Analytic representation of the Efimov effect in the helium trimer

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Exact solutions for the low-temperature helium dimer and trimer, $^4He_2$ and $^4He_3$, are derived, based on our δ function model for the interatomic potential. For the trimer, the Faddeev equations are shown to be separable in hyperspherical coordinates, with the *S*-wave alone giving an exact solution. The parameters λ_0 and r_0 are fitted to accurate computations on the dimer and trimer. Excited states of the trimer are shown to exhibit the Efimov effect, whereby artificially reducing the strength of the two-body potential causes an infinite number of weakly-bound levels to condense out of the continuum. All the features anticipated by Efimov are quantitatively reproduced within our model. Since short-range details of the intermolecular forces are not relevant, our results can be considered to be universally applicable.

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I. INTRODUCTION

In 1970 Efimov [1] proposed that a three-body system with short-range interactions can have an increasingly large number of weakly-bound states if, for at least two of the subsystems, the scattering length becomes much larger than than the range of the two-body potential. In the limiting case of a resonant system, when the energies of the two-body interactions approach zero, the number of Efimov states can become infinite.

The Efimov effect has been extensively studied in noble-gas trimers—notably $^4He_3$ [2–4]. The dimer $^4He_3$ supports a single bound state with a miniscule binding energy corresponding of 1.310 mK. The $^4He_3$ trimer is found nevertheless to have a bound state two orders of magnitude more stable. Accurate computations give a ground-state energy in the range 125−135 mK, plus a bound excited state of the order of 1−2 mK, which is typically greater than the binding energy of the the dimer. A number of workers [5] have characterized the excited level as an Efimov state. To confirm that this is actually so, it is necessary to consider the behavior as the two-body potentials are appropriately "tuned." This has been done computationally and might become possible experimentally by observing trimers in electric fields.

Several earlier studies have explored the effect of varying the strength of the diatomic potential energy function on the stability of the helium trimer. Cornelius and Glöckle [6] used the HFDHE2 helium diatomic potential of Aziz *et al.* [7] scaled by a parameter λ to solve the Faddeev equations in momentum space. The present authors have studied models for low-temperature helium dimers and trimers based on approximations of the interatomic potentials by δ functions [8]. Within these models, we have obtained exact solutions of the Schrödinger equation for both $^4He_2$ and $^4He_3$. In this paper we will derive an explicit analytic account of the Efimov effect.

II. HELIUM DIMER

For the dimer, the potential is idealized as a "Dirac bubble potential." Assuming a state of zero orbital angular momentum, the relative motion of a pair of helium atoms can be represented by

$$\frac{1}{2\mu}\left[-\psi''(r)-\frac{2}{r}\psi'(r)-\frac{\lambda}{r_0}\delta(r-r_0)\psi(r)\right]=E\psi(r) \quad (1)$$

with $E=-\kappa^2/2\mu$. The reduced mass $\mu=M/2$, where $M=7296.293$ atomic units for the ^{4}He atom. For $r\neq r_0$, Eq. (1) has solutions $\psi_1(r)=\sinh(\kappa r)/r$ and $\psi_2(r)=e^{-\kappa r}/r$, finite for $r\to 0$ and $r\to\infty$, respectively. The complete wave function must be continuous but kinked at $r=r_0$, so that the first derivative is discontinuous there. The second derivative will then contribute a term to match the δ function in the potential energy operator. The (unnormalized) solution to Eq. (1) can accordingly be written

$$\psi(r)=\frac{\sinh(\kappa r_<)e^{-\kappa r_>}}{r}, \quad \{r_<,r_>\}\in\{r,r_0\}. \quad (2)$$

The boundary condition at $r=r_0$ is satisfied by matching the $\delta(r-r_0)$ contributions from the kinetic and potential energies. This leads to the relation

$$\lambda_0=\kappa r_0[1+\coth(\kappa r_0)], \quad (3)$$

which determines the ground state energy. Accurate computations by Gentry and co-workers [9] predicted a $^4He_2$ ground-state energy of $\varepsilon=-1.310$ mK. Energies in these low-temperature species are most conveniently expressed in millikelvins, with the conversion factor 1 mK=3.166 829 $\times 10^{-9}$ hartree. A deltafunction potential supports only a single $J=0$ bound state, which makes it an appropriate model for the actual $^4He_2$ dimer. The parameters λ_0 and r_0 can be adjusted to agree with the ground-state energy. In earlier work, we found the best fit with $\lambda_0=1.074\,34, r_0=13.15$ bohr. A small readjustment of these parameters will optimize agreement with the trimer as well.

