PHYSICAL REVIEW A VOLUME 49, NUMBER 3 MARCH 1994

Pathologies in three-body molecular clusters when using δ-shell potentials

Young-Ju Jee, Sigurd Y. Larsen, and Robert L. Intemann
Department of Physics, Temple University, Philadelphia, Pennsylvania 19122

M. Fabre de la Ripelle
Division de Physique Théorique, Institut de Physique Nucléaire, 91406 Orsay, France

(Received 19 August 1993)

In this work the calculation of the binding energy of three ^{4}He atoms is carried out using δ-shell binary potential models, hyperspherical harmonic expansions, and adiabatic approximations. The results obtained with a one δ-shell potential are well within the range of those obtained by other workers using different techniques. The ones with the two δ-shell potentials are not. We show that attractive δ-shells lead to pathologies in calculations of the eigenpotentials, and in the resulting binding energies—and that those effects are expected to become more important for the two δ-shell binary potentials.

PACS number(s): 36.40.+d

I. INTRODUCTION

Noble-gas clusters have been observed experimentally in the cases of helium [1], argon [2], and xenon [3]. Recently even the very weakly bound helium dimer [4] has been observed experimentally. Many workers have tried to calculate the binding energies of two, three, and four helium atom clusters using a variety of methods. Among these have been the Green's-function Monte Carlo method, the variational Monte Carlo method [5], variational wave functions [5], amalgamation of two-body correlations into the multiple-scattering process [6], Faddeev-Yakubovsky theory [7,8], and separable approximations [9] to the two-body t matrix–all of these using various potentials [10–12]. In addition, Pandharipande, Zabolitzky, Pieper, Wiringa, and Helmbrecht (PZPWH) [5] and Pandharipande, Pieper, and Wiringa [13] have used a droplet model for a number of particles $A \geq 4$ to calculate the binding energies per atom E/A using the Hartree-Fock-dispersion He-He interatomic potential (HFDHE2) [14].

A hyperspherical harmonic (HH) approach [15–17] has been used with considerable success in the study of the few-body problem. We note, in the work of some of our collaborators, the study of bound-state problems in nuclear physics by Das, Coelho, and Fabre de la Ripelle (DCF) [18], by Ballot, Fabre de la Ripelle, and Levinger (BFL) [19], and by Fabre de la Ripelle, Jee, Klemm, and Larsen (FJKL) [20], as well as selected scattering problems [21,23,24].

With respect to the use of δ functions, a number of calculations in one dimension have been reported. In particular, McGuire [25], Yang [26], and Yang and Yang [27] used equal-strength δ functions for an N-body system; they also were used by Dodd [28] for three particles. Hyperspherical harmonic and adiabatic results were obtained by Gibson, Larsen, and Popiel (GLP) [29] for the binding energy of the three-body system, and Popiel [30] and Popiel and Larsen [31] showed that the first three coefficients in an expansion of the three-body S matrix could be obtained exactly by an extension of these hyperspherical harmonic and adiabatic techniques.

Since the latter authors were able to do much of their investigation analytically, it appears to be highly desirable to investigate the binding energy of clusters of ^{4}He atoms as a function of the number of ^{4}He atoms by the use of the hyperspherical harmonics method and δ-shell interatomic potentials. It was anticipated that the δ shells might yield, in three dimensions, the "separability" of the matrix elements without the divergences associated with δ functions at the origin [32]. To set the stage for the sections that follow, we conclude this Introduction with a brief outline of our model and our methods of calculation.

The one δ-shell model consists of a single attractive δ function of the form for the interatomic binary potential:

$$V(r_{ij}) = -V_1 r_1 \delta(r_{ij} - r_1) , \tag{1}$$

whereas the two δ-shell model consists of two δ functions, one attractive and one repulsive:

$$V(r_{ij}) = V_0 r_0 \delta(r_{ij} - r_0) - V_1 r_1 \delta(r_{ij} - r_1) . \tag{2}$$

It should be noted that all of these δ functions are located off the origin.

To determine suitable values for the parameters V_1 and r_1 in the one δ-shell case, and V_0, V_1, r_0, and r_1 in the two δ-shell case, we adopt the well-known Mason-Rice 1 (MR1) interatomic binary potential [33], already used by Blatt, Lyness, and Larsen (BLL) [12] to obtain three-body energies, which has one bound state of 0.034 K for the two helium-atom cluster [36]. We then obtain the parameters for the one and two δ-shell cases, by fitting to the wave function and the binding energy of the Mason-Rice potential—sometimes also using details of the potential itself—using a procedure which is described in detail in the following section.

