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Regularization of a three-body problem with zero-range potentials

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Abstract

We propose a coordinate-space regularization of the three-body problem with zero-range potentials. We include the effective range and the shape parameter in the boundary condition of the zero-range potential. The proposed extended zero-range model is tested against atomic helium trimers and is shown to provide an adequate quantitative description of these systems.

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1. Introduction

The zero-range potential [1] has been extensively used over many years as a practical and convenient form of effective interaction. The concept employs the separation of scales in a physical problem and allows a qualitative and often quantitative description of the low-energy properties of a physical system in a simple and transparent way (see, e.g., [2]).

However, the application of the zero-range potential to a three-body system presents a problem; a *collapse* of the system known as the Thomas effect [3]. The three-body system with zero-range potentials has no ground state but infinitely many bound states with vanishing spatial extension and an exceedingly large binding energy.

Several attempts have been made to alleviate this problem by adding some sort of cutoff to the potential in momentum space [4–6] or by switching to a finite-range potential in certain areas of configuration space [7].

We introduce an alternative coordinate space approach where the collapse is removed by a suitable modification of the boundary condition of the zero-range potential. The boundary condition is extended to include the higher-order parameters of the effective range expansion. The three-body system then acquires a well defined ground state while all the simplicity and transparency of the zero-range model is retained.

We apply this formalism to some rather involved three-body systems, helium trimers, and show that the extended zero-range model provides an accurate description of these systems.

2. The zero-range model and regularization

2.1. Zero-range potentials

The quantum mechanical two-body problem with a zero-range potential can be formulated [1] as the free Schrödinger equation for the s -state wavefunction ψ with the relative coordinate r and wavenumber k ,

$$\left(-\frac{d^2}{dr^2} - k^2\right)r\psi = 0 \quad (1)$$

with the solution

$$r\psi = \sin(kr + \delta(k)) \quad (2)$$

and a boundary condition at $r = 0$ expressed in terms of the scattering length a as

$$\frac{1}{r\psi} \frac{d(r\psi)}{dr} \Big|_{r=0} = k \cot \delta(k) = \frac{1}{a}. \quad (3)$$

For a negative scattering length a bound state solution exists

$$r\psi \propto \exp(-\kappa r) \quad (4)$$

where $\kappa > 0$ can be found from the boundary condition (3), $\kappa = 1/|a|$.

The zero-range model for a three-body system can be formulated as a *free* three-body wavefunction Ψ which satisfies the three boundary conditions

$$\frac{1}{|\mathbf{r}_j - \mathbf{r}_k| \Psi} \frac{\partial |\mathbf{r}_j - \mathbf{r}_k| \Psi}{\partial |\mathbf{r}_j - \mathbf{r}_k|} \Big|_{|\mathbf{r}_j - \mathbf{r}_k|=0} = \frac{1}{a_i} \quad i = 1, 2, 3 \quad (5)$$

where \mathbf{r}_i is the coordinate of the i th particle, a_i is the scattering length in the two-body system of particles j and k with $\{i, j, k\}$ being a positive permutation of $\{1, 2, 3\}$.

The derivatives in the boundary condition (5) are most suitably formulated in terms of the hyper-spheric coordinates $\{\rho, \alpha_i\}$ (defined in the appendix):

$$\frac{\partial}{\partial |\mathbf{r}_j - \mathbf{r}_k|} \Big|_{|\mathbf{r}_j - \mathbf{r}_k|=0} = \frac{\sqrt{\mu_i}}{\rho} \frac{\partial}{\partial \alpha_i} \Big|_{\alpha_i=0}. \quad (6)$$

The boundary condition (5) can then be rewritten as

$$\frac{1}{\alpha_i \Psi} \frac{\partial (\alpha_i \Psi)}{\partial \alpha_i} \Big|_{\alpha_i=0} = \frac{\rho}{\sqrt{\mu_i}} \frac{1}{a_i}. \quad (7)$$

