Mass-imbalanced three-body systems in two dimensions

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Abstract
We consider three-body systems in two dimensions with zero-range interactions for general masses and interaction strengths. The momentum-space Schrödinger equation is solved numerically and in the Born–Oppenheimer (BO) approximation. The BO expression is derived using separable potentials and yields a concise adiabatic potential between the two heavy particles. The BO potential is Coulomb-like and exponentially decreasing at small and large distances, respectively. While we find similar qualitative features to previous studies, we find important quantitative differences. Our results demonstrate that mass-imbalanced systems that are accessible in the field of ultracold atomic gases can have a rich three-body bound state spectrum in two-dimensional geometries. Small light–heavy mass ratios increase the number of bound states. For 87Rb–87Rb–6Li and 133Cs–133Cs–6Li we find respectively three and four bound states.

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

1. Introduction
Manipulating quantum systems on large, small and intermediate scales is no longer a distant dream. Ultracold quantum gas experiments have realized Bose–Einstein condensates [1] and degenerate Fermi gases [2] and study truly remarkable many-body states, but it has also proven its worth in exploring the physics of few-body systems [3]. Moreover, these studies can be conducted in different geometries as two- and one-dimensional quantum systems are produced regularly in laboratories [1].

The so-called Efimov three-body bound states were predicted over four decades ago [4]. They arise when a three-body system, composed of equal mass particles, has all its two-body subsystems at the threshold of binding. In this case, infinitely many bound states with energies geometrically separated are expected. These are the Efimov states and this effect is called the Efimov effect. The effect is related to a long-range effective force and can occur even when the individual two-body forces have zero range, as shown in an analytically solvable model by Fonseca, Redish and Shanley [5]. This is an example of how long-range forces can arise in the three-body problem in a way unpredictable by two-body intuition. In the early work of [5], the Efimov problem was handled through the adiabatic approximation, more precisely the Born–Oppenheimer (BO) approximation that is commonly used in molecular physics. The BO approximation considers a system composed of two heavy and one light particle. The terms heavy and light have relative meaning: two particles are heavier than the third one. In this approximation the heavy particles move very slowly while the light particle orbits around them. In fact, it is enough to assume that the kinetic energy of heavy particles is (much) smaller than the kinetic energy of light particles.

These results relating the Efimov effect and the adiabatic approximation were obtained for three-dimensional (3D) systems. The dynamics and properties of quantum systems drastically change when the system is restricted to lower dimensions. For example, the scattering length is not well
defined for two-dimensional (2D) systems [6] and the kinetic energy operator gives a negative centrifugal barrier for 2D systems with zero total angular momentum while the centrifugal barrier is always non-negative for 3D systems. Furthermore, it was shown that any infinitesimal amount of attraction produces a bound state in 2D [7–10], while a finite amount of attraction is necessary for binding a 3D system.

Another important difference between 2D and 3D systems is the occurrence of the Efimov effect. The effect does not occur in 2D neither for equal mass three-body systems [11] or unequal mass systems [12]. While the BO approximation was implemented in [12] to look for the Efimov effect in 2D imbalanced mass three-body systems, the mass-dependence of such systems was not addressed. The importance of the mass-dependence in the 2D imbalanced mass three-body systems was stressed in [13, 14], where an increasing number of bound states was found for a decreasing mass of one particle. This situation, where one particle is much lighter than the other ones, is suitably handled in the adiabatic approximation.

In this work we study the BO approximation of 2D three-body systems from the mass-dependence perspective in a systematic fashion. We consider a 2D three-body system with zero-range interactions for general masses and interaction strengths. The momentum-space Schrödinger equation is solved numerically both in full generality and in the BO approximation. The BO expression is derived using separable potentials and yields a concise adiabatic potential between the two heavy particles in the heavy–heavy–light system when the light particle coordinate is integrated out. The adiabatic potential is mass-dependent and it reveals an increasing number of bound states for the decreasing mass of the light particle. We find a transcendental equation that describes the adiabatic potential and an approximate analytic expression as well as the asymptotic form. Furthermore, we show that the approximate analytic form of the potential is very close to the full adiabatic potential.

Furthermore, we estimate the number of bound states for a heavy–heavy–light system as a function of the light–heavy mass ratio. Infinitely many bound states are expected as this ratio approaches zero. However, for each given mass configuration, we still have a finite number of bound states. Our results demonstrate that mass-imbalanced systems that are accessible in recent ultracold atomic gases experiments can have a rich three-body bound state spectrum in 2D geometries, where small mass ratios increase the number of bound states. For $^{87}$Rb–$^{87}$Rb–$^6$Li and $^{133}$Cs–$^{133}$Cs–$^6$Li we find, respectively, three and four bound states.

