Efimov Effect in Coordinate Space Faddeev Equations

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A novel mathematically simple and physically transparent derivation of the Efimov effect is presented by means of a new efficient method for solving coordinate space Faddeev equations. The method, which is directly applicable on small computers, is used to obtain energies and wave functions of the Efimov states.

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The Efimov effect [1] appears in a system of three particles interacting by short-range two-body potentials. The system can have infinitely many bound states, if two or three of the binary subsystems have a bound state at zero energy. A variety of different systems may possibly exhibit this unusual behavior [2].

The effect was first found by using the Schrödinger equation in an analysis of the asymptotic behavior of the three-body wave function [1]. This derivation is only concerned with the very large distances and the formulation therefore does not allow calculations of either energies or wave functions of the system. The effect was later confirmed in terms of momentum space Faddeev equations, where the rather complicated formulation exploited the fact that the kernel of the integral equation is not compact in certain points [3]. The effect was also investigated by use of the Born-Oppenheimer approximation, which is applicable only to a system of one light and two heavy particles [4].

The purpose of this Letter is to (i) provide a novel mathematically simple and physically transparent formulation of the Efimov effect, (ii) compute higher order corrections to Efimov's fundamental equation, (iii) introduce a new efficient method, directly applicable on small computers, for solving coordinate space Faddeev equations, and (iv) employ the method numerically to obtain energies and wave functions of the Efimov states.

Faddeev equations.—The three-body system may be described by any of the three sets of coordinates shown in Fig. 1. They are related to the usually employed Jacobi coordinates by a mass-dependent scaling. The total wave function of the system is written as a sum of three components, each expressed in terms of one of the three different sets of coordinates:

$$\Psi = \psi(\mathbf{x},\mathbf{y}) + \psi'(\mathbf{x}',\mathbf{y}') + \psi''(\mathbf{x}'',\mathbf{y}''). \tag{1}$$

This three component wave function is rather flexible and allows a description of different three-body structures by means of few angular momenta in each component. These wave functions satisfy the Faddeev set of equations [5]

$$\begin{aligned}(T-E)\psi + V_1(\psi+\psi'+\psi'') &= 0,\\ (T-E)\psi' + V_2(\psi+\psi'+\psi'') &= 0,\\ (T-E)\psi'' + V_3(\psi+\psi'+\psi'') &= 0,\end{aligned} \tag{2}$$

where E is the total energy, T is the kinetic energy operator, and V_1 (V_2, V_3) is the interaction between the particles 2 and 3 (1 and 3, 1 and 2). For simplicity we consider $V_1 = V_2 = V_3$ and particles of equal mass m. The hyperspherical coordinates are then defined by

$$\begin{aligned}\rho &= (1/2\,x^2 + 2/3\,y^2)^{1/2},\\ \alpha &= \arctan(\sqrt{1/2}\,x/\sqrt{2/3}\,y)\end{aligned} \tag{3}$$

for each set of coordinates leaving invariant ρ, but not the hyperangle α.

As in [1] only zero orbital angular momentum, responsible for the Efimov effect, is allowed in each component. Furthermore, in our case of an attractive l-independent central potential this component accounts for more than 98% of the norm of the wave function [6]. The Faddeev equations in Eq. (2) then reduce to the three identical equations

$$\left(T_\rho + \frac{1}{\rho^2}T_\alpha - \epsilon\right)\psi(\rho,\alpha) + v(\rho\sin\alpha)\{\psi(\rho,\alpha)+\psi(\rho,\alpha')+\psi(\rho,\alpha'')\} = 0\,, \tag{4}$$

where $\epsilon = 2mE/\hbar^2$, $v(z) \equiv 2mV_1(z\sqrt{2})/\hbar^2$, and the kinetic energy operators are

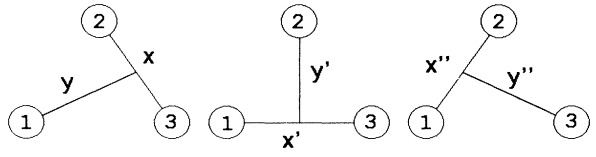

FIG. 1. Three possible sets of coordinates describing the positions of the particles of equal mass labeled by 1, 2, and 3. The relative coordinates are called x and y, respectively, between two particles and between their center of mass and the third particle. Thus $\mathbf{x} = \mathbf{r}_2 - \mathbf{r}_3$, $\mathbf{y} = -\mathbf{r}_1 + (\mathbf{r}_2 + \mathbf{r}_3)/2$, where $\mathbf{r}_i$ is the coordinate of the ith particle. The prime and double prime coordinates are analogously defined.