2.2. Hyper-spheric expansion

We shall employ the hyper-spheric adiabatic expansion [8] of the three-body wavefunction

$$\Psi(\rho, \Omega) = \frac{1}{\rho^{5/2}} \sum_n f_n(\rho) \Phi_n(\rho, \Omega) \quad (8)$$

in terms of the complete basis $\Phi_n(\rho, \Omega)$ of the solutions of the hyper-angular eigenvalue equation

$$\left(\Lambda + \frac{2m\rho^2}{\hbar^2} \sum_{i=1}^3 V_i\right) \Phi_n(\rho, \Omega) = \lambda_n(\rho) \Phi_n(\rho, \Omega) \quad (9)$$

where V_i is the potential between particles j and k , m is the mass scale used in the definition of the hyper-spheric coordinates and Λ is the angular part¹ of the kinetic energy operator (see appendix).

For potentials without strong repulsive cores the lowest term in the expansion (the so-called hyper-spheric adiabatic approximation) already gives a very good approximation to the precise solution [10]. Again it is the lowest term that causes the Thomas collapse of a three-body system with zero-range potentials and thus in the following for the sake of simplicity we shall consider only this problematic lowest term of the hyper-spheric expansion. The inclusion of the higher terms is straightforward.

The wavefunction then simplifies to

$$\Psi(\rho, \Omega) = \frac{1}{\rho^{5/2}} f(\rho) \Phi(\rho, \Omega) \tag{10}$$

where the hyper-radial wavefunction $f(\rho)$ satisfies the equation

$$\left(-\frac{\partial^2}{\partial \rho^2} + \frac{\lambda(\rho) + \frac{15}{4}}{\rho^2} - Q(\rho) - \frac{2mE}{\hbar^2} \right) f(\rho) = 0 \tag{11}$$

where $\lambda(\rho)$ is the lowest eigenvalue in equation (9), E is the total energy and

$$Q(\rho) = \int d\Omega \Phi(\rho, \Omega) \frac{\partial^2}{\partial \rho^2} \Phi(\rho, \Omega). \tag{12}$$

2.3. Faddeev equations

For short- and zero-range potentials the Faddeev decomposition of the angular wavefunction $\Phi(\rho, \Omega)$ provides a convenient framework for an analysis of the three-body system [9]

$$\Phi(\rho, \Omega) = \sum_{i=1}^3 \frac{\varphi_i(\rho, \alpha_i)}{\sin(2\alpha_i)} \tag{13}$$

where the three components $\varphi_i(\rho, \alpha_i)$ satisfy a system of Faddeev equations [11]

$$(\Lambda - \lambda(\rho)) \frac{\varphi_i(\rho, \alpha_i)}{\sin(2\alpha_i)} + \frac{2m\rho^2}{\hbar^2} V_i \Phi(\rho, \Omega) = 0. \tag{14}$$

Since the zero-range potentials act only on the s-waves only the latter are included in each of the three components φ_i .

All three components of the wavefunction Φ in (14) must be ‘rotated’ into the same Jacobi system. This is done by substituting the variables and subsequently projecting onto the s-waves. The transformation of φ_k into the j th Jacobi system is given as

$$\varphi_{j \leftarrow k}(\alpha_j) = \frac{1}{\sin(2\phi_{jk})} \int_{|\phi_{jk}-\alpha_j|}^{\frac{\pi}{2}-|\frac{\pi}{2}-\phi_{jk}-\alpha_j|} \varphi_k(\alpha_k) d\alpha_k \tag{15}$$

where

$$\phi_{jk} = \arctan \left(\sqrt{\frac{m_i(m_1 + m_2 + m_3)}{m_j m_k}} \right). \tag{16}$$

The expansion of $\varphi_{j \leftarrow k}(\alpha_j)$ for small angles $\alpha_j \ll 1$ reads

$$\varphi_{j \leftarrow k}(\alpha_j) = \alpha_j \frac{2\varphi_k(\phi_{jk})}{\sin(2\phi_{jk})} + O(\alpha_j^2). \tag{17}$$

¹ Here Ω is any of three possible sets of angles.

