Three-body halos in two dimensions

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Abstract

A method to study weakly bound three-body quantum systems in two
dimensions is formulated in coordinate space for short-range potentials.
Occurrences of spatially extended structures (halos) are investigated. Bor-
romean systems are shown to exist in two dimensions for a certain class
of potentials. An extensive numerical investigation shows that a weakly
bound two-body state gives rise to two weakly bound three-body states,
a reminiscence of the Efimov effect in three dimensions. The properties
of these two states in the weak binding limit turn out to be universal.
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Introduction. Characteristic properties of halo systems are binding energies
much smaller than the typical energy of the interaction and spatial extensions
much larger than the range of the potential \cite{1,2}. Three-body halos in \textit{three dimensions} exhibit many interesting features. Borromean systems, discovered now experimentally, are bound three-body structures where none of the two-body
subsystems are bound \cite{3,4,5}. The Thomas and Efimov effects are anomalies
due to a singularity which occurs in a three-body system when the ratio
of scattering length and effective range is infinitely large \cite{6,7,8,9,10}. Then
the effective three-body potential behaves as the inverse square of the distance
which results in infinitely many three-body bound states.

The Thomas effect corresponds to an infinitely small effective range. The
Efimov effect is associated with an infinitely large scattering length where the
wave functions of excited states reside in the tail region of the effective three-
body potential. Physical examples of these might possibly exist in nature \cite{10,11,12}.

The three-body halos in \textit{two dimensions} are less studied and the present
investigations \cite{13,14,15,16} are limited in various ways. It has been proven
\cite{10} that the number of bound states is always finite. However, the possibility of
existence of a Borromean state has not been examined and therefore the number
of bound states is not established. Moreover the properties of these states have
not been investigated in detail.
In this letter we shall for simplicity only consider a system of three identical bosons in two dimensions. The purpose is to (i) formulate an efficient method to solve the coordinate space Faddeev equations in two dimensions, applicable for arbitrary short-range two-body potentials, (ii) derive asymptotic equations for the effective three-body potential which alleviate crucially the numerical investigations of weakly bound systems, (iii) discuss the possible existence of Borromean systems, halos, Efimov and Thomas effects and (iv) illustrate numerically the universal properties of the three-body halos.

The method. We shall use the method developed for three dimensions [9].

Let \( r_{jk} = (r_j - r_k) \) be the distance between particles \( j \) and \( k \), \( r_{i(jk)} = -r_i + (r_j + r_k)/2 \) the distance between particle \( i \) and the center of mass of particles \( j \) and \( k \). All particles have the same mass \( m \). The Jacobi coordinates are then introduced as \( x_i = r_{jk}/\sqrt{2}, y_i = r_{i(jk)}\sqrt{2/3} \). The hyperspherical coordinates in two dimensions are given by \( \{\rho, \Omega_i\} \equiv \{\rho, \alpha_i, \theta_{xi}, \theta_{yi}\} \), \( \rho = \sqrt{x_i^2 + y_i^2}, \alpha_i = \arctan(x_i/y_i) \), \( \theta_{xi} \) and \( \theta_{yi} \) are the azimuthal angles of \( x_i \) and \( y_i \). The volume element in hyperspherical coordinates is \( \rho^3 \sin^2(\alpha_i) d\rho d\theta_{xi} d\theta_{yi} \sin \alpha_i \cos \alpha_i d\alpha_i \) and the kinetic energy operator is

\[
T = \frac{\hbar^2}{2m} \left( -\rho^{-3/2} \frac{\partial^2}{\partial \rho^2} \rho^{3/2} + \frac{3}{4} \frac{1}{\rho^2} + \frac{\hat{\Lambda}^2}{\rho^2} \right),
\]

(1)

\[
\hat{\Lambda}^2 = -\frac{\partial^2}{\partial \alpha_i^2} - 2 \cot(2\alpha_i) \frac{\partial}{\partial \alpha_i}
\]

(2)

\[
- \frac{1}{\sin^2(\alpha_i)} \frac{\partial^2}{\partial \theta_{xi}^2} - \frac{1}{\cos^2(\alpha_i)} \frac{\partial^2}{\partial \theta_{yi}^2}.
\]

The total wavefunction is now expanded in a complete set of hyperangular functions

\[
\Psi(\rho, \Omega) = \frac{1}{\rho^{3/2}} \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\rho, \Omega),
\]