The fitted δ-shell potentials are then used to obtain the binding energy of a three-^{4}He-atom cluster. To do this, we use HH expansions to transform the Schrödinger equation for a cluster of three helium atoms, interacting via the δ-shell potentials, into a set of coupled differential equations. We decouple these equations using the adiabatic approximations (an extreme adiabatic approximation yields a lower bound to the binding energy and an uncoupled adiabatic approximation yields an upper bound) to obtain diagonal eigenpotentials. After carrying out extensive analytical and numerical calculations of these eigenpotentials, we use them to obtain binding energies by integrating the resulting uncoupled radial equations.

II. THE δ-SHELL POTENTIAL MODEL

In our approach the one δ-shell potential for a two-body interaction is given by Eq. (1). From the Schrödinger equation, $H\Psi=E_0\Psi$, the two-body equation for the s-wave bound state is

$$\left\{-\frac{\hbar^2}{m}\frac{d^2}{dr^2}+V(r)-E_0\right\}u(r)=0\ , \tag{3}$$

where $r=r_{ij}$ and $\Psi=u(r)/r$. Hence, if we let the binding energy be $E_0=-\hbar^2k^2/m$, and define $x\equiv kr$, we obtain the following reduced equation:

$$\left\{-\frac{d^2}{dx^2}+\frac{1}{|E_0|}V(x/k)+1\right\}u(x)=0\ . \tag{4}$$

Integrating this equation twice, we find that the solution of Eq. (4) will have the form

$$u(x)=\begin{cases}\sinh x, & x\le x_1\\ Ce^{-x}, & x\ge x_1\ .\end{cases} \tag{5}$$

At $x=x_1(\equiv kr_1)u(x)$ is continuous and $C=e^{x_1}\sinh x_1$. For $x\ge x_1$, therefore, $u(x)=e^{x_1}\sinh x_1 e^{-x}$.

At the point x_1 the wave function undergoes a change of slope. Integrating Eq. (4) between $x_1\pm\epsilon$, where ϵ is infinitesimally small, we obtain a relation between V_1 and x_1 of the form

$$\frac{V_1x_1}{|E_0|}=1+\frac{\cosh x_1}{\sinh x_1}\ . \tag{6}$$

We can then determine V_1, given x_1, if the energy $|E_0|$ is known. Different values have been proposed for this binding energy. See, for example, BLL [12], Poulat, Larsen, and Novaro [34], and Uang and Stwalley [35]. Here we will adopt the value 0.034 K from the calculation of the binding energy of two ^{4}He atoms using the Mason Rice 1 potential. The general Mason-Rice potential has the form

$$V(r_{ij})=\frac{\epsilon}{1-6/\alpha}\left[\frac{6}{\alpha}e^{\alpha(1-r_{ij}/r_m)}-\left[\frac{r_m}{r_{ij}}\right]^6\right]\ , \tag{7}$$

where the constant ϵ is the depth of the potential minimum, r_m is the value of r at the minimum, and α determines the hardness of the repulsive core. As discussed by MR, the choice of values

$$\alpha=12.4,\ \frac{\epsilon}{k}=9.16\text{ K},\ r_m=3.135\text{ Å}\ , \tag{8}$$

defines the Mason-Rice 1 potential.

We choose x_1 in such a way that the mean squared radius a^2, which is defined by

$$a^2=\frac{\int_0^\infty[u(x)]^2r^2dr}{\int_0^\infty[u(x)]^2dr}\ , \tag{9}$$

has the same value for the one δ-shell potential as it has for the Mason-Rice 1 potential. [For the δ-shell potential the mean square radius a is a function of r_1 since the integration of $u(x)$ depends on r_1.] Once x_1 is determined from Eq. (9) in this way, the value of V_1 can be determined from Eq. (6). Our one δ-shell potential is then completely determined.

The two δ-shell binary potential, as defined by Eq. (2), includes a repulsive δ-shell term in addition to the attractive one. In the same way as for the one δ-shell potential, we have for the solution of Eq. (4): $u(x)=\sinh x$ for $x\le x_0$, and $u(x)=Ce^{-x}$ for $x\ge x_1$, as in Eq. (5). In the region between the δ shells, $x_0\le x\le x_1$, one can write

$$u(x)=\sinh x+B\sinh(x-x_0)\ . \tag{10}$$

By integrating Eq. (4) between $x_0\pm\epsilon$, where ϵ is very small, we obtain the coefficient B so that

$$u(x)=\sinh x+\frac{V_0}{|E_0|}x_0\sinh x_0\sinh(x-x_0) \tag{11}$$

for $x_0\le x\le x_1$. From

$$u(x_1+\epsilon)=u(x_1-\epsilon) \tag{12}$$

at $x=x_1$, we obtain the coefficient C so that

$$u(x)=\left\{\sinh x_1+\frac{V_0}{|E_0|}x_0\sinh x_0\sinh(x_1-x_0)\right\}e^{-(x-x_1)} \tag{13}$$

for $x\ge x_1$.