The zero-range potentials vanish identically except at the origin and we are therefore left with the free Faddeev equations

$$\left(-\frac{\partial^2}{\partial \alpha_i^2} - v^2(\rho)\right) \varphi_i(\rho, \alpha_i) = 0 \quad (18)$$

which are obtained from (14) with $l_x = l_y = 0$ and $V_i=0$, and where $v^2 = \lambda + 4$. The solutions are

$$\varphi_i(\rho, \alpha_i) = A_i(\rho) \sin \left[v(\rho) \left(\alpha_i - \frac{\pi}{2} \right) \right] \quad (19)$$

with the boundary condition $\varphi_i(\rho, \frac{\pi}{2}) = 0$.

The factors A_i are to be determined from the boundary condition (7) which can now be reformulated in terms of the angular function Φ as

$$\left. \frac{\partial (\alpha_i \Phi(\rho, \Omega))}{\partial \alpha_i} \right|_{\alpha_i=0} = \frac{\rho}{\sqrt{\mu_i}} \frac{1}{a_i} \alpha_i \Phi(\rho, \Omega) \Big|_{\alpha_i=0}. \quad (20)$$

The required wavefunction, $\alpha_i \Phi$, and its partial derivative, $\partial(\alpha_i \Phi)/\partial \alpha_i$, are easily obtained from (13) and (17):

$$2\alpha_i \Phi = \varphi_i(\alpha_i) + \alpha_i \sum_{j \neq i} \frac{2\varphi_j(\phi_{ij})}{\sin(2\phi_{ij})} + O(\alpha_j^2) \quad (21)$$

$$2 \left. \frac{\partial(\alpha_i \Phi)}{\partial \alpha_i} \right|_{\alpha_i=0} = \left. \frac{\partial \varphi_i(\alpha_i)}{\partial \alpha_i} \right|_{\alpha_i=0} + \sum_{j \neq i} \frac{2\varphi_j(\phi_{ij})}{\sin(2\phi_{ij})}. \quad (22)$$

Substituting the free solutions (19) leads to

$$2\alpha_i \Phi|_{\alpha_i=0} = -A_i \sin \left(v \frac{\pi}{2} \right) \quad (23)$$

$$2 \left. \frac{\partial(\alpha_i \Phi)}{\partial \alpha_i} \right|_{\alpha_i=0} = A_i v \cos \left(v \frac{\pi}{2} \right) + \sum_{j \neq i} A_j \frac{2 \sin \left[v \left(\phi_{ij} - \frac{\pi}{2} \right) \right]}{\sin(2\phi_{ij})}. \quad (24)$$

The boundary condition (20) then becomes a system of linear equations for the three factors A_i

$$A_i v \cos \left(v \frac{\pi}{2} \right) + \sum_{j \neq i} A_j \frac{2 \sin \left[v \left(\phi_{ij} - \frac{\pi}{2} \right) \right]}{\sin(2\phi_{ij})} = -\frac{\rho}{\sqrt{\mu_i}} \frac{1}{a_i} A_i \sin \left(v \frac{\pi}{2} \right). \quad (25)$$

A non-trivial solution exists only when the determinant of the corresponding matrix $M(v, \rho)$ is zero

$$\det M(v, \rho) = 0 \quad (26)$$

where the matrix elements are

$$\begin{aligned} M_{ii} &= v \cos \left(v \frac{\pi}{2} \right) + \sin \left(v \frac{\pi}{2} \right) \frac{\rho}{\sqrt{\mu_i}} \frac{1}{a_i} \\ M_{i \neq j} &= \frac{2 \sin \left[v \left(\phi_{ij} - \frac{\pi}{2} \right) \right]}{\sin(2\phi_{ij})}. \end{aligned} \quad (27)$$

The solution $v(\rho)$ of equation (26) provides the adiabatic potential $(v^2(\rho) - 1/4)/\rho^2$ for the hyper-radial equation (11) from which one obtains the hyper-radial wavefunction of the three-body system.

