rho) \sin \left( \nu \left[ a_i - \frac{\pi}{2} \right] \right) \tag{9} \]

is a solution to (4), \( \nu^2 = \lambda + 4 \) and \( N(\rho) \) is a normalization factor, we find the eigenvalue equation

\[ \nu \cos \left( \frac{\nu \pi}{2} \right) - \frac{8}{\pi^3} \sin \left( \frac{\nu \pi}{2} \right) = \sqrt{2} \rho \frac{1}{a}, \tag{10} \]

after rotating two of the Faddeev components into the coordinate system of the third [25]. For large positive \( \rho/a \) there is an asymptotic solution of the form \( \nu \to i \sqrt{2} \rho/a \) yielding a dimer binding energy of

\[ E_D = \frac{\lambda + 15}{8 \rho^2} = \frac{\nu^2 - \frac{1}{8}}{2 \rho^2} \approx -\frac{1}{\rho^2}, \tag{11} \]

(in units where \( h = m = 1 \)). For negative \( a \) there are no bound dimers. The limit \( \rho/a \to 0 \) yields the solution \( \nu = 1_0 \) with \( s_0 = 1.00624 \). These are the basic properties of the simplest single-parameter zero-range model when applied to a system of three identical bosons.

2.1.2. Effective range expansion. The first method for including finite-range effects beyond the scattering length is the effective range expansion (range expansion or boundary condition model for short). It is a generalization of the boundary condition (7). From scattering theory the effective range expansion of the phase shift \( \delta \) as a function of the wave number \( k \) is

\[ \lim_{k \to 0} k \cot \delta(k) = -\frac{1}{a} + \frac{1}{2} R k^2, \tag{12} \]

where \( a \) is the scattering length and \( R \) is the effective range. As it stands \( R \) is an additional parameter. However, later we will take \( R \) to be dependent on the scattering length \( a \), i.e. \( R = R(a) \), since this is the physical reality of Feshbach resonances, where both \( a \) and \( R \) are dependent on the external magnetic field (this effect arises naturally in the two-channel model described below). When we use \( R(a) \) in the effective range expansion we will be assuming the same functional dependence on \( a \) as found in the two-channel model (see equation (21)) since this is a generic feature of many Feshbach resonance models [6].

The boundary condition (7) now becomes (see [25])

\[ \frac{\partial (\alpha_i \Phi)}{\partial a_i} \bigg|_{a_i=0} = \sqrt{2} \rho \left[ -\frac{1}{a} + \frac{1}{2} \frac{R_i}{2 \rho^2} \right] \alpha_i \Phi \bigg|_{a_i=0}, \tag{13} \]

where \( R_i \) is the effective range between particles \( j \) and \( k \), and the momentum in (12) is given by \( k = \sqrt{2} \rho \) [25]. Again assuming that all particles are equal, the eigenvalue equation (10) becomes

\[ \frac{\nu \cos \left( \frac{\nu \pi}{2} \right) - \frac{8}{\pi^3} \sin \left( \frac{\nu \pi}{2} \right)}{\sin \left( \frac{\nu \pi}{2} \right)} = \sqrt{2} \rho \left[ -\frac{1}{a} + \frac{1}{2} R \left( \frac{\nu}{\sqrt{2} \rho} \right) \right]^2. \tag{14} \]

Inclusion of the effective range yields the dimer binding energy

\[ E_D = -\frac{1}{R^2} \left( 1 - \sqrt{1 - \frac{2 a}{\nu}} \right)^2 \approx -\frac{1}{a^2} \left( 1 + \frac{R}{a} \right), \tag{15} \]

for \( |R| \ll a \). Thus the dimer system can be more or less bound depending on the sign of the effective range. In the case of atomic Feshbach resonances the effective range is negative [6], yielding less bound dimers.