A bound state for the dimer will exist only for values $\lambda>1$. The limiting case $\lambda=1$ represents a zero-energy resonance. Such a hypothetical state is of particular importance in connection with the Efimov effect in the trimer. For $\kappa\approx 0$, Eq. (3) is approximated by

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$$\kappa r_0 \approx \lambda - 1 \approx \frac{r_0}{a}, \tag{4}$$

where $a \approx 1/\kappa$ is an estimate of the scattering length.

Our δ function model is particularly fortuitous for studying the Efimov effect since details of the short-range potential are largely irrelevant [10].

III. FADDEEV EQUATIONS FOR TRIMER

Generalizing the δ function model to the $^4He_3$ trimer, we will assume that the three particles interact through pairwise δ function potentials of the same form:

$$V(r_{ij}) = -\frac{\lambda_0}{M r_0}\delta(r_{ij} - r_0). \tag{5}$$

For compactness of notation, we write the three interatomic separations as $r_1 \equiv r_{23}, r_2 \equiv r_{31}, r_3 \equiv r_{12}$. The three-particle kinetic energy operator, expressed in terms of the relative interatomic coordinates, is given by $T = T_0/M$ with

$$T_0 = -\frac{\partial^2}{\partial r_1^2} - \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{r_3^2 - r_1^2 - r_2^2}{4 r_1 r_2}\frac{\partial^2}{\partial r_1 \partial r_2} + \frac{r_2^2 - r_3^2 - r_1^2}{4 r_1 r_3}\frac{\partial^2}{\partial r_1 \partial r_3} + (\text{cyclic permutations}). \tag{6}$$

With a potential energy consisting entirely of pairwise interactions, it is most convenient to use Faddeev's method. The Faddeev equations for this system can be written

$$(T - E)\psi_a + V_a(r_1)\Psi = 0,$$

$$(T - E)\psi_b + V_b(r_2)\Psi = 0,$$

$$(T - E)\psi_c + V_c(r_3)\Psi = 0. \tag{7}$$

These three equations add up to give the three-particle Schrödinger equation

$$(H - E)\Psi = 0 \tag{8}$$

with

$$H = T + V_a + V_b + V_c, \quad \Psi = \psi_a + \psi_b + \psi_c. \tag{9}$$

For the homonuclear helium trimer, each Faddeev equation (7) has the identical form

$$(T_0 + k^2)\psi_a - \frac{\lambda_0}{r_0}\delta(r_1 - r_0)\Psi = 0. \tag{10}$$

The advantage of the Faddeev equation (10) over the full Schrödinger equation (8) is that only a single δ function boundary condition need be considered. The function ψ_a can be associated with the channel in which atoms 2 and 3 form a diatomic molecule, with atom 1 as a spectator.

Equation (10) is separable in the hyperspherical coordinates R, α_1, β_1. The hyperradius is defined by

$$R \equiv \sqrt{\frac{2r_1^2 + 2r_2^2 + 2r_3^2}{3}}, \tag{11}$$

while

$$\alpha_1 \equiv \arcsin(r_1/R), \quad 0 \leqslant \alpha_1 \leqslant \pi/2 \tag{12}$$

and β_1 is the angle between the Jacobi vectors $\mathbf{r}_3 - \mathbf{r}_2$ and $\mathbf{r}_1 - \frac{1}{2}(\mathbf{r}_3 + \mathbf{r}_2)$. As we will show, an exact analytic solution to the Faddeev equations can be obtained with a separable function

$$\psi_a(R, \alpha_1, \beta_1) = f(R)\phi(\alpha_1)P_L(\cos\beta_1), \tag{13}$$

where $P_L(\cos\beta_1)$ is a Legendre polynomial. The quantum number L represents the internal angular momentum of atom 1 about the diatomic fragment 2-3.