The paper is structured as follows. The introduction in section 1 is followed by the 2D three-body system formalism for zero-range interactions and general masses in the BO approximation in section 2. The BO approximation and the adiabatic potential are shown in section 3. The results are presented in section 4 and a discussion is given in section 5.

2. Formalism

The general setup that we consider has particles that are always confined to a 2D plane of motion, i.e. the kinematics is always 2D. However, we do not rule out systems with long-range interactions across many 2D planes (as done in recent experiments with polar molecules [15]). Both of these situations are shown in figure 1 for the most general case with three different particles $A$, $B$ and $C$. The only assumptions concerning the interactions is that they are dependent only on the relative distance of the particles under consideration. We can then assume that the three-particle dynamics effectively happens in a single plane, since we may consider the layer index as an additional quantum number that specifies a few-body state.

Here we only consider zero-range interactions since we are interested in the model-independent low-energy universal limit. This limit emphasizes universal behaviour that should be independent of the particular system under study. In general, the validity of the approximation can be established by comparing the typical energy scale of the two-body interactions at short-range, i.e. for atomic systems this would typically be the van der Waals length, $r_{vdW}$. In order for the bound states to be universal and the zero-range interaction limit to apply, we need the binding energy, $|E_3|$, to satisfy $|E_3| \ll \frac{\hbar^2}{mr_{vdW}}$. We will assume that we are in this universal regime throughout the paper. The zero-range limit provides a simplification of the Faddeev equation for the three-body bound state due to the separability of the zero-range interaction. In the case where we have long-range interaction across different layers and we have to assume that at low
energy, the long-range forces may be approximated by a short-range pseudopotential that reproduces the two-body properties of the full potential. As discussed in [16], this can be done for potentials that decay faster than $r^{-2}$ for $r \to \infty$. This includes the case of dipolar $r^{-3}$ interactions, which we will return to at the end of this paper.

The 2D Hamiltonian for the three-particle $ABC$ system with pairwise two-body potentials is

$$H = H_0 + V_{AB} + V_{AC} + V_{BC}$$

(1)

where the three particles are, in principle, assumed to be bosons. However, for three different mass particles there is no symmetry requirements. Our formalism takes the symmetry fully into account when two particles are identical bosons.

The kinetic energy operator is

$$H_0 = \frac{q_A^2}{2\mu_{A,B,C}} + \frac{q_B^2}{2\mu_{B,C}} + \frac{q_C^2}{2\mu_{C,AB}} + \frac{p_A^2}{2\mu_{A,B}} + \frac{p_B^2}{2\mu_{B,C}} + \frac{p_C^2}{2\mu_{C,AB}}$$

(2)

where we use Jacobi relative momenta given in terms of rest frame momenta, $k_i$ with $i = \alpha, \beta, \gamma$, as

$$q_i = k_i - \mu_{\alpha\beta} \left( \frac{k_{\alpha}}{m_{\alpha}} - \frac{k_{\beta}}{m_{\beta}} \right)$$

(3)

where $(\alpha, \beta, \gamma)$ is the cyclic permutations of particles $A$, $B$ and $C$ with masses $m_A$, $m_B$, and $m_C$. The reduced masses are $\mu_{\alpha\beta} = \frac{m_{\alpha} m_{\beta}}{m_{\alpha} + m_{\beta}}$ and $\mu_{\gamma,\alpha\beta} = \frac{m_{\gamma}(m_{\alpha} + m_{\beta})}{m_{\alpha} + m_{\beta} + m_{\gamma}}$. We use a separable potential with operator form

$$V_{\alpha\beta} = \lambda_{\alpha\beta} \langle \chi_{\alpha\beta} \rangle \langle \chi_{\alpha\beta} \rangle,$$

(4)

where the form factor is $\langle p_i \rangle \langle \chi_{\alpha\beta} \rangle = g(p_i)$, depends only on the relative momentum of the two particles $\alpha$ and $\beta$. The limit to zero-range interaction is simply $g(p) = 1$.