This model breaks down for sufficiently large positive effective ranges since there does not exist any solution to the eigenvalue equation (14) for \( \rho \lesssim R \) if \( R \) is positive. To remedy this deficiency an additional parameter known as the shape parameter, \( P \), can be included in (12) [25],

\[ \lim_{k \to 0} k \cot \delta(k) = -\frac{1}{a} + \frac{1}{2} \frac{Rk^2 + PR^3k^4}{a}, \tag{16} \]

and (13) gets a similar additional term. Typical values of \( P \) are around 0.1. However, we note that results from binding energy calculations are largely insensitive to the exact value of \( P \) [25]. We therefore fix \( P = 0.1 \) in this study. We again stress that when using (16) we take \( R = R(a) \) given in (21) in order to model Feshbach resonances.

2.1.3. Two-channel model. The other model for including finite-range effects that we consider is a two-channel contact interaction model that takes the internal degrees of freedom of the atoms into account. This model has background scattering lengths in open and closed channels that we denote by \( a_{\text{open}} \) and \( a_{\text{closed}} \), respectively. The full scattering length and effective range parameters of this model are (all details of this model are described in our previous work [36])

\[ \frac{1}{a} = \frac{1}{a_{\text{open}}} + \frac{\beta^2}{\kappa - \frac{1}{a_{\text{closed}}}}, \tag{17} \]

\[ R = \frac{-\beta^2}{\kappa (\kappa - \frac{1}{a_{\text{closed}}})}, \tag{18} \]

where \( \beta \) parametrizes the coupling between the channels and \( \kappa \) is given by the energy separation \( E^* - h^2k^2/2m_r \) between the channels, where \( m_r = \frac{m}{2} \) is the two-body reduced mass. The expressions are valid when \( a \gg \kappa^{-1} \) (equivalently \( E^* \gg h^2/2m_r a^2 \)), which is always the case near a Feshbach
resonance. At the resonance, i.e. \( a = \infty \), the effective range is [6]

\[
R_0 = - \frac{1}{a_{bg}} \frac{\hbar^2}{m_r \Delta \mu \Delta B},
\]

where \( \Delta B \) is the width of the resonance, \( \Delta \mu \) the difference in magnetic moments of the channels and \( a_{bg} \) the background scattering length (the value away from the given Feshbach resonance). The resonance width \( \Delta B \) and position \( B_0 \) as given in the phenomenological expression [6]

\[
a(B) \approx a_{bg} \left(1 - \frac{\Delta B}{B - B_0}\right),
\]

which can be derived in the two-channel model. The parameters \( a_{open}, a_{closed}, \beta \) and \( E^* \) can now be replaced by \( \Delta B, B_0 \), the difference in magnetic momenta \( \Delta \mu \) and the off-resonance scattering length \( a_{bg} \) to relate all quantities to physically measured values. Since we address neutral atom systems here, the long-range atom–atom interaction is of the van der Waals length, \( r_{vdW} \). It has been shown that the scattering length in a potential with a van der Waals tail is \( \sim 0.956 r_{vdW} \) [37]. For simplicity we will assume that \( a_{bg} = r_{vdW} \) and use the two interchangeably. This also means that we are working with \( a_{bg} > 0 \) throughout this paper. We have checked that the case with \( a_{bg} < 0 \) gives the same qualitative results. Off resonance the model predicts the effective range \( R \) in terms of \( R_0 \) and \( a \),

\[
R(a) = R_0 \left(1 - \frac{a_{bg}}{a}\right)^2,
\]

similar to the results obtained in [38–42]. Since the \( a \)-dependence of \( R \) of \( \text{(21)} \) should be generic for Feshbach resonances (independent of the particular scattering model used), we will use \( R = R(a) \) in both the effective range expansion model \( \text{(12)} \) and the two-channel model.