For the helium trimer, the ground state and the Efimov states all have total rotational angular momenta of zero. This does not preclude contributions from $L > 0$ terms in a hyperspherical partial-wave expansion. For the δ function model, however, exact solutions exist with just the S partial-wave, $L = 0$. This is possible because of the way δ function factors simplify the right-hand sides of the Faddeev equations. The implication is that, in addition to the 2-3 diatomic being in an S state, the orbit of atom 1 about the diatomic fragment is also spherically symmetrical. Indeed solutions involving higher partial waves do exist, but these almost certainly represent excited states of the model. (For more realistic potentials, higher partial waves have been found to make small but nonvanishing contributions to the ground state.)

With $L = 0$, $P_L(\cos\beta_1) = 1$, and the requisite solutions to the Faddeev equations become separable functions of just R and α_1. For $r_1 \neq r_0$, the Faddeev equation (10) describes a free-particle state:

$$(T_0 + k^2)f(R)\phi(\alpha_1) = 0. \tag{14}$$

The other two Faddeev component equations are analogous, with α_1 replaced by α_2 and α_3, respectively. Equation (14) reduces to two ordinary differential equations

$$f''(R) + \frac{5}{R}f'(R) + \frac{s^2 + 4}{R^2}f(R) = k^2 f(R) \tag{15}$$

and

$$\phi''(\alpha) + 4\cot(2\alpha)\phi'(\alpha) - (s^2 + 4)\phi'(\alpha) = 0, \tag{16}$$

where $s^2 + 4$ is a convenient separation constant. Integration over the domain of R and α involves the differential element $R^5 \sin(2\alpha) dR d\alpha$.

Solutions to Eq. (15), for real s, involve modified Bessel functions of imaginary order, $K_{is}(kR)$ and $I_{is}(kR)$. These are oscillatory functions with exponentially increasing frequency as $kR \to 0$. The solution $f(R) = R^{-2}K_{is}(kR)$ is a real function, well-behaved at both $R \to 0$ and $R \to \infty$. The second solution $R^{-2}I_{is}(kR)$ is well behaved only for $0 \leqslant R \lesssim R_0$.

Equation (16) has solutions $\phi(\alpha)=\csc(2\alpha)\sinh(s\alpha)$ finite at $\alpha=0$ and $\phi(\alpha)=\csc(2\alpha)\sinh[s(\pi/2-\alpha)]$ finite at $\alpha=\pi/2$. A continuous solution ψ_a to the Faddeev equation (17), with the requisite kink at $r_1=r_0$, can thus be constructed as follows:

$$\psi_a = R^{-2} I_{is}(kR_<) K_{is}(kR_>) \csc(2\alpha) \times \sinh(s\alpha_<) \sinh\left[s\left(\frac{\pi}{2} - \alpha_> \right) \right], \tag{17}$$

where $\alpha=\arcsin(r_1/R)$, $\alpha_0=\arcsin(r_0/R)$ and $R_0=\sqrt{2}\, r_0$.

The solution to the Faddeev equation is obtained by matching the δ function contributions from the kinetic- and potential-energy operators. *After* evaluating the derivatives, we set $r_1=r_2=r_3=r_0$, which represents the instantaneous equilateral-triangle configuration of the trimer, with hyperradius R_0.