2.4. Asymptotic behaviour of the eigenvalues

For a system of three identical bosons, where $\varphi_{ij} = \pi/3$, equation (26) simplifies to

$$\frac{-v \cos(v\frac{\pi}{2}) + \frac{8}{\sqrt{3}} \sin(v\frac{\pi}{6})}{\sin(v\frac{\pi}{2})} = \frac{\rho}{\sqrt{\mu}} \frac{1}{a}. \tag{28}$$

For large distances, $\rho \gg a$, there is a solution that asymptotically approaches $v(\infty) = 2$. Expanding (28) in terms of $1/\rho$ around $v = 2$ gives the leading terms

$$v = 2 - \frac{12}{\pi} \frac{\sqrt{\mu}a}{\rho} \quad \lambda = -\frac{16}{\pi} \frac{3\sqrt{\mu}a}{\rho^3} \tag{29}$$

which is the lowest solution when no bound two-body subsystems are present. In this case the effective potential is a $1/\rho^3$ type.

However, when there is a two-body bound state another kind of solution exists for large ρ which asymptotically behaves as $v \sim i\rho$. The leading terms are then

$$v = i \frac{\rho}{\sqrt{\mu}} \frac{1}{|a|} + i \frac{8}{\sqrt{3}} \exp\left(-\frac{\rho}{\sqrt{\mu}} \frac{1}{|a|} \frac{\pi}{3}\right) \tag{30}$$

$$\lambda = -\frac{\rho^2}{\mu a^2} - \frac{\rho}{\sqrt{\mu}} \frac{1}{|a|} \frac{16}{\sqrt{3}} \exp\left(-\frac{\rho}{\sqrt{\mu}} \frac{1}{|a|} \frac{\pi}{3}\right) - 4. \tag{31}$$

The effective potential is then of the Yukawa type:

$$\frac{\lambda + 15/4}{\rho^2} = -\frac{2mB}{\hbar^2} - \frac{1}{4\rho^2} - \frac{16\sqrt{3}}{\pi} \frac{b}{\rho} \exp\left(-\frac{\rho}{b}\right) \tag{32}$$

where $B = \hbar^2/(2\mu ma^2)$ is the two-body binding energy and $b = 3\sqrt{\mu} |a|/\pi$. The corresponding angular wavefunction (19) is asymptotically

$$\sin\left[v\left(\alpha - \frac{\pi}{2}\right)\right] = \sin\left[\frac{i\rho}{\sqrt{\mu}} \frac{1}{|a|} \left(\alpha - \frac{\pi}{2}\right)\right] \propto \exp\left(-\frac{\rho\alpha}{\sqrt{\mu} |a|}\right). \tag{33}$$

This wavefunction is non-vanishing only when $\alpha \sim \sqrt{\mu} |a|/\rho \ll 1$. In this region the Jacobi coordinates x and y (defined in the appendix) are approximately, up to the linear terms in α , given by $x \approx \rho\alpha$ and $y \approx \rho$. This solution corresponds to a bound two-body state with momentum $k_0 = i/|a|$ and binding energy B . The three-body wavefunction then factorizes as

$$\Phi \propto \frac{1}{x} \exp\left(-\frac{x}{\sqrt{\mu} |a|}\right) f(y) \tag{34}$$

and describes a dimer in the bound state $\frac{1}{x} \exp(-\frac{x}{\sqrt{\mu} |a|})$ and a third particle with a relative coordinate y and wavefunction $f(y)$. The corresponding radial equation asymptotically describes a two-body system with a Yukawa potential

$$\left[-\frac{\partial^2}{\partial \rho^2} - \frac{2m}{\hbar^2} (E + B) - \frac{16\sqrt{3}}{\pi} \frac{b}{\rho} \exp\left(-\frac{\rho}{b}\right) \right] f(\rho) = 0. \tag{35}$$

The term $-1/(4\rho^2)$ in this equation cancelled the leading order term of $Q(\rho)$. Indeed the normalized angular Faddeev component is (asymptotically)

$$\varphi(\rho, \alpha) = \sqrt{\frac{2\rho}{\sqrt{\mu} |a|}} \exp\left(-\rho \frac{\alpha}{\sqrt{\mu} |a|}\right) \tag{36}$$

and therefore

$$Q(\rho) \rightarrow \int_0^\infty \varphi(\rho, \alpha) \frac{\partial^2}{\partial \rho^2} \varphi(\rho, \alpha) d\alpha = -\frac{1}{4\rho^2}. \tag{37}$$

We have thus a correct asymptotic wavefunction corresponding to a dimer and a third particle in a relative s-wave.