(3)

where \( \Phi_n(\rho, \Omega) \) for each \( \rho \) are chosen as eigenfunctions of the hyperangular part of the Schrödinger equation

\[
\left( \hat{\Lambda}^2 + \frac{2m}{\hbar^2} \rho^2 \sum_{i=1}^{3} V(r_i) \right) \Phi_n = \lambda_n(\rho) \Phi_n.
\]

(4)

Here \( V \) is the two-body potential and the expansion coefficients \( f_n(\rho) \) satisfy the system of coupled equations

\[
\left( -\frac{\partial^2}{\partial \rho^2} + \frac{\lambda_n + 3/4}{\rho^2} - Q_{nn} \frac{2mE}{\hbar^2} \right) f_n(\rho)
\]

\[
= \sum_{n' \neq n} \left( Q_{nn'} + 2P_{nn'} \frac{\partial}{\partial \rho} \right) f_{n'}(\rho),
\]

(5)
\[ Q_{nn'}(\rho) = \int d\Omega \Phi^*_n(\rho,\Omega) \frac{\partial^2}{\partial \rho^2} \Phi_{n'}(\rho,\Omega) \]  
\[ P_{nn'}(\rho) = \int d\Omega \Phi^*_n(\rho,\Omega) \frac{\partial}{\partial \rho} \Phi_{n'}(\rho,\Omega). \]

The wavefunction \( \Phi_n \) is written as a sum of three components, each expressed in the corresponding system of Jacobi coordinates

\[ \Phi_n = \sum_{i=1}^{3} \phi^{(i)}_n(\rho,\Omega_i). \]

these components satisfy the three Faddeev equations

\[ \hat{\Lambda}^2 \phi^{(i)}_n + \frac{2m}{\hbar^2} \rho^2 V(r_i) \Phi_n = \lambda_n(\rho) \phi^{(i)}_n, \quad i = 1, 2, 3. \]

The physical solutions are equivalent to the solutions of the Schrödinger equation in Eq. (4) but these equations are better suited for descriptions of subtle correlations.

The s-wave motion is responsible both for the long distance behavior and the Thomas and Efimov effects. We therefore restrict to s-waves where the wavefunction \( \phi^{(i)}_n \) only depends on \( \rho \) and \( \alpha_i \). The Faddeev components in Eq. (9) must all be expressed in the same set of Jacobi coordinates. This amounts for s-waves to rewriting one set of coordinates in terms of the other and a subsequent integration over the angular variables \( \theta_x \) and \( \theta_y \), i.e.

\[ \phi(\rho,\alpha') \rightarrow \frac{1}{2\pi} \int_0^{2\pi} \phi(\rho,\alpha'(\alpha,\beta)) \, d\beta, \]

where \( \alpha' \) is given by \( \alpha \) and the variable \( \beta \), describing the rotation between two sets of Jacobi coordinates, given by

\[ \sin^2 \alpha' = \frac{1}{4} \sin^2 \alpha + \frac{3}{4} \cos^2 \alpha \pm \frac{\sqrt{3}}{2} \sin \alpha \cos \alpha \cos \beta, \]

where the choice of \( \pm \) is independent of \( \beta \). For three identical bosons (\( \phi \equiv \phi^{(i)}_n \)) the Faddeev equations then reduce to the three identical equations

\[ \left( -\frac{\partial^2}{\partial \alpha^2} - 2 \cot(2\alpha) \frac{\partial}{\partial \alpha} - \lambda \right) \phi(\rho,\alpha) = \]

\[ -\frac{2m}{\hbar^2} \rho^2 V(\sqrt{2} \rho \sin \alpha) \left( \phi(\rho,\alpha) + \frac{1}{\pi} \int_0^{2\pi} \phi(\rho,\alpha') \, d\beta \right). \]
Large-distance behavior. We define an angle $\alpha_0$ such that $|2m\rho^2 V(\sqrt{2}\rho \sin \alpha_0)/\hbar^2| = |\lambda(\rho)|$ and we assume that the potential is of short range, that is $\alpha_0$ approaches zero with increasing $\rho$. If $\alpha > \alpha_0$ the potential is then negligible for large $\rho$ and Eq. (12) becomes

$$\left(-\frac{\partial^2}{\partial \alpha^2} - 2 \cot(2\alpha) \frac{\partial}{\partial \alpha} - \lambda\right) \phi(\alpha) = 0.$$  