IV. TRIMER GROUND STATE

Efimov [1] concluded that the trimer has not only an infinite number states with real values of the parameter s, but also a single deep bound state with a pure imaginary value of s. We will show that the appropriate value for the latter state is $s=-\frac{1}{2}\, i$. The Faddeev component ψ_a in Eq. (17) can be reduced to

$$\psi_a = R^{-3} \sinh(kR_<) e^{-kR_>} \csc(2\alpha) \sin\left(\frac{\alpha_<}{2} \right) \sin\left(\frac{\pi}{4} - \frac{\alpha_>}{2} \right), \tag{18}$$

making use of the simple analytic forms for $I_{1/2}(x)$ and $K_{1/2}(x)$ in terms of spherical Bessel functions. By virtue of the δ-function-bubble potential, each pair of helium atoms has zero interaction energy when $r_{ij}<r_0$. Thus the dimer can hypothetically be obtained from the trimer simply by merging two of the helium atoms (do not try this with a more realistic potential function). This is accomplished by setting $r_1=r_2=r$ and $r_3=0$. Correspondingly, we have $R=2r/\sqrt{3}$, $R_0=2r_0/\sqrt{3}$ and $\alpha=\alpha_0=\pi/4$. The trimer function then reduces to the form

$$\psi_a(r) = r^{-3} \sinh(\kappa r_<) e^{-\kappa r_>} \tag{19}$$

identical to Eq. (2), apart from a factor of r from the change in coordinate system. Because all interatomic potentials vanish when $r_{ij}=0$ for our delta-shell model, the three-body singularity ("Thomas collapse") is avoided.

Using Eq. (18) in the Faddeev equation (10), we find, for the ground state of the trimer,

$$\lambda_0 = \frac{1}{3} \cot\left(\frac{\pi}{8} \right) + \frac{1}{9} kR_0 e^{kR_0} \operatorname{csch}(kR_0). \tag{20}$$

The parameters λ_0 and r_0 can be fitted to the accurately-calculated energies of the dimer and trimer ground states: $\varepsilon^{\text{dimer}}=-1.31$ mK and $\varepsilon_0^{\text{trimer}}\approx -130$ mK. Energy on the millikelvin scale is given by $\varepsilon=-3.1577\times 10^8\, k^2/M$ mK. The values consistent with Eqs. (3) and (20) are $\lambda_0=1.080\,44, r_0=14.2486$ bohr. In agreement with Efimov, we find no other bound states with imaginary values of s. As we shall show in the following section, real values of s give the Efimov states.

The Thomas effect also follows easily from Eq. (20). Thomas [11] showed that as the *range* r_0 of the two-body potential is decreased, the three-body binding energy can become very large. Since λ_0 determines the quantity kR_0 and k is proportional to $\sqrt{-\varepsilon}$, it follows that $\varepsilon=-\text{const}/r_0^2$ and thus its magnitude increases without limit as $r_0\to 0$. Thomas was able to estimate the range of nuclear forces by relating the energies of two- and three-nucleon systems.

V. EFIMOV STATES

For real values of the parameter s, the Bessel function $K_{is}(kR)$ is an acceptable solution to the hyperradial equation (15) over the entire range of R. The discontinuous derivative necessary to produce a deltafunction can be obtained from the dependence on α alone, such that

$$\psi_a = R^{-2} K_{is}(kR) \csc(2\alpha) \sinh(s\alpha_<) \sinh\left[s\left(\frac{\pi}{2} - \alpha_> \right) \right]. \tag{21}$$

Solution of the Faddeev equation fulfilling the deltafunction boundary condition can be obtained with

$$\lambda = \frac{2}{3} s \coth\left(\frac{s\pi}{4} \right) \tag{22}$$

and

$$K_{is}(kR_0) = 0. \tag{23}$$

We are no longer restricting λ to λ_0, its optimal value in $^4\text{He}_3$, in order to demonstrate the most general aspects of the Efimov effect. Using the trimer parameters λ_0 and r_0 determined above, Eq. (22) gives $s_0=1.184$. The lowest energy root of Eq. (23) corresponds then to the first excited state of the trimer with $\varepsilon_1=-1.34$ mK, of the right general magnitude and below the dimer energy of -1.31 mK.