In order to relate the separable potential ansatz above to physical properties of the two-body system we use the two-body T-matrix. For negative energies and zero-range potentials it is defined by

$$T_{\alpha\beta}(E) = \langle \chi_{\alpha\beta} \rangle \tau_{\alpha\beta}(E) \langle \chi_{\alpha\beta} \rangle,$$

(5)

where the matrix element of the 2D transition matrices are given by (see e.g. [17] for the case of identical particles)

$$\tau_{\alpha\beta}(E) = \frac{-4\pi \mu_{\alpha\beta} \hbar^2}{E} \ln \left( \frac{E}{E_{\alpha\beta}} \right)^{1},$$

(6)

where $\alpha, \beta = A, B$ or $C$ and $\alpha \neq \beta$. $E_{\alpha\beta}$ is the energy of the $\alpha\beta$ two-body bound state. We will measure all three-body energies in units of the two-body energy. In general systems where $A$, $B$, and $C$ are different, one only needs to make a specific choice between the $E_{\alpha\beta}$. We will explicitly state our units in these cases. Also it is important to know that $E_{\alpha\beta} = 0$ corresponds to a non-interacting $\alpha\beta$ system since $\tau_{\alpha\beta} \rightarrow 0$ in this case. This is different from 3D where a two-body bound state at zero energy happens at unitarity, i.e. where the interactions are as strong as allowed by the unitary limit of quantum mechanics applied to the s-wave scattering amplitude.

In order to solve for three-body bound states, the wave function $|\Psi_{ABC}\rangle$ is decomposed in terms of the Faddeev components as

$$|\Psi_{ABC}\rangle = |\Psi_A\rangle + |\Psi_B\rangle + |\Psi_C\rangle,$$

(7)

where $|\Psi_{\gamma}\rangle = G_0(E)|\chi_{\alpha\beta}\rangle|\Psi_{ABC}\rangle$ with the resolvent $G_0(E) = (E - H_0)^{-1}$ which is nonsingular for bound states. The bound state equation can be solved by the method described in [13] for AAB systems with some straightforward generalizations to the ABC structure. We therefore refer to [13] for the details of the formalism and do not repeat them here. Instead we now proceed to discuss the adiabatic approximation.

3. The adiabatic approximation

We now consider two heavy particles with masses $m_A$ and $m_B$. These particles are fixed and their centres are separated by a distance $R$. The additional light particle has mass $m_C$ and coordinate $r$ relative to the centre-of-mass of the heavy subsystem. The configuration and coordinates are depicted in figure 2. We assume that the particles interact with each other through short-range potentials. The notation for the potential is that $v_C$ means the interaction between particles $A$ and $B$ and $v_A$ and $v_B$ are analogously defined. The three-body Hamiltonian is given by

$$H = \frac{p_A^2}{2\mu_{A,B}} + \frac{q_C^2}{2\mu_{C,AB}} + v_A + v_B + v_C,$$

(8)

where the Jacobi relative momenta and reduced mass definitions are given in (3). The Schrödinger eigenvalue equation is $H\Psi(r, R) = E\Psi(r, R)$ where $H$ is given by

$$H = -\frac{\hbar^2}{2\mu_{A,B}} \nabla_r^2 + \frac{\hbar^2}{2\mu_{C,AB}} \nabla^2_R + v_A \left( \frac{r - \mu_{A,B}}{m_A} R \right) + v_B \left( \frac{\mu_{A,B}}{m_B} R \right) + v_C(R).$$

(9)
The adiabatic approximation now instructs a split of the three-body eigenvalue equation into the solution of two two-body problems: the light particle motion is considered with respect to the heavy–heavy system and the heavy–heavy system motion is separated out. These eigenvalue equations will be useful whenever the motion of the light particle is rapid compared to the motion of the heavy ones, so that the light particle dynamics can be solved while the heavy particles are instantaneously at rest. The wave function is written as

\[ \Psi(r, R) = \psi(r, R)\phi(R), \]

where \( \psi(r, R) \) is the wave function describing the motion of the light particle for fixed \( R \) and \( \phi(R) \) is the heavy–heavy system wave function. The approximation is valid when the kinetic energy, \(-\frac{\hbar^2}{2\mu_{AB}}\nabla^2_{\psi} + \nu_A(r - \frac{\mu_{AB}}{m_B} R) + v_B(r + \frac{\mu_{AB}}{m_A} R)\), plays the role of an effective potential in the equation describing the heavy–heavy particle system, i.e.

\[ \left( -\frac{\hbar^2}{2\mu_{AB}}\nabla^2_{\psi} + \nu_C(R) + \epsilon(R) \right) \phi(R) = E\phi(R). \]

(11)

Assuming that the potentials in (11) are separable and have the same strength, i.e. \( \nu_a = \lambda |\chi_{a0}\rangle \langle \chi_{a0}| \), the light particle wave function in (11) in momentum space reads

\[ \tilde{\psi}(p) = \lambda \frac{g(p)}{\epsilon(R) - \frac{\hbar^2}{2\mu_{AB}}p^2} \left[ e^{\frac{\lambda_{AB} p}{\hbar} A_+} + e^{-\frac{\lambda_{AB} p}{\hbar} A_-} \right]. \]