(13)

The solution which satisfies the boundary condition of vanishing derivative at $\alpha = \pi/2$ is

$$\phi(\alpha) = \pi \cos \pi \nu P_{\nu}(\cos 2\alpha) - 2 \sin \pi \nu Q_{\nu}(\cos 2\alpha),$$  

(14)

where $\lambda \equiv 4\nu(\nu + 1)$ and $P$ and $Q$ are Legendre functions. At small $\alpha$ this solution behaves as

$$\phi(\alpha) = 2 \sin(\nu \pi) \left(\gamma + \log \alpha + \psi(1 + \nu)\right) + \pi \cos(\nu \pi) + O(\alpha^2),$$  

(15)

where $\psi$ is the digamma function and $\gamma$ is Euler’s constant. Without interactions the solution in Eq. (14) with the boundary condition of zero derivative at $\alpha = 0$ provides the quantization rule $\nu = 0, 1, 2, ...$, see Eq. (15).

For a non-zero short-range potential the integral in Eq. (12) can be expanded for $\alpha < \alpha_0 \ll 1$ as

$$\frac{1}{\pi} \int_0^{2\pi} \phi(\rho, \alpha') d\beta = 2\phi(\frac{\pi}{3}) + O(\alpha^2).$$  

(16)

Then Eq. (12) simplifies to a differential equation with an inhomogeneous term

$$\left(-\frac{\partial^2}{\partial \alpha^2} - 2 \cot(2\alpha) \frac{\partial}{\partial \alpha} + \frac{2m}{\hbar^2} \rho^2 V(\sqrt{2}\rho \sin \alpha) - \lambda\right) \phi(\alpha) = -\frac{2m}{\hbar^2} \rho^2 V(\sqrt{2}\rho \sin \alpha)\phi(\pi/3).$$  

(17)

The homogeneous part of this equation reduces for small $\alpha$ by the substitution $r = \rho \alpha \sqrt{2}$ to the two dimensional Schrödinger equation for two particles. Thus, assuming that $\lambda$ can be neglected compared to $2m\rho^2 V/\hbar^2$, the large-distance ($\alpha < \alpha_0 \ll 1$) solutions to the homogeneous part of Eq. (17) simply are the zero-energy two-body solutions. Then for $\alpha \simeq \alpha_0$ the physical solution is approximately $C \log \left(\frac{\sqrt{2} \rho \alpha}{a}\right)$, where $C$ is an arbitrary constant and $a$ is the scattering length defined as the distance where the two-body wave function for zero energy is zero. One solution to the inhomogeneous part of the equation is now $-2\phi(\pi/3)$. The complete physical solution to the inhomogeneous equation is therefore ($\alpha \simeq \alpha_0$)

$$\phi(\alpha) = C \log \left(\frac{\sqrt{2} \rho \alpha}{a}\right) - 2\phi(\frac{\pi}{3}).$$  

(18)
Matching the two solutions, Eqs. (14) and (18), and their derivatives at $\alpha = \alpha_0$ gives the equation

$$2 \sin(\nu \pi) \log \left( \frac{\sqrt{2} \rho}{a} \right) = 2 \sin(\nu \pi) (\gamma + \psi(1 + \nu)) + \pi \cos(\nu \pi) + 2 \phi \left( \frac{\pi}{3} \right).$$  \hfill (19)

Both for $\rho \gg a$ and $\rho \ll a$ the logarithm at the left hand side is large. The quantity $\nu$ must therefore approach an integer $l$ to compensate for this divergence. The leading order of an expansion in powers of $\rho$ for the lowest $\nu$ gives

$$\nu \approx \frac{3}{2} \left[ \log \left( \frac{4 \sqrt{2} \rho}{3a} \right) \right]^{-1} \rightarrow 0 .$$  \hfill (20)

Therefore this eigenvalue $\lambda \equiv 4 \nu(\nu+1)$ is approaching zero in both these limiting cases in contrast to three dimensions where a negative constant asymptotically is approached when the scattering length is infinitely large. The effective radial potential in Eq. (19) has therefore a repulsive centrifugal term and no collapse of the wave function in the center is possible.