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$$T_\rho = -\rho^{-5/2}\frac{\partial^2}{\partial\rho^2}\rho^{5/2} + \frac{15}{4}\rho^{-2}\,,$$
$$T_\alpha = -\frac{1}{\sin(2\alpha)}\frac{\partial^2}{\partial\alpha^2}\sin(2\alpha) - 4 + \frac{\hat{l}_x^2}{\sin^2\alpha} + \frac{\hat{l}_y^2}{\cos^2\alpha}\,, \quad (5)$$

where $\hat{l}_x$ and $\hat{l}_y$ are the orbital angular momentum operators with respect to $\mathbf{x}$ and $\mathbf{y}$.

To solve Eq. (4) we choose to work in the first coordinate system. The two functions defined in the second and the third system must therefore be "rotated" into the first system. This rotation, which expresses one set of coordinates by another and subsequently integrates out the four angular variables of $\mathbf{x}$ and $\mathbf{y}$, is performed by an operator R given as [7]

$$R[\psi] = \frac{1}{\sin(2\phi)}\frac{1}{\sin(2\alpha)} \times \int_{|\phi-\alpha|}^{\pi/2-|\pi/2-\phi-\alpha|} d\alpha'\,\sin(2\alpha')\psi(\rho,\alpha')\,, \quad (6)$$

where all angular momenta are assumed to be zero and the angle ϕ depends only upon the masses of the particles and equals $\pi/3$ when the masses are equal. The Faddeev equation, after integration over the four angular variables, becomes

$$\left(T_\rho + \frac{1}{\rho^2}T_\alpha - \epsilon\right)\psi(\rho,\alpha) + v(\rho\sin\alpha)\left\{\psi(\rho,\alpha) + \frac{2}{\sin(2\phi)}\int_{|\phi-\alpha|}^{\pi/2-|\pi/2-\phi-\alpha|} d\alpha'\frac{\sin(2\alpha')}{\sin(2\alpha)}\psi(\rho,\alpha')\right\} = 0\,. \quad (7)$$

Method of solving.—We solve this integro-differential Faddeev equation by applying the method previously used to solve the three-body Schrödinger equation [8]. The wave function ψ is expanded in a complete set of hyperangular functions Φ_λ,

$$\psi(\rho,\alpha) = \sum_\lambda \frac{f_\lambda(\rho)}{\rho^{5/2}}\frac{\Phi_\lambda(\rho,\alpha)}{\sin\alpha\cos\alpha}\,, \quad (8)$$

where Φ_λ are the eigenfunctions of the α-dependent part of the Faddeev equation

$$-\frac{\partial^2\Phi_\lambda(\rho,\alpha)}{\partial\alpha^2} + \rho^2 v(\rho\sin\alpha)\left\{\Phi_\lambda(\rho,\alpha) + \frac{2}{\sin(2\phi)}\int_{|\phi-\alpha|}^{\pi/2-|\pi/2-\phi-\alpha|} d\alpha'\Phi_\lambda(\rho,\alpha')\right\} = \lambda(\rho)\Phi_\lambda(\rho,\alpha)\,. \quad (9)$$

The wave functions f_λ are solutions to a coupled set of radial differential equations. The convergence in λ is extremely fast and the lowest λ alone gives a very good approximation, except in the presence of avoided crossings [9], which does not occur in our case. We shall therefore restrict ourselves to the lowest value of λ, which as we shall demonstrate later is responsible for the appearance of the Efimov effect. The diagonal radial equation, where $\lambda(\rho)$ now serves as an effective potential, is then

$$\left(-\frac{\partial^2}{\partial\rho^2} - Q_\lambda(\rho) + \frac{\lambda(\rho)-1/4}{\rho^2} - \epsilon\right)f(\rho) = 0\,, \quad (10)$$

where the term $Q_\lambda(\rho) \equiv \langle\Phi_\lambda|\frac{\partial^2}{\partial\rho^2}|\Phi_\lambda\rangle$ is small and at large distances proportional to $1/\rho^4$.