(13)

where

\[ \begin{align*}
A_+ &= \int d^2r' \tilde{\psi}(r') \left( r' + \frac{\mu_{AB}}{m_B} R \right) \Psi(r') \\
A_- &= \int d^2r' \tilde{\psi}(r') \left( r' - \frac{\mu_{AB}}{m_B} R \right) \Psi(r')
\end{align*} \]

(14)

(15)

Rewriting (13) in terms of \( A_{\pm} \), we find the system of equations

\[ A_{\pm} = \lambda \int d^2p \frac{|g(p)|^2}{\epsilon(R) - \frac{\hbar^2}{2\mu_{AB}}p^2} \left( e^{\gamma_{AB} R} A_+ + A_- \right). \]

(16)

The non-trivial solution of (16), i.e. \( A_\pm \neq 0 \), gives a transcendental equation for the energy, which reads

\[ \frac{1}{\lambda} = \int d^2p \frac{|g(p)|^2}{\epsilon(R) - \frac{\hbar^2}{2\mu_{AB}}p^2} \left[ 1 + \cos \left( \frac{p \cdot R}{\hbar} \right) \right]. \]

(17)

We now use the binding energy of the two-particle heavy–light subsystem, \( E_2 \), and the T-matrix to eliminate \( \lambda \) [6]. This yields

\[ \int d^2p |g(p)|^2 \left[ 1 + \cos \left( \frac{p \cdot R}{\hbar} \right) \right] \frac{1}{\epsilon(R) - \frac{\hbar^2}{2\mu_{AB}}p^2} + \frac{1}{|E_2| + \frac{\hbar^2}{2\mu_{AB}}p^2} = 0. \]

(18)

Since we are interested in low-energy, model-independent bound states, we describe the heavy–light particle system interacting through zero-range interactions. In momentum space this means that \( g(p) = 1 \), so (18) is finite and its two terms can be integrated to give the transcendental equation

\[ \log \frac{|\epsilon(R)|}{|E_2|} = 2K_0 \left( \frac{2\mu_{AB}\epsilon(R)|R|}{\hbar^2} \right), \]

(19)

where \( K_0 \) is the zero order modified Bessel function of the second kind. Equation (19) is a powerful tool in understanding mass-imbalanced three-body systems in two dimensions. We are able to solve it to obtain an analytic form for the small and large distance behaviour of the adiabatic potential. We can also numerically solve it to test the validity of the analytical expressions.

When the separation, \( R \), between the two heavy particles is large, i.e. \( |R| \to \infty \), the light particle only feels the interaction from one of the heavy particles. In this limit, the three-body problem becomes a two-body problem and we expect that \( |E| = |E_2| \). Thus, defining \( |\epsilon(R)| = |E_2| + V(R) \), this condition is fulfilled when \( V \to 0 \) for \( |R| \to \infty \). Inserting these definitions into equation (19) and expanding both sides up to first order in \( V(R) \), we obtain

\[ V(R) = \frac{2|E_2| |K_0(s(R))|}{1 + s(R) K_1(s(R))}, \]

(20)

for \( R \to 0 \) (where \( \gamma \) is Euler’s constant). For large arguments, \( R \to \infty \), the adiabatic potential becomes

\[ \frac{|\epsilon_{\text{asymp}}(R)|}{|E_2|} \to 1 + \frac{2K_0(s(R))}{1 + s(R) K_1(s(R))} \quad \text{for} \quad R \to \infty. \]

(22)

Once the adiabatic potential is known, we can solve equation (12) and determine the bound state spectrum. In order to write a Sturm–Liouville eigenvalue equation for the heavy–heavy system in a \( L_z = 0 \) state, we set \( \phi = \frac{\lambda}{\sqrt{\lambda}} \) and equation (12) becomes

\[ \left[ -\frac{\hbar^2}{2\mu_{AB}} \frac{\partial^2}{\partial R^2} + v_C(R) + \epsilon(R) \right] \psi(R) = E \psi(R). \]

(23)
with the adiabatic potential from equation (19) given in the limits of \( R \to 0 \) and \( R \to \infty \) by (21) and (22), respectively.

Due to the behaviour of the adiabatic potential at small \((1/R \text{ Coulomb-like})\) and large distances (exponential decrease with \(\sqrt{m_C}\)), we expect to find an increasing number of bound states when particle \( C \) is much lighter than the other ones (\(m_C \to 0\)). In this limit, the adiabatic potential becomes more attractive and these states will accumulate both at \( R \to 0 \) as the strength of the \(1/R \) Coulomb-like potential increases, see (21), and at \( R \to \infty \), where more states are allowed because the exponential cut off moves to larger distances, see (22). However, for finite \( m_C \), the number of bound states is still finite.