Note that the effective range is always negative since \( R_0 \) is always negative for an atomic Feshbach resonance [6], which in turn means that the two-channel model studied here will have \( R(a) < 0 \) always. Multi-channel calculations of resonance properties have shown that some Feshbach resonances can have positive \( R \) in the vicinity of the resonance (see for instance [10] for an example in \( ^7 \text{Li} \)). This is typically only found for broad resonances (with \( \Delta B \) large and correspondingly small \( |R_0| \)). For narrow resonances with \( \Delta B \) small, \( |R_0| \) is large and can potentially cause non-negligible corrections to the zero-range models; this is the case we are interested in here. Around the latter type of resonance the effective range, \( R(a) \), is found to be negative. The two-channel model we employ here is only applicable to those Feshbach resonances where the effective range is negative.

### 2.2. Model comparison

Before we consider the recombination rates and the binding energies in the different models, we first make a comparison of the two-body potential models in terms of their predictions for the \( \nu^4 = \lambda + 4 \) coefficient that provides the effective potential for the three-body system in the hyperradial equation (5). We compare the models by explicitly plotting their associated eigenvalues in figure 1. At large \( \rho \) all models have the same asymptotic value \( \nu^4 = -2 \rho^2 / a^2 \). This is because we have a two-body bound state for \( a > 0 \), i.e. the structure is that two particles are bound and have a small interparticle distance while the third particle is far away. This is more clearly illustrated in the inset of figure 1 where the horizontal axis extends up to \( \rho / a_{bg} = 1000 \). For intermediate distances \( \rho \lesssim 2 |R_0| \), the finite-range models show surprisingly similar forms given their quite different formalism. What is particularly important to note is the fact that an inner pocket develops in the two-channel model, but at the same time a barrier with respect to the zero-range model is also seen. For \( \rho < |R_0| \), the effective range expansion model eigenvalue goes to zero, and thus effectively becomes regularized. There is no need for a three-body parameter (in the form of a high-momentum cut-off in momentum-space or a short-distance cut-off in coordinate space). This is not the case for the two-channel model we use here. It requires a cut-off at small distance when calculating e.g. bound state energies \( \text{(25)} \) and the recombination rate \( \text{(24)} \). This can be understood by considering that the two-channel model consists of two single-channel models that are coupled together by a coupling potential of zero range. This means that there is no scale coming from the coupling that can regularize the three-body problem and in turn one still needs to introduce a short-distance cut-off as discussed in [36].

### 3. Finite-range effects in the recombination rate

We now proceed to consider three-body observables starting with the recombination rate on the positive \( a \) side of the Feshbach resonance. On this side of the resonance the recombination takes place by the transition of two of the three particles into the channel with a bound two-body dimer with the universal binding energy proportional to \( -a^{-2} \). On the \( a < 0 \) side where there is no bound dimer, the decay goes directly into some strongly bound two-body state of the atom–atom potential and depends on the short-range details. This latter case will not be considered here.
The recombination rate for $a > 0$ is calculated using the semi-classical WKB method of hidden crossing theory where the recombination coefficient $\alpha$ is [18]

$$\alpha = 8(2\pi)^2 3\sqrt{\frac{\hbar}{m_r}} \lim_{k \to 0} \frac{P(k)}{k^4},$$

(22)

with the wave number $k$ defined by $E = \hbar^2 k^2 / 2m_r$. The transition probability $P(k) \equiv |S_{01}(k)|^2$, with $S_{01}$ the transition matrix element between adiabatic channels 0 and 1, is [18]

$$P(k) = 4 e^{-2\pi} \sin^2 \Delta,$$

(23)

$$\Delta + i\Sigma = \int_C d\rho \sqrt{k^2 - \frac{v(\rho)^2}{\rho^2}},$$

(24)

where the integral is taken along a contour $C$ in the complex $\rho$-plane connecting the adiabatic channel corresponding to three free particles, $n = 1$, to the channel describing a dimer and a free particle, $n = 0$. The integration path $C$ goes around a so-called branchpoint $\rho_b$ that connects the two channels. Additional details can be found in [36]. Note that since $v_0^2(0) < 0$ for the zero-range and two-channel models, there is no classical turning point in the open ($n = 1$) channel; thus we employ a regularization cut-off in order to avoid a divergent integral.