Integrating Eq. (4) between $x_1\pm\epsilon$, we get the relation between V_1 and V_0

$$\frac{V_1x_1}{|E_0|}=1+\frac{\cosh x_1+\dfrac{V_0}{|E_0|}x_0\sinh x_0\cosh(x_1-x_0)}{\sinh x_1+\dfrac{V_0}{|E_0|}x_0\sinh x_0\sinh(x_1-x_0)}\ . \tag{14}$$

The binding energy, $E_0=-(\hbar^2/m)k^2$, which determines the wave number k, is to be the same as that given by the Mason-Rice 1 potential. We can then obtain x_0 (or r_0) by choosing it so that for the Mason-Rice 1 potential $V(x_0)=0$ [or $V(r_0)=0$]. The position of x_1 (or r_1) is determined in such a way that r_1 is fixed as the position of the minimum of the Mason-Rice 1 potential.

As before, we have to choose V_0 in such a way that the mean squared radius a^2 has the same value for our two δ-shell potential as for the Mason-Rice 1 potential, using the definition, Eq. (9). The two δ-shell potential is then completely defined, the continuity condition at x_1, Eq. (14), determining the value of V_1.

III. HYPERSPHERICAL HARMONICS

The hyperspherical formalism [15–17,20,21,22,37] provides a method for solving the Schrödinger equation to obtain the binding energies of the three-body system, or for that matter any A-body system. In our work we will use Fabre de la Ripelle's hyperspherical formalism [22] to obtain the coupled equations and the matrix elements.

The Schrödinger equation for a system of A identical particles can be expressed as

$$\left\{-\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla_{x_i}^2+\sum_{i,\,j>i}V(\vec{r}_{ij})-E\right\}\Psi(\mathbf{x})=0\ , \tag{15}$$

where $\mathbf{x}$ stands for the set of coordinates x_i of the particles and $V(r_{ij})$ is a two-body interaction potential. Using Jacobi coordinates

$$\vec{\xi}_n=\left[\frac{2n}{n+1}\right]^{1/2}\left[\vec{x}_{n+1}-\frac{1}{n}\sum_{i=1}^{n}\vec{x}_i\right],\quad n=1,\ldots,N$$

where $N=A-1$, one can eliminate the center of mass. The Schrödinger equation, in the center of mass system, is then

$$\left\{-\frac{\hbar^2}{m}\nabla^2+V(\vec{\xi})-E\right\}\Psi(\vec{\xi})=0\ .$$

In our formalism, we expand the wave function of the ground state in a potential hyperspherical harmonics basis with the hyperradius,

$$r=\left[\frac{2}{A}\sum_{i,\,j>i}(\vec{x}_i-\vec{x}_j)^2\right]^{1/2}\ ,$$

giving us

$$\Psi(\vec{\xi})=r^{-(D-1)/2}\sum_{K=0}^{\infty}C_K\sum_{i,\,j>i}\mathcal{P}_{2K}^{0}(\Omega_{ij})u_K(r)\ ,$$

where C_K is a normalization constant determined by Eqs. (19) and (20), and where

$$\mathcal{P}_{2K}^{0}(\Omega_{ij})=Y_0^0(\omega_{ij})^{(N)}P_{2K}^{0,0}(\phi_N)Y_0(D-3)$$

and ${}^{(N)}P_{2K}^{0,0}(\phi_N)$ and $Y_0(D-3)$ will be defined shortly by Eqs. (27) and (23), respectively. This is an approximation to an expansion using a full basis, but it is much simpler and preserves one and two-body correlations. It gives rise to the coupled equations

$$\left\{-\frac{d^2}{dr^2}+\frac{\mathcal{L}_K(\mathcal{L}_K+1)}{r^2}-\frac{m}{\hbar^2}E\right\}u_K(r)+\frac{m}{\hbar^2}\sum_{K'}V_K^{K'}(r)u_{K'}(r)=0\ , \tag{16}$$

where

$$\mathcal{L}_K=2K+\frac{D-3}{2} \tag{17}$$

and

$$D=3(A-1),\ K=0,1,2,3,\ldots\ .$$

The potential matrix in Eq. (16) is given by

$$V_K^{K'}(r)=f_Kf_{K'}\langle\mathcal{P}_{2K}^{0}(\Omega_{ij})|V(r_{ij})|\mathcal{P}_{2K'}^{0}(\Omega_{ij})\rangle \tag{18}$$