Efimov effect.—Let us now consider the asymptotic behavior of λ for small and large ρ in a short-range potential, i.e., a potential which falls off faster than the inverse square of the distance. For $\rho = 0$ the lowest solution of Eq. (9), which obeys the boundary conditions of being zero for both $\alpha = 0$ and $\pi/2$, is $\sin(2\alpha)$ with an eigenvalue of 4. The eigenvalue λ for small ρ is now obtained in first order perturbation theory as

$$\lambda = 4 + 3v(0)\rho^2\,. \quad (11)$$

To solve Eq. (9) for large ρ we divide the α space into two regions I and II, where $\rho^2 v(\rho\alpha)$ respectively is more than and less than λ. The dividing point equals r_0/ρ, where r_0 is defined by $\rho^2 v(r_0) = \lambda$. [For potentials equal to zero outside a finite radius, r_0 approaches this radius as ρ increases, for exponentially decreasing potentials r_0 diverges logarithmically, and for potentials behaving like $r^{-\nu}$ ($\nu > 2$), r_0 diverges like $\rho^{2/\nu}$. These types of potential provide asymptotically decreasing r_0/ρ.] For $\rho \gg r_0$ the potential in Eq. (9) vanishes unless $\alpha < r_0/\rho$ and then the equation to first order in r_0/ρ reduces to

$$\left\{-\frac{\partial^2}{\partial\alpha^2} - \lambda(\rho)\right\}\Phi_\lambda(\rho,\alpha) + \rho^2 v(\rho\alpha)\left\{\Phi_\lambda(\rho,\alpha) + \alpha\frac{4\Phi_\lambda(\rho,\phi)}{\sin(2\phi)}\right\} = 0\,. \quad (12)$$

In region I, where $\alpha > r_0/\rho$, the potential is negligible and this equation becomes

$$\left(-\frac{\partial^2}{\partial\alpha^2} - \lambda\right)\Phi_\lambda^{(\mathrm{I})}(\rho,\alpha) = 0\,, \quad (13)$$

with the solution $\sin[(\alpha-\pi/2)\sqrt{\lambda}]$ vanishing at $\pi/2$ independent of λ.

In region II, where $\alpha < r_0/\rho$, we have instead the equation

$$\left\{-\frac{\partial^2}{\partial(\rho\alpha)^2} + v(\rho\alpha)\right\}\Phi_\lambda^{(\mathrm{II})}(\rho,\alpha) = -v(\rho\alpha)\alpha\frac{4\Phi_\lambda^{(\mathrm{I})}(\rho,\phi)}{\sin(2\phi)}\,, \quad (14)$$

where the small term λ/ρ^2 has been neglected. If λ/ρ^2 is not small at large ρ, the resulting configuration does not exhibit the Efimov effect; see below. The total solution to Eq. (14), the homogeneous plus the inhomogeneous, is now

$$\Phi_\lambda^{(\mathrm{II})}(\rho,\alpha) \propto \psi_0(\rho\alpha) - \alpha\frac{4\Phi_\lambda^{(\mathrm{I})}(\rho,\phi)}{\sin(2\phi)}\,, \tag{15}$$

where the homogeneous solution $\psi_0(\rho\alpha)$ is the wave function describing the state of zero energy in the potential $v(\rho\alpha)$, which outside the potential ($\rho\alpha > r_0$) has the form $\rho\alpha + a$, where a is the scattering length.