The perhaps more familiar form $\alpha = C(a) a^2 / m$ (as for instance found in [4]) can be found from the above equations in the universal limit ($a = \infty$) of the single-channel model (where $v(\rho) = 1/\rho_0$). Here $C(a)$ is a log-periodic function of $a$. We can now split the integral into two parts: one from the cut-off $\rho_{cut}$ to the real part of the branchpoint $\rho_b$ and another from the rest. If we denote the first part by $\Delta_1 + i\Sigma_1$, then we have the result $\Delta_1 = s_0 \log(\text{Re}(\rho_b)/\rho_{cut})$ and $\Sigma_1 = 0$. The vanishing of the imaginary part comes about since the potential is negative in the lower branch and $k^2$ is positive, thus yielding a purely real integrand. Now, the branchpoint is simply related to $a$ by $\rho_b = (1.8327 + 2.1029 a) a$ in the single-channel model and thus $\text{Re}(\rho_b) \propto a$. When plugging this into (23) the log-periodic dependence is established. The rest of the integration path only leads to a constant phase-shift independent of $a$ since $v(\rho)$ only depends on the ratio $\rho / a$, see equation (10). The $a^4$ dependence is most easily seen by dimensional analysis, $k$ has units of inverse length and the only available length scale in the zero-range model is the scattering length $a$.

The recombination coefficients for different values of the effective ranges and different models are shown in figure 2. The scattering length values $a_1^\ast$ and $a_2^\ast$ indicate locations of minima in the recombination rate. The minima are caused by the vanishing of bound trimers into the atom-dimer continuum. The cut-offs were chosen such that the minimum at $a_2^\ast$ is the same for all models. We can thus compare the models at the other minimum. For the zero-range model, the ratio of $a_2^\ast$ to $a_1^\ast$ is 22.7, showing that this calculation scheme agrees with the universal result. For the other models this ratio is reduced, and the minimum at $a_1^\ast$ moves towards higher $a$. In order to make this more clear we plot the ratios of the minima positions as a function of the effective range, $R$, in figure 3. We see that the two-channel and range expansion models give similar qualitative predictions but there are overall quantitative differences. We cannot extend the curves in figure 3 all the way to $R = 0$ due to numerical difficulties, but the trends should be clear. What we also see is that the scale factor reduces quite drastically at large $R_0$ for both models. This corresponds to narrow Feshbach resonances, where there are currently not enough experimental data to make a detailed comparison.

3.1. Cut-off effects on binding energy

As we noted above, we need to put a cut-off on the WKB integral in order to render it finite. We therefore need to consider the behaviour of the results as we change this cut-off. In particular, the choice of cut-off affects the trimer binding energy. The WKB approximation yields a simple estimate of bound state energies (similar to the Bohr–Sommerfeld quantization rule)

$$\int_{\rho_{cut}}^\hbar d\rho \sqrt{2E_n - \frac{v_0(\rho)^2}{\rho^2}} = \pi \left( n - \frac{1}{4} \right),$$

(25)

where $n = 1, 2, \ldots$ indicate the ground state, first excited, etc. $\rho_{cut}$ is defined at the end of section 2. It is required since the potential $v_0^2/\rho^2$ diverges as $\rho \to 0$ and $\rho_{cut}$ acts as the
innermost turning point in the WKB approximation. Likewise \( \rho_0 \) is the outermost turning point where \( 2E_n = v_0(\rho_0)^2 / \rho_0^2 \).