The term Q is generally small and only is important for ensuring the correct asymptotic behaviour. In the following practical application for simplicity we shall always use only the leading term $-1/(4\rho^2)$ instead of the full Q similar to the Langer correction term in [7].

2.5. The Thomas effect and regularization

For $\rho \ll a$ the equation (28) for ν reduces to

$$-\nu \cos\left(\nu \frac{\pi}{2}\right) + \frac{8}{\sqrt{3}} \sin\left(\nu \frac{\pi}{6}\right) = 0 \quad (38)$$

which has the well known imaginary roots $\nu_0 = \pm ig$, where $g \cong 1.006$, which cause the Thomas and also the Efimov [12] effects.

These imaginary roots lead to an effective potential in the hyper-radial equation which in the small distance region, $\rho \ll a$, is equal to $(\nu_0^2 - 1/4)/\rho^2 \cong -1.262/\rho^2$ and the radial equation becomes

$$\left(-\frac{\partial^2}{\partial \rho^2} + \frac{\nu_0^2 - 1/4}{\rho^2} - \frac{2mE}{\hbar^2}\right) f(\rho) = 0. \quad (39)$$

The (negative) energy $E = -\hbar^2 \kappa^2/(2m)$ is negligible compared to the effective potential when the distance is sufficiently small, $\rho \ll \kappa^{-1}$, and the corresponding radial equation

$$\left(-\frac{\partial^2}{\partial \rho^2} + \frac{\nu_0^2 - 1/4}{\rho^2}\right) f(\rho) = 0 \quad (40)$$

has, in this region, solutions of the form $f(\rho) \sim \rho^n$, where $n = \frac{1}{2} \pm \nu_0$. For imaginary $\nu_0 = \pm ig$ the exponent n also acquires an imaginary part $\pm ig$ leading to

$$f(\rho) \propto \sqrt{\rho} \exp(\pm ig \ln \rho). \quad (41)$$

This wavefunction has infinitely many nodes at small distances or, correspondingly, infinitely many low-lying states at smaller distances. This is called the Thomas effect.

A suitable modification of the boundary condition (7) is necessary in order to eliminate the problematic imaginary root ν_0 at $\rho = 0$ which causes the Thomas effect. Intuitively one could generalize the zero-range potential by introducing the higher-order terms of the effective-range theory

$$\frac{1}{r\psi} \frac{d(r\psi)}{dr} \Big|_{r=0} = \frac{1}{a} + \frac{1}{2} Rk^2 + PR^3k^4 \quad (42)$$

where R is the effective range and P is the shape parameter of the two-body system. This would lead to the following modification of the matrix elements in the eigenvalue equation (26):

$$M_{ii} = \nu \cos\left(\nu \frac{\pi}{2}\right) + \sin\left(\nu \frac{\pi}{2}\right) \frac{\rho}{\sqrt{\mu_i}} \left[\frac{1}{a_i} + \frac{1}{2} R_i \left(\frac{\sqrt{\mu_i} \nu}{\rho}\right)^2 + P_i R_i^3 \left(\frac{\sqrt{\mu_i} \nu}{\rho}\right)^4 \right] \quad (43)$$

and equation (7) for three identical bosons is then replaced by an extended equation

$$\frac{-\nu \cos(\nu \frac{\pi}{2}) + \frac{8}{\sqrt{3}} \sin(\nu \frac{\pi}{6})}{\sin(\nu \frac{\pi}{2})} = \frac{\rho}{\sqrt{\mu}} \left[\frac{1}{a} + \frac{1}{2} R \left(\frac{\sqrt{\mu} \nu}{\rho}\right)^2 + PR^3 \left(\frac{\sqrt{\mu} \nu}{\rho}\right)^4 \right]. \quad (44)$$

This extended equation at $\rho = 0$ has a real root $\nu(0) = 0$ and the Thomas collapse is therefore removed.