The eigenvalue equation for λ now arises by matching of the derivative of the logarithm of the two solutions at the point $\alpha = r_0/\rho$. To first order in r_0/ρ we then immediately obtain

$$-\sqrt{\lambda}\cos\left(\sqrt{\lambda}\frac{\pi}{2}\right) + \frac{8}{\sqrt{3}}\sin\left(\sqrt{\lambda}\frac{\pi}{6}\right) = \frac{\rho}{a}\sin\left(\sqrt{\lambda}\frac{\pi}{2}\right)\left(1+\lambda\frac{r_0}{\rho}\frac{r_0+a}{\rho}\right), \tag{16}$$

where we inserted $\phi = \pi/3$. Neglecting the first order term in r_0/ρ we get the zero order equation investigated by Efimov [1]. For infinite scattering length ($a = \infty$) it has a solution $\lambda_\infty = -1.012\,51$, which substituted into Eq. (10) implies that the radial equation asymptotically has an effective attractive potential given by $-1.262\,51/\rho^2$, which in turn results in an infinite number of bound states.

The simple derivation above makes it easy to compute various correction terms. For example, the next term in the expansion of λ in powers of r_0/ρ for $a = \infty$ is

$$\lambda = -1.012\,51 - 1.375\,22\frac{r_0}{\rho}\,, \tag{17}$$

where r_0 is defined by $v(r_0) = \lambda_\infty/\rho^2$. As another example, for finite $a \gg r_0$, the first two terms of λ in powers of a/ρ are

$$\lambda = 4\left(1 - \frac{12}{\pi}\frac{a}{\rho}\right). \tag{18}$$

These two different expansions explicitly show that the large distance limit of λ has a singular point at $a = \infty$.

Recently Efimov studied other types of corrections by use of the three-particle zero-range theory [10]. He calculated the corrections to the three-body binding energy and to the effective long-range radial potential to first order in the effective range r_e of the short-range two-body potential. He showed that in the special cases, where $r_e \ll \rho \ll a$, the correction to the effective radial potential has the form r_e/ρ^3. The derivations are based on perturbation theory and restricted to large ρ values. The procedure is complicated and lacking all numerical values.

The effective range differs from our expansion parameter r_0, which has a simple geometric interpretation and, for example, in a square well potential is equal to its radius. For a given scattering length, r_e is proportional to r_0 with a proportionality factor depending on the shape of the short-range potential. Thus Eq. (17) (divided by ρ^2) is consistent with the results of [10] with the difference being that our method enables us to calculate the proportionality coefficient as well as the expansions in the other cases [see Eqs. (11) and (18)].

Our practical procedure, where we calculate the radial potential strictly for all distances, provides the tool to calculate the three-body binding energy directly without use of perturbation theory unlike [10] where the energy perturbation is furthermore a correction of an unknown energy determined by the unknown potential at small distances.

Numerical illustration.—The numerical implemetation of the method, treating one radial point at a time, requires then rather little computer memory. This consequently allows dense grids and therefore improved accuracy and stability, still with modest time requirements. It is also worth mentioning that this method allows us to calculate both discrete and continuum spectrum wave functions of a three-body system by specifying appropriate boundary conditions in the radial equation.

For illustration we show in Fig. 2 the lowest eigenvalue of Eq. (9) as a function of ρ for a two-body Gaussian potential. The strength of the potential is varied and the results for three different scattering lengths are shown. The $\rho = 0$ limit is 4 in all cases; see Eq. (11). For positive a the eigenvalue returns to 4 at infinity [see Eq. (18)], whereas negative a, corresponding to a finite binding energy of the binary subsystem, leads to a parabolic dependence of ρ. This dependence, $\lambda(\rho) = -\epsilon_x\rho^2$, leads (after dividing by ρ^2) to a constant potential $-\epsilon_x$ in the radial