In the universal limit \( a \to \infty \) where \( v_0(\rho) = i\kappa_0 \), \( E_n \) is given by

\[
E_n \approx -\frac{2\pi^2}{\rho_{\text{cut}}^2} \exp\left( -\frac{2\pi n}{x_0} + \frac{\pi}{2x_0} - 2 \right),
\]

(26) clearly showing the geometric scaling \( E_{n+1} = e^{-2\pi / n} E_n \approx E_n / 22.7 \) and the Thomas effect \( E_n \to -\infty \) for \( \rho_{\text{cut}} \to 0 \).

Now we show that the cut-offs chosen such that the recombination minima at \( a^*_n \) in figure 2 coincide for the three models lead to similar trimer binding energies. Solving (25) numerically for finite scattering length gives trimer binding energies at e.g. \( a = 500, R = -10, n = 2 \) (in units of \( \hbar^2 / ma_{bg}^2 \)):

- Zero-range : \( E_T = -0.002 \, 060 \)
- Two-channel : \( E_T = -0.002 \, 441 \)
- Effective range : \( E_T = -0.002 \, 062 \),

which shows that the chosen cut-offs give similar bound state energies for the different models. The effect of this choice of cut-off is thus under control.

4. Bound trimers

In order to further study the three-body physics and its dependence on two-body interaction models, we now consider the three-body bound state spectrum when finite-range effects are included. When the scattering length \( a \) is large, (25) yields the same binding energy values as the radial equation (5). However, for the following discussion we will solve the radial equation numerically (5) to obtain accurate results also when the binding energy is close to zero. We solve the radial equation (5) numerically for \( f(\rho) \) with the boundary condition \( f(\rho_{\text{max}}) = 0 \) for some large hyperradius \( \rho_{\text{max}} \). The value of \( \rho_{\text{max}} \) is chosen such that the bound state energy converges to the desired degree of accuracy. Also, the aforementioned cut-off \( \rho_{\text{cut}} \) is used in the boundary condition \( f(\rho_{\text{cut}}) = 0 \).

For the three models in question we have calculated \( E(\alpha) \) for the three lowest trimers, and the result is shown in figure 4. For positive \( \alpha \) the dashed line indicates the atom-dimer threshold which is given by the dimer binding energy \(-1/\alpha^2\) for the zero-range model and by (15) for the effective range expansion model. For the two-channel model this can be calculated only numerically, yet it agrees surprisingly well with the analytical formula for the effective range expansion model (15). The cut-offs (on the coordinate-space hyperspherical potential) were chosen such that the second trimer (\( n = 2 \)) energies coincide at \( |\alpha| = \infty \). The three spectra for \( n = 3 \) are virtually identical. This is reasonable since the binding energy is very small for \( n = 3 \) and the state is almost completely insensitive to finite-range effects. However, for the ground state \( n = 1 \) a clear distinction between the models appears. At \( |\alpha| = \infty \) the finite-range models give practically the same trimer energy, a factor of \( \sim 25.3^2 \) times higher than the \( n = 2 \) state. In comparison, the zero-range model trimer energy is only a factor of \( 22.7^2 \) times higher.

We have already seen that the ratio of \( a \)-values corresponding to recombination minima in figure 2 differs from the universal value 22.7. This is directly related to the change in the atom-dimer threshold shown in figure 4 since the ratio between \( a \) corresponding to trimer energy termination points on the threshold line is no longer 22.7 for the models incorporating effective range effects.

For negative \( \alpha \), the value of \( a^*(-\alpha) \) indicates the threshold scattering length for creation of the lowest Efimov trimer, as indicated in figure 4. When written in units of \( r_{\text{vdW}} \), this quantity is the subject of much recent discussion since it seems to have a universal value of \( a^* \sim -9r_{\text{vdW}} \) for different cold atomic systems [15]. Here we want to address finite-range effects on the value of \( a^* \) for the two models. Some other recent works that address finite-range effects on this threshold value can be found in [30] and [19].