Equation (23) has an infinite number of roots. For values of $\lambda\leqslant 1$, these correspond, in principle, to trimer energy levels which are *not* absorbed into the dimer+monomer continuum. These can be quite accurately determined from the $x\to 0$ asymptotic form of the Bessel function

$$K_{is}(x) \approx \frac{\Gamma(-is)}{2} \left(\frac{x}{2} \right)^{is} + \frac{\Gamma(is)}{2} \left(\frac{x}{2} \right)^{-is}. \tag{24}$$

The recursive relation $k_{n+1}=k_n\, e^{-\pi/s}$ is implied for the roots $x_n=k_nR_0$ of Eq. (23). This leads to Efimov's exponential sequence of energy levels

$$\varepsilon_{n+1} = \varepsilon_n e^{-2\pi/s}, \quad n=1,2,3\ldots, \tag{25}$$

with a point of accumulation at $\varepsilon=0$ as $n\to\infty$.

In representing the trimer ground state, $is=\frac{1}{2}$ is assumed only for $\lambda\geqslant 1$, so the hypothetical alchemy to a bound dimer described above can be carried out. For $\lambda<1$, the parameter

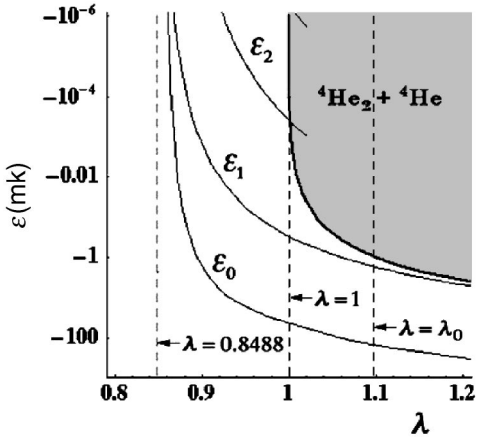

FIG. 1. Quantitative version of Efimov diagram based on the δ function potential. The energy levels of the helium dimer and trimer are plotted as functions of the pairwise interaction strength. The shaded region represents the dimer+monomer continuum. Note the logarithmic energy scale. For $0.8488 \leq \lambda \leq 1$, there is an infinite number of bound Efimov states, with a point of accumulation at $\varepsilon = 0$.

is is chosen to minimize the energy. In accordance with Eq. (20), the parameter *is* decreases from $\frac{1}{2}$ to 0 as λ is reduced to $8/3\pi \approx 0.8488$.

VI. SUMMARY OF RESULTS

Figure 1 represents the dependence of dimer and trimer energies as functions of λ. This is a quantitative version, based on our deltafunction model, of the schematic energy diagrams given in Efimov's papers. As λ is increased to approximately 0.8488, an infinite number of trimer bound states $\varepsilon_0, \varepsilon_1, \varepsilon_2 \ldots$ condense out of the continuum. According to Eq. (25), the energy levels are exponentially spaced, with a point of accumulation at $\varepsilon = 0$. This is the essence of the famous "Efimov effect." These bound levels persist up to $\lambda = 1$, which corresponds to the zero-energy resonance of the dimer. It is unlikely that more than two or three Efimov levels are experimentally accessible, since higher levels involve energies in the nanokelvin range. As λ is further increased above 1, the discrete states are successively absorbed into the continuum—the shaded region in Fig. 1—as the trimer fragments into a dimer+monomer. The model is consistent with the survival of just two bound states at the empirical value of λ_0.

For λ slightly greater than 1, the highest bound state ε_N must have an energy comparable to that of the dimer for the same value of λ. Equation (4) implies, to logarithmic accuracy, that

$$\ln \varepsilon_N \approx \ln(\lambda - 1) \approx \ln\left(\frac{r_0}{a}\right), \tag{26}$$

so that the number of Efimov levels is approximated by

$$N \approx \frac{s}{\pi} \ln\left(\frac{a}{r_0}\right), \tag{27}$$

where a/r_0 is the ratio of the scattering length to the range of the interatomic potential.

Our model for the Efimov effect agrees with results deduced by other workers using more realistic potentials. See, for example, the detailed studies of three-body systems with short range interactions by Federov, Jensen and co-workers [12,13]. Efimov states are exhibited in the limiting behavior of real resonant systems. By contrast, our results follow from *exact* solutions for an idealized model of the trimer.

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