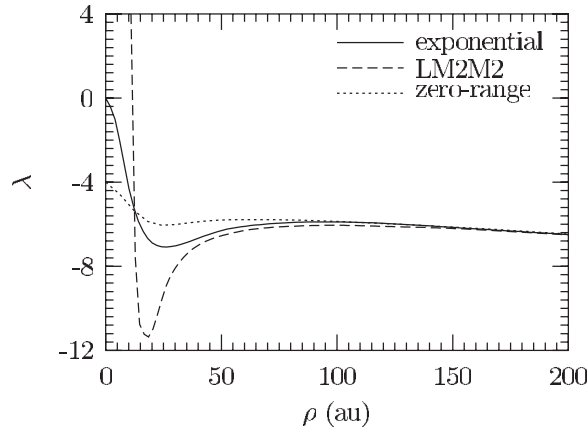


Figure 1. The angular eigenvalue λ as function of ρ for the ${}^4\text{He}$ -trimer for different potential models: exponential [10], realistic LM2M2 [10], and zero-range with $P = 0.13$. All models have the same scattering length $a = -189.05$ au and effective range $R = 13.843$ au.

Although the second-order term with the effective range is, in principle, enough for the elimination of the imaginary root, the fourth-order term is necessary to ensure the correct analytic properties of the roots of the equation.

Unlike the scattering length and effective range the parameter P has to be interpreted as a regularization parameter which somehow accounts for all the higher-order terms in the k^2 expansion, rather than a true shape parameter of the two-body scattering. The scattering length and effective range are important for the correct asymptotic behaviour of the eigenvalue λ at large distances while the P parameter accounts for the pocket region and is in this model supposed to absorb all the remaining short distance properties of the system.

3. Application to helium trimers

The helium trimer ${}^4\text{He}_3$ is a challenging three-body system since there is a weakly bound dimer state, ${}^4\text{He}_2$, where the scattering length $a = -189.054$ au is much larger than the effective range $R = 13.843$ au (the atomic unit of length is equal to the Bohr radius $a_B = 0.529177$ Å). Numeric computations with a realistic LM2M2 potential show that there is a ground state and an extremely weakly bound excited state interpreted as an Efimov state (see, e.g., [10, 13] and references therein).

For our calculations we use as in [10] the mass scale $m = 1822.887$ au (the atomic unit of mass is equal to the electron mass $m_e = 0.510999$ MeV c^{-2}). The mass of the ${}^4\text{He}$ atom is $m({}^4\text{He}) = 4.002603m$. The angular eigenvalue $\lambda(\rho) = v^2(\rho) - 4$ is obtained directly by numeric solution of the transcendental equation (44).

On figure 1 we compare the angular eigenvalues obtained from the zero-range model with $P = 0.13$ and from two finite-range models: the realistic LM2M2 potential and an exponential potential with all models having the same scattering length and effective range.

At large distances, $\rho \gg R$, the angular eigenvalues from all models approach each other since it is only the scattering length and effective range that determine the asymptotic behaviour of λ .