Let us now consider diverging solutions $\lambda(\rho)$ to Eq. (19). Then large imaginary values of $\nu \propto -i \rho$ are necessary and the outer function in Eq. (14) approaches

$$\phi(\alpha) \approx \frac{1}{\sqrt{\nu}} \sqrt{\frac{2\pi}{\sin 2\alpha}} \sin \left( (\nu + \frac{1}{2})(2\alpha - \pi) + \frac{\pi}{4} \right) ,$$  \hfill (21)

which for large $\rho$ is exponentially small at $\alpha = \pi/3$ compared to it’s value at $\alpha = \alpha_0$. For large imaginary $\nu$ the equation in Eq. (19) then becomes

$$\log \left( \frac{\sqrt{2} \rho}{a} \right) = \gamma + \log \nu + \frac{1}{2\nu} - \frac{1}{12\nu^2} + i \frac{\pi}{2} ,$$  \hfill (22)

which has the asymptotic solution

$$\nu = -\frac{1}{2} - ie^{-\gamma} \frac{\sqrt{2} \rho}{a} - \frac{i}{12} \left( e^{-\gamma} \frac{\sqrt{2} \rho}{a} \right)^{-1} + O(\rho^{-2}) \hfill (23)$$

$$\lambda \equiv 4\nu(\nu+1) = -\frac{4}{3} - \frac{8}{e^{2\gamma} a^2} + O(\rho^{-2}) .$$  \hfill (24)

This parabolic behavior of $\lambda$ is the signature of a bound two-body state with the binding energy $B$ and wave number $k$ given by $4e^{-2\gamma}a^{-2} = 2m^*B/h^2 \equiv k^2$, where $m^* = m/2$ is the reduced mass of the two particles. We can verify this by solving the two-body problem, where the $s$-wave radial solution outside the potential is $K_0(kr) \approx -\log(kr/2) - \gamma$ which must be matched with the solution
inside the potential at \( r_0 = \rho a \sqrt{2} \). For small binding we can use the zero-energy solution which at \( r \simeq r_0 \) is \( \log (r/a) \). This matching gives the above \( B \) and \( k \) and the result is accurate to the order \( r_0/a \). For attractive zero-range potential it is therefore exact. For the potentials without two-body bound state, where \( r_0/a \) is not small, this particular solution does not exist.

The wavefunction is exponentially small everywhere except in a small region close to \( \alpha = 0 \), see Eq. (21). In this region the zero-range wave function obtained from Eq. (17) is proportional to \( K_0(kr = k\rho a \sqrt{2}) \) and after normalization approximately given by

\[
\phi(\alpha) \approx 2k\rho K_0 \left( \sqrt{2} k \rho a \right).
\] (25)

The related diagonal part of \( Q_{11} \) is then by use of Eq. (6) computed to be \( Q_{11} = -\frac{1}{3} \), which in combination with Eq. (24) gives the first diagonal equation in Eq. (5) as

\[
\left( -\frac{\partial^2}{\partial \rho^2} - \frac{1}{4\rho^2} - \frac{2m}{\hbar^2} (E + B) \right) f(\rho) = 0.
\] (26)

This is the characteristic large-distance behavior of a two-body radial Schrödinger equation in two dimensions.

**Efmov and Thomas effects.** The eigenvalue equation for large distances is in *three dimensions* given by

\[
\sin(\tilde{\nu} \frac{\pi}{2}) \frac{\sqrt{2} \rho}{a} = -\tilde{\nu} \cos(\tilde{\nu} \frac{\pi}{2}) + \frac{8}{\sqrt{3}} \sin(\tilde{\nu} \frac{\pi}{6}),
\] (27)

where \( \lambda = \tilde{\nu}^2 - 4 \). For \( \rho \gg a \) the lowest solution is \( \tilde{\nu} = 2 \) (\( \lambda = 0 \)) that is a regular free solution whereas for \( \rho \ll a \), \( \lambda \to \lambda_\infty = -5.012... \), which leads to a strongly attractive \( \rho^{-2} \) potential in the radial equation. Physically the \( \rho^{-2} \) behavior is limited at small distances by a finite range \( R \) of the potential, and at large distances by a finite scattering length \( a \). However, in the limit \( R/a \to 0 \) such a potential gives rise to the so called "falling towards the center" phenomenon with infinitely many bound states. When \( R \to 0 \), the phenomenon is called the Thomas effect and when \( a \to \infty \) it is called the Efimov effect.