Although we cannot address the limit \(|E_2| \to 0\) in (21) and (22) in the current paper, it is worthwhile to point out that the limit where all subsystems interacting through zero-range interactions are unbound \((|E_2| \to 0)\) does not support three-body bound states in two dimensions [11, 12, 14]. However, recent studies show that these so-called Borromean states are possible in 2D, but only for potentials with an outer barrier and an inner attractive pocket [19, 20].

4. Results

4.1. Adiabatic potentials

We found analytical forms for the small, (21), and large, (22), distance behaviour of the adiabatic potential. Once we are able to numerically compute the exact adiabatic potential from equation (19), we must show that our asymptotic behaviours in (21) and (22) are consistent with the exact adiabatic potential.

The exact potential, \(\epsilon_{\text{exact}}(s)\), obtained numerically from equation (19) is shown in figure 3 and compared to \(\epsilon_{\text{asymp}}(s)\) of equations (21) and (22). The asymptotic behaviour does indeed work very well for most of the coordinate space. The largest deviations are found in the region \(0.3 < s < 3\), where the difference between \(\epsilon_{\text{asymp}}(s)\) and \(\epsilon_{\text{exact}}(s)\) still never exceeds 9%. Notice that the approximation accuracy increases a lot when higher order terms are included in the expansions. One could go to more precise adiabatic potential representations taking higher order expansions of equation (19). However, the results of the approximate and full adiabatic potentials are almost indistinguishable in practice.

4.2. Bound states

It is known that the number of bound states increases as one particle becomes much lighter than the other ones [13, 14]. Here, we have calculated the adiabatic potential asymptotic forms (21) and (22) and found a differential equation, equation (23), applicable to the case where two particles are much heavier than the third. In the following, we specialize to identical heavy particles i.e. \(m_A = m_B = M\) and \(E_{BC} = E_2\). From now on, we also adopt units such that \(M = h = |E_2| = 1\) for simplicity. The mass ratio between light and heavy particles is then denoted \(m = \frac{m_C}{M}\) as in [13]. In this case, the reduced mass \(\mu_{C,AB}\) is written as

\[
\frac{2m}{m + 2} \quad \text{and} \quad \mu_{C,AB} \to m \quad \text{for} \quad m \to 0.
\]

With these definitions and denoting the three-body energy by \(E = E_3\), a useful adiabatic potential expression is given by

\[
\epsilon(R) = -\frac{2e^{-\gamma}}{\sqrt{4m + 2}} R = \left(1 - \frac{e^{-\gamma}}{4m + 2} R \ln\left(\frac{e^{-\gamma}}{\sqrt{4m + 2}} R\right)\right)^{-1}
\]

for \(\sqrt{4m + 2} R \leq 1.15\) and

\[
\epsilon(R) = -1 - \sqrt{2\pi} \frac{e^{-\sqrt{\frac{mC}{m}}} R}{\sqrt{\frac{4m}{m+C}}} \quad \text{for} \quad \sqrt{4m + 2} R \geq 1.15.
\]

This approximation is very accurate when \(2R \approx 1.15\sqrt{1 + 2/m}\), where the largest deviation of 9% is reached. Proper bound three-body states are present when \(E_3 - E_2 \leq 0\), or equivalently \(|E_3| > |E_2|\).

We numerically solve the differential equation, equation (23), with the adiabatic potential (25) and (26) to estimate the number of bound states \(N_B\) for a system with mass ratio \(m\) when the heavy particles do not interact with each other. Letting \(E_{AB}\) be the binding energy of the heavy–heavy system, we can choose \(\nu_C = 0\) in (23) and get \(E_{AB} = 0\). If \(\nu_C\) is attractive and able to support bound states, the three-body system would effectively be reduced to the lightest particle moving around a heavy–heavy dimer. The corresponding additional much deeper-lying bound states are, however, not interesting in the present context. Such states are not the universal three-body structures that we address in the current study, but should rather be regarded as bound two-body states.
dressed by an orbiting third particle. The numerical solution is obtained by writing the eigenvalue equation, equation (23), in matrix form. After discretization of the operators and the wave function of the radial equation, we get a tridiagonal matrix, which can be diagonalized to obtain the energies and the number of bound states. As always, one needs to introduce both a short- and long-range cut-off to numerically solve the differential equation in equation (23). But changing the cut-offs in a systematic manner (making the short-range cut-off smaller and the long-range cut-off larger) we have checked that our results for the number of bound states are properly converged (we discuss this quantitatively below).