At short distances the behaviour is different. The realistic LM2M2 model with a strong repulsive core produces a strongly repulsive eigenvalue. The eigenvalue from the exponential

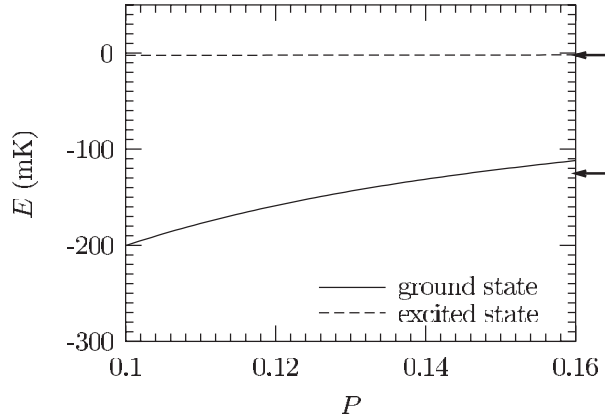


Figure 2. The energies of the ground and the excited state of ${}^4\text{He}$ -trimer as function of the P parameter of the extended zero-range model. The arrows indicate the results of the realistic LM2M2 model [10].

Table 1. The bound-state energies of the helium trimers ${}^4\text{He}_3$ and ${}^4\text{He}_2 {}^3\text{He}$ for finite-range potential models [10], and for the zero-range model with $P = 0.13$. The ${}^4\text{He}$ - ${}^4\text{He}$ scattering length is $a = -189.054$ au and effective range $R = 13.843$ au. For ${}^4\text{He}$ - ${}^3\text{He}$ system $a = 33.261$ au, $R = 18.564$ au. The mass of ${}^3\text{He}$ is $m({}^3\text{He}) = 3.016026$. For the Gaussian, exponential and zero-range models the energies shown are calculated within the adiabatic (one-channel) approximation (10). For these simple potentials the relative accuracy of the adiabatic approximation is better than 1%. The LM2M2 energies are obtained with the full expansion (8).

Potential	$E_0({}^4\text{He}_3)$ (mK)	$E_1({}^4\text{He}_3)$ (mK)	$E_0({}^4\text{He}_2 {}^3\text{He})$ (mK)
LM2M2	-125.2	-2.269	-13.66
Gaussian	-150.2	-2.462	-18.41
Exponential	-173.9	-2.714	-24.27
Zero-range	-143.7	-2.21	-34.0

potential converges to $\lambda(0) = 0$ as it does for all potentials which diverge slower than r^{-2} at the origin [8]. The eigenvalue from the zero-range model converges to $\lambda(0) = -4$ according to (44). This is precisely sufficient to eliminate the Thomas effect.

Although the zero-range model gives a stronger attraction at small distances the correct large distance behaviour and a good overall agreement make it a solid alternative to finite-range potentials. One would expect that a weakly bound three-body state, not sensitive to the short-range details of the potential, should be reasonably well described by the zero-range model while one would expect some over-binding for strongly bound states.

3.1. Bound states

The extended zero-range model correctly predicts the number of ${}^4\text{He}$ -trimer bound states (two states) for large variations in the P parameter, see figure 2. The energy of the weakly bound excited state, predicted rather accurately, is largely independent of the P parameter since it mostly resides in the outer region which is determined exclusively by the scattering length and effective range. The stronger bound ground state is more sensitive to the inner part of the effective potential and therefore to the P parameter. On average the zero-range model gives a description similar to finite-range models, see table 1.

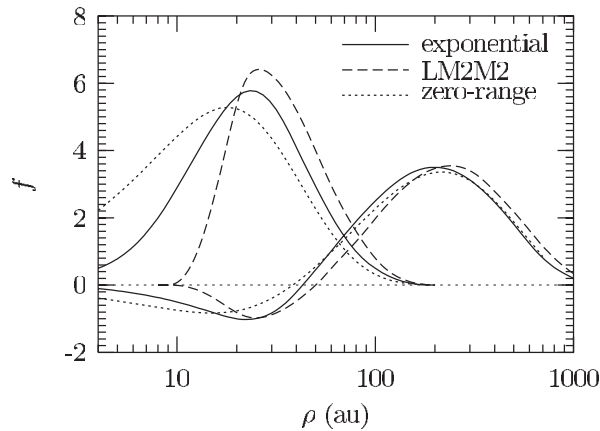


Figure 3. The arbitrarily normalized radial wavefunctions f as function of ρ for the ground and the excited states of the ${}^4\text{He}$ trimer for the potential models from figure 1.