Eq. (27) is in two dimensions replaced by Eq. (19) and the Efimov effect is therefore not present in two dimensions. Furthermore, the hyperradial potential has even for zero-range potentials a repulsive centrifugal barrier at small distance. Then the Thomas collapse is not possible and the three-body system must for zero-range potentials have a finite number of bound states.

Equations (19) and (27) can be formally written in terms of hypergeometric function as one general equation for \( d \)-dimensions, where \( d \) is a real number. The asymptotic solution \( \lambda_\infty \) of this equation leads to the Efimov and Thomas effects in the region \( 2.3 < d < 3.8 \).
Bound states. The solutions to the zero-range potentials are similar to those of purely attractive weak potentials. The two-body system has at least one bound state and for such interactions Borromean systems do not exist in two dimensions. The three-body ground state is more bound and an excited state is in addition always present. In Fig.1 is shown the effective radial potential together with the resulting two bound-state wave functions. The corresponding root mean square radii are in units of the scattering length respectively \(< (r/a)^2 >^{1/2} = 0.111, 0.927\). Their large sizes are reminiscent of the three-dimensional Efimov states with an extension comparable to the scattering length.

The energies \(E_3\) of these states are given in terms of the two-body bound-state energy \(E_2\) as \(E_3/E_2 = 16.52, 1.267\). We have numerically tried to find a third bound state with weaker binding energy and larger radial extension by calculating the zero-energy wavefunction and looking at the number of nodes. Even a careful search to about \(10^3\) times the scattering length did not reveal another bound state. This strongly indicates that only two bound states exist. The large proportionality factor for the ground state energy can be considered a reminiscence of the Thomas effect. These relations are still valid for arbitrary weakly attractive, finite-range potentials. This is because weak binding corresponds a scattering length much larger than the range of the potential, which is the limit of a zero-range potential.

In Fig.2 we show the ratio \((E_3 - E_2)/E_2\) as function of \(|E_2|\) for different potentials. We first notice that there are always two states which in the weak binding limit approach the results for zero-range potential (marked with small circles). The purely attractive potentials (solid lines) as well as repulsive core potentials (dashed lines) fall approximately on the same universal curves. This is
Figure 2: Ratio of three- to two-body energies as function of the two-body energy for different two-body potentials $V(r) = \frac{k^2}{2mb^2} \left[ S_1 \exp\left(-\frac{1}{2}r^2/b^2\right) + S_2 \exp\left(-2r^2/b^2\right) \right]$. The unspecified strength parameter $S_i$ is used to vary the two-body binding.

equivalent to the observation in three dimensions that only low-energy scattering properties like the scattering length are important in the weak binding limit.

The potentials with a short-range repulsive barrier (dash-dot and dotted lines), unlike the repulsive core, produce energies deviating in the middle of the plot from the universal curves. The reason is that a sufficiently large barrier and a sufficiently large attraction produce a three-body ground state confined inside the barrier, that yields three bound states in total. As $|E_2|$ then decreases towards zero two cases are possible. If the potential does not allow the spatially confined ground state the third bound state disappears and the first two approach the zero-range limit (dotted lines). If, however, the potential allows a spatially confined ground state, all three states survive in the small $|E_2|$ limit (dash-dot lines). Now the second and the third bound states approach the zero-range limit, while the ground state energy remains finite. In this case the ground state persists even into the region where two-body state is unbound, creating thus a Borromean phenomenon. This is only possible with a repulsive confining barrier which therefore also limits the spatial extension of the three-body system. The properties of Borromean systems are therefore different in two and three dimensions.

Conclusions. Based on the hyperspherical expansion of the Faddeev equations we have investigated the possible structure of three weakly bound identical bosons in two dimensions. For purely attractive two-body potentials and the potentials with repulsive cores the Borromean systems do not exist. For two-body potentials with a short-range repulsive barrier the two-body system may not have a bound state while a three-body bound state exists. Borromean
systems are therefore possible in two dimensions.

We find numerically that a weakly bound two-body state is always accompanied by two bound three-body states, resembling the Efimov states in three dimension. If a Borromean state is present there are therefore in total three bound three-body states. For all types of potentials, two of these three-body bound states have energies and radii following a universal curve in the weak binding limit. Their sizes scale with the two-body scattering length and can therefore become arbitrarily large in analogy to s-state halos in three dimensions.

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