The number of bound states as a function of mass ratio, \( m \), is shown in figure 4, where a comparison between the adiabatic result of equation (23) and the full numerical solution is made. Comparing both results in figure 4, we see that the adiabatic approximation picks up the small mass behaviour very well, even for mass ratios up towards 1. There is a small error in the threshold for the number of available bound states for \( 0 < N_B < 14 \), but it decreases as \( m \to 0 \). The adiabatic approximation has an accuracy better than 10% for \( m = 0.01 \), as can be seen in the inset of figure 4. Due to the numerical difficulties, it is very hard to count the number of bound states for \( N_B > 14 \) by solving the full problem numerically. Fortunately, it is very easy to do it through the differential equation, equation (23), with the adiabatic potentials (25) and (26). We also see clearly in figure 4 that \( N_B \to \infty \) for \( m \to 0 \), as pointed out in [13].

A fit to the results presented in figure 4 shows that the dependence of the number of bound states, \( N_B \), with the mass ratio, \( m \), is rather well described by

\[
N_B \approx \frac{0.731}{\sqrt{m}}. \tag{27}
\]

This behaviour can be explained by the old quantum theory (perhaps better known as the semi-classical JWKB approximation of Jeffreys, Wentzel, Kramers and Brillouin). What we need to consider is the number of nodes in the wave function at zero energy, since this measures the number of allowed bound states. Within the old semi-classical quantum theory, the usual way to estimate the number of bound states in a one-dimensional quantum problem is

\[
\int p \, dq = N \pi \hbar. \tag{28}
\]

This is the JWKB estimate of the number of bound states in a given potential. Taking into account the effective potential in (23) and proper units, the number of bound states can be estimated from the formula

\[
N = \frac{1}{\pi \sqrt{2m}} \int_0^\infty dx \sqrt{\frac{m}{2x^2} - V(x)} = 0.733 \frac{\pi}{\sqrt{m}}, \tag{29}
\]

where \( V(x) \) is the adiabatic potential (25) and (26) with \( x = \sqrt{\frac{m}{2\hbar^2} R} \). One may object that the integral in (29) diverges in both limits and cannot be performed. Introducing a lower and upper cut-off in the integral, which are the same as those used in the numerical calculation (10^{-2} and 10^{2}, respectively), we obtain that \( N = 0.736 \frac{\pi}{\sqrt{m}} \). This result approaches the estimate in (27) once the diverging term in (29) becomes less important as \( m \) becomes smaller. The integral in (29) is \( m \)-independent for \( m \leq 0.001 \) with a 10^{-2} cut-off, implying that the term \( m/x^2 \) is negligibly small itself. The apparent divergences are due to the semi-classical estimate, and accurately removed by a cut-off at both small and large \( x \). The true quantum mechanical number of states can then be fully recovered.

The estimates of the number of bound states in (27) and (29) agree very nicely. These estimates are less than the upper 2D limit for a 2D system with total angular momentum equal to zero, which is given in [21]. For the adiabatic potential in (25) and (26), this upper limit is given by \( N = \frac{0.44}{m} \). The difference between the estimates is shown in figure 5. It is known that any three-body system in two dimensions will achieve its maximum number of bound states when all two-body subsystems are bound and have the same two-body
binding energy [14]. We thus expect that the estimate given by the dashed curve in figure 5 will hold for the adiabatic potential in (25) and (26) when $E_{AB} = E_2$. Also, the number of bound states for a system with $0 \leq |E_{12}| \leq 1$ is in the window between the solid and dashed curves shown in figure 5. The large difference between these curves is necessarily due to states that have non-zero angular momentum that we are not concerned with in the present study but that are included in the strict mathematical bound cited above.

As we expected, the results confirm that the bound states accumulate at both $R \to 0$ and $R \to \infty$ as $m \to 0$. From our numerical calculations we find that the energy of the lower states (which reside at small distances) seems to increase without bounds when $m \to 0$. Furthermore, in the same limit, the wave function vanishes slower at large distances, allowing more bound states also at large distances. This can be interpreted as an Efimov-like effect for the 2D case. However, an important distinction between the 2D and 3D cases must be made. While the Efimov effect says that three identical particles can have infinitely many bound states when $E_2 \to 0$ in three dimensions, this limit leads to an unbound three-body system. We expected to have infinitely many bound states in two dimensions, when $m = 0$ and two interactive interactions. But we must stress that for finite $m$ we still have a finite number of bound states.

4.3. Experimentally relevant systems

Experiments with ultracold atoms are able to produce quasi-2D samples of $^{23}$Na [22], $^{40}$K [23, 24], $^{87}$Rb [25], $^{133}$Cs [26–28], and $^6$Li [29]. It was recently reported that mixtures of $^{133}$Cs and $^6$Li were successfully trapped and that very favourable Feshbach resonances, which can be used for tuning the interaction strengths between the atoms have now been found [30, 31]. We note that the zero-range model of interactions that we use in the current study is applicable for broad Feshbach resonances where finite-range corrections are negligible. Many heteronuclear systems typically have narrow Feshbach resonances where finite-range corrections are expected to play a larger role [32]. However, the recent results of [30] and [31] demonstrate that broad resonances are also available for highly mass-imbalanced cases. We will therefore not consider finite-range corrections and narrow resonances in this work.