3.2. Radial functions

Figure 3 compares the radial functions from different models. Due to the softness of the zero-range model at short distances the ground state wavefunction is shifted to the left in comparison to the exponential and LM2M2 potentials. However, it is still rather similar to those obtained from the finite-range models. The wavefunctions for the excited state are roughly identical for all models since the spatially extended weakly bound states are less sensitive to the individual features of the underlying potential model.

3.3. Non-identical particles

Another bound atomic trimer ${}^4\text{He}_2\text{}^3\text{He}$ is obtained by substituting ${}^3\text{He}$ for one of the ${}^4\text{He}$ atoms. The scattering length in the subsystem ${}^3\text{He}\text{-}{}^4\text{He}$ is $a = 33.261$ au and the effective range is $R = 18.564$ au. In order to obtain $v(\rho)$ for the system of non-identical particles we have to solve the general equation (26).

Although the P parameter for the ${}^3\text{He}\text{-}{}^4\text{He}$ subsystem should generally speaking be also different, we choose the same value $P = 0.13$ for the sake of simplicity. With these parameters the zero-range model correctly predicts that there is only one bound state in this system. The binding is somewhat larger than for finite-range potentials but within the same range of accuracy, see table 1. Again, we did not make any attempt to fit the binding energy by varying P .

4. Conclusion

Zero-range potential is a very useful form of effective interaction whose applications to three-body systems are, however, severely hampered by the Thomas collapse. We propose a coordinate space regularization of the zero-range potential which leads to a removal of the Thomas collapse. The new model on one hand retains all the simplicity of the zero-range potential and on the other hand provides a fully regularized solution for the three-body system. Compared to finite-range potentials the computational load is greatly reduced and amounts to solving a transcendental equation for the effective potential and the subsequent ordinary differential equation for the radial wavefunction. We applied the proposed model to atomic

helium trimers and showed that it works well and produces results comparable to finite-range models.

Appendix. Hyper-spheric coordinates

If m_i and \mathbf{r}_i refer to the i th particle then the hyper-radius ρ and the hyper-angles α_i are defined in terms of the Jacobi coordinates \mathbf{x}_i and \mathbf{y}_i as [14]

$$\begin{aligned} \mathbf{x}_i &= \sqrt{\mu_i}(\mathbf{r}_j - \mathbf{r}_k) & \mathbf{y}_i &= \sqrt{\mu_{jk}} \left(\mathbf{r}_i - \frac{m_j \mathbf{r}_j + m_k \mathbf{r}_k}{m_j + m_k} \right) \\ \mu_i &= \frac{1}{m} \frac{m_j m_k}{m_j + m_k} & \mu_{jk} &= \frac{1}{m} \frac{m_i(m_j + m_k)}{m_i + m_j + m_k} \\ \rho \sin(\alpha_i) &= x_i & \rho \cos(\alpha_i) &= y_i \end{aligned} \quad (45)$$

where $\{i, j, k\}$ is a cyclic permutation of $\{1, 2, 3\}$ and m is an arbitrary mass. The set of angles Ω_i consists of the hyper-angle α_i and the four angles $x_i/|x_i|$ and $y_i/|y_i|$. The kinetic energy operator T is then given as

$$\begin{aligned} T &= T_\rho + \frac{\hbar^2}{2m\rho^2} \Lambda & T_\rho &= -\frac{\hbar^2}{2m} \left(\rho^{-5/2} \frac{\partial^2}{\partial \rho^2} \rho^{5/2} - \frac{1}{\rho^2} \frac{15}{4} \right) \\ \Lambda &= -\frac{1}{\sin(2\alpha_i)} \frac{\partial^2}{\partial \alpha_i^2} \sin(2\alpha_i) - 4 + \frac{l_{x_i}^2}{\sin^2(\alpha_i)} + \frac{l_{y_i}^2}{\cos^2(\alpha_i)} \end{aligned} \quad (46)$$

where l_{x_i} and l_{y_i} are the angular momentum operators related to \mathbf{x}_i and \mathbf{y}_i .

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