Our results within the different models for \( a^*(-\alpha) \) as a function of \( R_0/a_{bg} \) are shown in figure 5. Most notable is the lowering of \( a^*(-\alpha) \) for the finite-range models compared to the zero-range model. This is partly due to the lower binding energy \( E_T^{(\infty)} \) at \( |\alpha| = \infty \). The product \( a^*(-\alpha)^2 \) (where \( -\hbar^2 \kappa^2 / 2m_e = E_T^{(\infty)} \) is universal in the zero-range model with the value \(-1.5076 \) [43]. Thus increasing \( E_T^{(\infty)} \) will reduce \( |a^*(-\alpha)| \). This effect is, however, not enough to account for the deviation from the zero-range result. The product is further reduced for decreasing \( R_0 \), indicating a lower value of \( a^*(-\alpha) \).

Both finite-range models show the same trend. However, the value of the change is different for the two models when \( R_0 \) gets sufficiently large. The plot also shows that for the two-channel model the effect depends on the cut-off. The cut-off, chosen for the purpose of illustration but with reasonable values, is 0.5, 0.6 and 0.7 for the top, middle and bottom blue curves, respectively, in figure 5. The effective range expansion model shows only a very small dependence on the cut-off (the three green curves in figure 5 show very little deviation). The opposite behaviour, i.e. \( a^*(-\alpha)^2 \) gets larger for the larger effective range, is found for \( R_0 > 0 \). To obtain results for this case we use the
boundary condition including the shape parameter (16) in the effective range expansion model in order to extend it to the positive effective range. Indeed, we find that the change is now opposite, see figure 5. This is similar to the product $a^{(-)} \kappa^*$ found in [22]. We note, however, that it is found in [22] that the trimer binding energies for $|a| = \infty$ get smaller and the value of $|a^{(-)} |$ gets larger for the large effective range. This is not seen in our calculations. This can be connected to the use of finite-range potentials with positive effective range.

In order to better understand the behaviour of the trimer energies and $a^{(-)}$, figure 6 shows the ratio of trimer bound state energies on resonance ($|a| \to \infty$) for the two-channel and range expansion models for three different cut-offs, chosen for the purpose of illustration. The most notable feature is the rise and fall of the ratio of the ground state energy $E^{(1)}$ to the first excited state energy $E^{(2)}$ for the two-channel model for negative $R_0$. This non-monotonic behaviour can be understood if one assumes a three-body wavefunction that lives at large hyperradii, $\rho$. When the effective range is increased from zero (|$|\rho|\|$ increases) a barrier with respect to the pure zero-range model initially decreases the binding energy. This can be clearly seen in figure 1. As we increase the effective range further the wavefunction will leak into the attractive pocket at small $\rho$, which will again increase the binding compared to the pure zero-range result. This effect is strong for the ratio of the two lowest trimers but becomes weak for the ratio of the two highest trimers. This is understandable since the least bound trimer resides at very large hyperradii and is largely insensitive to the changes in the hyperradial potential at small $\rho$ due to the effective range correction.

With this interpretation the behaviour can now be better understood. In figure 7, we plot the solution to (4), which determines the effective three-body hyperradial potential for the different models and for different signs of the effective range. The finite-range corrections for the two-channel model and the effective range models are very different as one has the inner pocket and the other does not. This is the origin of the differences seen in figure 6. Initially, we see a repulsive effect compared to the pure zero-range model that drives the ratio upwards as all states are pushed out to large distance. However, for the two-channel model we eventually feel the presence of the inner pocket and states will leak into smaller hyperradii where the ratio of energies is in turn driven down. For the positive effective range case we see from figure 7 that the range expansion model will now have a pocket at small distance. The trimer states can leak into this pocket and the ratio of energies will again go down. The important point is that in the models we have presented here there is no reason to expect monotonic behaviour since the effective three-body hyperradial potentials have non-trivial structure with repulsive and attractive parts in comparison to the pure zero-range model with no effective range corrections.