In order to discuss some properties of mass-imbalanced three-body systems, we consider two different systems that can be probed in laboratories in the near future. These systems are $^{133}$Cs–$^{133}$Cs–$^6$Li, represented as circles in figures 7 and 8, and $^{87}$Rb–$^{87}$Rb–$^6$Li, represented as diamonds in the same figures.

Figures 7 and 8 are mass diagrams that show how many bound states a system composed of different particles supports for a given set of two-body binding energies in each subsystem. The energy symmetric case (all two-body binding energies equal) was discussed in [14]. In general, there are several ways to obtain a $^{133}$Cs–$^{133}$Cs–$^6$Li system if we assume that the interactions in the different subsystems give rise to different binding energies. The possibilities are shown in figure 6. If we consider a system of just one hyperfine state of $^6$Li and of $^{133}$Cs clearly two of the interactions will be identical (for instance $E_{AC} = E_{BC}$ on the left-hand side of figure 6). However, as has been discussed in the recent studies of Feshbach resonances in this mixed system [30, 31], different hyperfine states will, in general, give different interactions. This implies that with different hyperfine states we may be able to access the full range of parameter space. The adiabatic problem was handled for a non-interacting heavy–heavy system, i.e. $E_{AB} = 0$. This is close to the situation in $^{133}$Cs–$^6$Li experiments, where three-body bound states are expected to be found when the subsystem
energy scales related through [EAC] are fully imbalanced. We have selected a generic case with [EAC] case is then [EAC] for a rich energy spectrum in two dimensions. The systems [87Rb–87Rb–6Li (diamond) and 133Cs–133Cs–6Li demonstrates that also in a 2D setup, the 6Li–133Cs system is always the heavy–heavy particle energy. This region gives [EAC] = 0 and only regions 2 and 3 are symmetric. The systems [87Rb–87Rb–6Li (diamond) and 133Cs–133Cs–6Li (circles) have three and four bound states, respectively. This is the experimentally relevant case [30, 31], and our results demonstrates that also in a 2D setup, the 6Li–133Cs system will have several bound states.

It is known that the most favourable scenario for a spectrum with many bound states for 2D three-body systems is the symmetric energy case, where all of the subsystems are equally bound, i.e. [EAB = EAC = EBC] [14]. However, this scenario seems less likely in current experiments. A very promising scenario is shown in figure 7, where the heavy–heavy system does not interact and the two heavy–light systems have the same binding energy. Except for the energy-symmetric case in [14], this is the most favourable scenario for a rich energy spectrum in two dimensions.

Figure 8 shows the scenario where the two-body energies are fully imbalanced. We have selected a generic case with energy scales related through [EAB = 10EAC and EBC = 0.1EAC]. This may appear difficult to set up experimentally, but fortunately this scenario does not seem to have any advantage over the others. In region 1, where our reference system has the heavy–heavy system more strongly bound than the others, the [87Rb–87Rb–6Li and 133Cs–133Cs–6Li systems have only one bound state each. In this energy configuration, the region 2 should be the most similar to region 1 in figure 7, where the heavy–heavy system is not as bound as the others. However, regions 2 and 3 appear almost symmetric in figure 8, showing that both systems have two bound states each. Effectively, we see that the strongly bound heavy–light system changes the threshold of binding for the three-body system and effectively removes the most weakly bound three-body states.

5. Summary and conclusion

We consider three-body systems with zero-range interactions for general masses and interaction strength in two dimensions. The aim of this work is to study the limit where one particle is much lighter than the others ([mC ≪ mA = mB]) for non-interacting heavy particles, i.e. [EAB = 0]. This limit contains a rich energy spectrum and can be handled through the Born–Oppenheimer (BO) approximation. The BO approximation allows us to integrate out the light particle coordinate in order to derive the adiabatic potential between the heavy particles in the heavy–heavy–light system.

The adiabatic potential is found to be the solution of a transcendental equation. We are able to find analytical forms for the asymptotic behaviour for large and small [R], where [R] is the distance between the two heavy particles. Comparing both asymptotic behaviour and numerical solution of the adiabatic potential, we find that the analytic form precisely describes the adiabatic potential for any [R] and can be directly applied in 2D three-body system calculations. The analytic adiabatic potential explicitly shows the mass-dependence. The analytic adiabatic potential becomes more attractive and suffers less screening as the mass of the light particle [C] decreases ([mC → 0]). This potential explains the increasing number of bound states in this limit and we are able to demonstrate that the bound states accumulate both at [R → 0] and [R → ∞]. We thus see an Efimov-like effect when [mC = 0]. However, we still caution that for any finite [mC] there are only a finite number of bound three-body states.