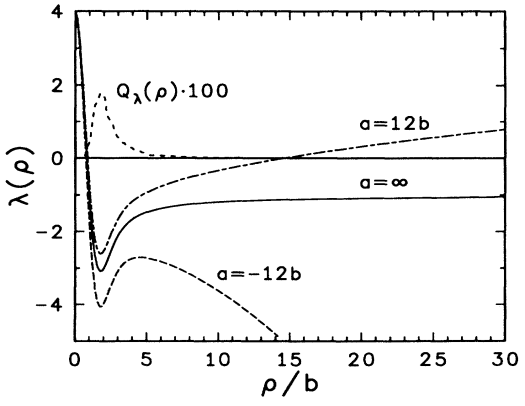

FIG. 2. The eigenvalue λ of Eq. (9) as a function of ρ for a Gaussian potential $S\exp(-r^2/b^2)$ of range b and depth S corresponding to scattering lengths of, respectively, $12b$ (dot-dashed curve), infinitely large (full curve), and $-12b$ (dashed curve). The term Q_λ in Eq. (10) is blown up by a factor of 100 and is also exhibited as a function of ρ.

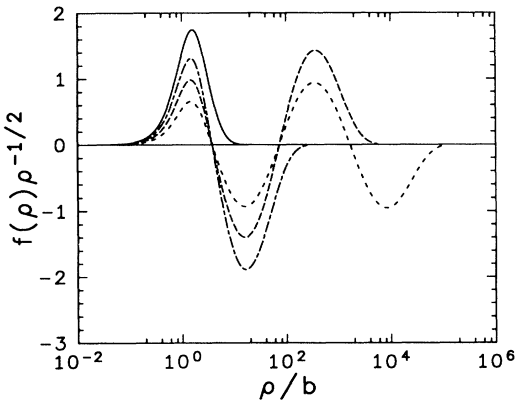

FIG. 3. The wave functions as a function of ρ for the four lowest Efimov states [energies -2.3×10^{-1} (solid), -4.2×10^{-4} (dot-dashed), -8.0×10^{-7} (dashed), and -1.6×10^{-9} (dotted) in units of $\hbar^2/2mb^2$] obtained from Eq. (10) and corresponding to the $a = \infty$ potential of Fig. 2. The plotted quantities are arbitrarily normalized for better visibility.

equation, which means that asymptotically the energy scale is shifted by $-\epsilon_x$. In fact, ϵ_x turns out to be the binding energy of the binary subsystem [11].

When a approaches infinity, the eigenvalue $\lambda(\rho)$ approaches λ_∞ as ρ increases until $\rho \approx a$ where it starts to deviate and eventually either reaches $+4$ [Eq. (18)] or diverges parabolically to $-\infty$. At finite distances we observe the attractive pocket in the effective potential, which employed in Eq. (10) may lead to one or more bound three-body states. In Fig. 2 is also plotted the term in Eq. (10) which arises from the variation of the eigenfunction Φ_λ with ρ. It is contributing at most on the 1% level and it has no influence on our general arguments.

The radial wave functions and the related total energies are now obtained from Eq. (10) for the potential of infinite scattering length used in Fig. 2. The small distance behavior is found by numerical integration and matched outside the potential to the known analytical solution, i.e., the modified Bessel function $K_{\sqrt{\lambda}_\infty}$ divided by $\sqrt{\rho}$. The resulting four lowest Efimov states are shown in Fig. 3. The first of these is an ordinary solution concentrated in the pocket region of the potential, whereas the higher lying states all extend far out into the asymptotic tail region. They are all, except the lowest, very sensitive to the asymptotic behavior of λ. The wave functions are similar before their exponential falloff where the last oscillation of the next eigenfunction continues. The nodes are regularly spaced in this logarithmic plot until $\rho \approx a$ where the deviation from the ρ^{-2} asymptotic behavior of λ prevents further continuation.

Summing up, the Efimov effect is derived from coordinate space Faddeev equations using the method of expansion in terms of hyperangular functions, and the energies and wave functions of several of the lowest Efimov states are calculated. The method appears to be general and applicable to any three-body system regardless of the particular type of interaction between the particles. However, in this Letter we restricted ourselves to l-independent attractive potentials; we assumed equal masses of the three particles and allowed only the dominating components in the expansion with zero angular momenta. These simplifications can be avoided without significant loss of numerical efficiency, but with an increased notational complexity. More detailed work is in progress.

The new derivation is self-contained and physically transparent and the method allows analytical investigation of the asymptotic behavior of three-body systems as well as efficient numerical calculation of energies and wave functions.

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