Figure 5. The product $\kappa^* a^{(-)}$ as a function of the effective range, $R_0$, where $-\hbar^2k^2/2m_0 = E_T^{(\infty)}$; $E_T^{(\infty)}$ is the trimer binding energy at resonance ($a = \infty$) and $a^{(-)}$ is the threshold scattering length for trimer creation (see figure 4). The universal value $\kappa^* a^{(-)} = -1.5076$ for the zero-range model is not correct for the lowest trimer, where the value is $-1.469$, independent of cut-off. The two-channel model curves are for different value coordinate-space cut-offs on the hyperradial potential. The cut-off is $0.5$, $0.6$ and $0.7$ in units of $a_0$ for the top, middle and bottom blue curves, respectively. For the effective range expansion model the dependence on the cut-off is insignificant. Note that the two-channel model only works for $R_0 < 0$.

Figure 6. Ratio of trimer bound state energies at resonance as a function of the effective range for several different cut-offs. The solid lines show the ratio of energies for the first and second state, and the dashed lines for the second and third state. The red, yellow and blue curves (top three in the legend) are for the two-channel model, while the green, cyan and magenta curves (bottom three in the legend) are for the range expansion model.

Figure 7. The eigenvalue solutions to (4) as a function of the hyperradius, $\rho$, for the zero-range, two-channel model and range expansion model for a representative case with $|R_0| = 5a_0$. The lowest adiabatic potentials multiplied by $\rho^2$ as functions of the hyperradius, $\rho$, for the zero-range one-channel model and three different effective ranges for the two-channel model.
5. Conclusion

We investigate finite-range effects in three-body recombination rates in cold atomic gases near Feshbach resonances as well as finite-range effects in the trimer bound state energy spectrum. We use two models which include the finite-range effects and compare their results with a contact interaction (i.e. zero-range) model. The first model is the range expansion model which is a straightforward extension of the zero-range contact interaction model. Here the effective range is included directly in the boundary condition on the three-body wavefunction following the effective range expansion of standard scattering theory. Variation of the scattering length through the Feshbach resonance is done phenomenologically as in the zero-range model. This model can also be used for positive effective range calculations. The second model is a two-channel contact interaction model which naturally includes both the finite effective range and the variation of the scattering length through the Feshbach resonance.

We show that with these well-tested two-body interaction models the three-body physics can display complicated non-monotonic behaviour as the effective range is varied. In particular, we find that the geometric scaling factor of 22.7 for equal mass particles changes when including range corrections, and that it can become both larger and smaller than 22.7 depending on the magnitude and sign of the effective range.

In the current setup this can be understood based on the functional form of the effective hyperradial potential. On resonance where the scattering length diverges, the lowest trimer bound state has the strongest dependence on the effective range since it lives at small hyperradii, whereas the excited states live at much larger hyperradii and the effective range contribution is much less pronounced. The adiabatic potential of the range expansion model is raised and lowered relative to the zero-range model potentials when the effective range is negative and positive, respectively. This leads to bound states being less or more bound, respectively. For the two-channel model the effective range is always negative which can only be achieved by using potentials with an outer barrier. The hyperradial potential reflects this fact and develops a pocket at small hyperradii that the lowest states will eventually leak into. This feature is similar to the range expansion model but for the case of a positive effective range.

Our results demonstrate that effective range corrections within the framework of contact model potentials can lead to non-trivial behaviour of trimer energies, thresholds and interference features in recombination rates. Effective range corrections are expected to be important for the case of narrow Feshbach resonances. The experimental data on Efimov states for narrow resonance systems are sparse and more measurements are needed in order to fully discriminate between different models that include finite-range corrections. However, what we can conclude is that care must be taken when a particular two-body scattering model is used for the trimer states that have the largest binding energies in a universal setup, i.e. for the lowest states that have binding energies related to the background short-range scales. For higher lying trimers it is less important since the states are largely insensitive to the short-distance behaviour of the effective three-body potential.

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