The results obtained with the analytic adiabatic potential agree with numerical solutions of the momentum-space Schrödinger equation. However, approaching the three-body problem in two dimensions with the analytic form of the adiabatic potential has the huge advantage that it is much less computationally demanding and allows for easy access to rich regions of the mass diagrams. Furthermore, we are able to show that the number of bound states calculated with the analytic adiabatic potential matches the estimate given by the semi-classical JWKB methods of the old quantum theory, i.e. the Bohr–Sommerfeld method.

In recent work it was shown that the richest 2D energy spectrum is found when the three-body mass-imbalanced system has all two-body subsystems bound with the same energy, namely [EAB = EAC = EBC] for [mC ≪ mA ≠ mB] [14]. However, as these conditions are difficult to obtain in experiment, we search for other configurations able to produce a rich energy spectrum. We numerically solve the momentum-space Schrödinger equation for general masses and interaction strengths in order to build mass–mass diagrams, which outline the expected number of bound states for a general three-body system. We find that systems with equal mass and
non-interacting heavy particles, i.e. $m_C \ll m_A = m_B$ and $E_{AB} = 0; E_{AC} = E_{BC}$, are the most promising candidates to achieve a rich three-body bound state spectrum in two dimensions. Incidentally, this promising configuration is the one that can be handled with great precision in the BO approximation as we have shown.

One of these promising configurations was recently reported as the experimental realization of $^{133}\text{Cs}^–^{133}\text{Cs}$ systems [30, 31]. It even looks as if three-body bound states can be expected when the subsystem $^{133}\text{Cs}^–^{133}\text{Cs}$ is almost non-interacting. We can estimate the number of bound states for such a system in a two-dimensional setup through the mass–mass diagrams in this work. For $^{87}\text{Rb}^–^{87}\text{Rb}^–^{6}\text{Li}$ and $^{133}\text{Cs}^–^{133}\text{Cs}^–^{6}\text{Li}$, we find, respectively, three and four bound states. It is very important to note that these numbers do not depend on the exact two-body energy in the $^{6}\text{Li}^–^{133}\text{Cs}$ subsystem. This two-body energy in the 2D setup are functions of the 3D low-energy scattering length [1] of the particular Feshbach resonance that is used in experiment to tune the interaction. However, as long as there is such a resonance, our results should apply when the system is squeezed into a 2D geometry.

For now, the system $^{133}\text{Cs}^–^{133}\text{Cs}^–^{6}\text{Li}$ prepared as in region 1 of figures 6 and 7 seems to be the most promising realistic combination to achieve a richer three-body energy spectrum in two dimensions. Some other mixtures under intense study at the moment with large mass imbalances are lithium–ytterbium [33] and helium–rubidium [34]. Of particular interest is that there are different isotopes available in those systems so that the quantum statistics of the components can also be changed. In the case of layered systems with long-range dipolar interactions, as shown in figure 1, it is also extremely promising for finding bound states [35–41], and we expect that some of these will have a universal low-energy character. The possibility of tuning the binding energy of each pair and performing experiments mixing molecules and atoms should open new avenues for even richer 2D three-body spectra. Another interesting discussion is what trace of the three-body parameter is in the corresponding 2D bound states. The three-body parameter determines the overall scale of the three-body spectrum in three dimensions and has recently been shown to be universally connected to the two-body van der Waals interaction [42–48]. The 2D three-body problem does not require a three-body parameter in order to study the universal limit with zero-range interaction due to the ever present two-body bound state with energy $E_2$ which makes the three-body problem regular and well defined even in the zero-range limit [11]. However, the fact remains that short-range physics due to the real atomic two-body potential (typically of Lennard-Jones type) is still present in the system. This clear physical origin of the three-body parameter indicates that it could still play a role in two dimensions in not only determining the precise physical value of $E_2$ for a given system but perhaps also have a quantitative influence on three-body energies.

In order to experimentally observe the presence of these three-body bound states one should be able to use similar techniques to those used for the study of Efimov states in three dimensions, i.e. loss measurements [49, 3] and photo-association [50, 51]. It may also be possible to use radio-frequency transition techniques as in recent experiments that studied two-body bound states and many-body pairing in 2D Fermi gases [52, 29]. Another possible experimental signature of 2D three-body systems is through the momentum distribution and the two- and three-body contact parameters which appear as coefficients [53–55]. These coefficients depend sensitively on the presence of two- and three-body bound states.

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