with the normalized symmetrical basis,

$$B_K^{(s)}=C_K\sum_{i,\,j>1}\mathcal{P}_{2K}^{0}(\Omega_{ij})\ , \tag{19}$$

where

$$\langle B_K^{(s)}|B_K^{(s)}\rangle=1\ . \tag{20}$$

The potential matrix is symmetric under exchanges between K and K'. The quantity f_K^2 is given by the following formula in which $C_{2K+1}^{D/2-2}(\tfrac{1}{2})$ is the Gegenbauer polynomial with $D=3N=3(A-1)$, as before:

$$\begin{aligned}f_K^2&=\left\langle\mathcal{P}_{2K}^{0}(\Omega_{21})\,\middle|\,\sum_{i,\,j>i}\mathcal{P}_{2K}^{0}(\Omega_{ij})\right\rangle\\&=1+4(N-1)\frac{(2K+1)!(D-5)!}{(2K+D-4)!}C_{2K+1}^{D/2-2}(\tfrac{1}{2})\\&\quad+\frac{(-1)^K}{2^{2K+1}}(N-1)(N-2)\frac{(2K+1)!}{K!}\\&\quad\times\frac{\Gamma((D-3)/2)}{\Gamma(K+(D-3)/2)}\ .\end{aligned} \tag{21}$$

For the calculation of the matrix in Eq. (18), we use

$$\mathcal{P}_{2K}^{0}(\Omega_{ij})=Y_0^0(\omega_{ij})^{(N)}P_{2K}^{0}(\phi_N)Y_0(D-3)\ , \tag{22}$$

where

$$\cos\phi_N=\frac{r_{ij}}{r}\ ,Y_0(D-3)=\left[\frac{\Gamma((D-3)/2)}{2\pi^{(D-3)/2}}\right]^{1/2}, \tag{23}$$

with the surface element given by

$$d\Omega=2^{-D/2}(1-z)^{(D-5)/2}(1+z)^{1/2}dz\,d\omega_{ij}\,d\Omega_{N-1}\ , \tag{24}$$

where

$$z=\cos^2\phi_N=2\frac{r_{ij}^2}{r^2}-1,\ 0\le r_{ij}\le r\ . \tag{25}$$

The potential matrix can now be written as

$$\begin{aligned}V_K^{K'}(r)&=f_Kf_{K'}2^{-D/2}\int_{-1}^{1}(1-z)^{(D-5)/2}(1+z)^{1/2}\\&\quad\times{}^{(N)}P_{2K}^{00}(\phi_N)^{(N)}P_{2K'}^{00}(\phi_N)V(r_{ij})dz\\&\quad\times\int|Y_0^0|^2d\omega_{ij}\int|Y_0(D-3)|^2d\Omega_{N-1}\ ,\end{aligned} \tag{26}$$

where

$$ {}^{(N)}P_{2K}^{00}=\left[\frac{2\left(2K+\frac{D-2}{2}\right)\Gamma\left(K+\frac{D-2}{2}\right)K!}{\Gamma\left(K+\frac{D-3}{2}\right)\Gamma\left(K+\frac{3}{2}\right)}\right]^{1/2} P_K^{(D-5)/2,1/2}(\cos 2\phi_N)\ , \tag{27} $$

with $P_K^{(D-5)/2,1/2}$ denoting a Jacobi polynomial. It may also be expressed as an integral over r_{ij}

$$ V_K^{K'}(r)=f_K f_{K'} C_K^N C_{K'}^N \int_0^r \left(1-\frac{r_{ij}^2}{r^2}\right)^{(D-5)/2} V(r_{ij})\frac{r_{ij}^2}{r^3} P_K^{(D-5)/2,1/2}\left(2\frac{r_{ij}^2}{r^2}-1\right) P_{K'}^{(D-5)/2,1/2}\left(2\frac{r_{ij}^2}{r^2}-1\right) dr_{ij}\ , \tag{28} $$

with

$$ C_K^N=\left[\frac{(\mathcal{L}_K+1)\Gamma(\mathcal{L}_K-K+\frac{1}{2})K!}{\Gamma(\mathcal{L}_K-K)\Gamma(K+\frac{3}{2})}\right]^{1/2}\ . \tag{29} $$

For the case of the δ-shell potential, i.e., the two δ-shell potential $V(r_{ij})=V_0 r_0 \delta(r_{ij}-r_0)-V_1 r_1 \delta(r_{ij}-r_1)$, the potential matrix then becomes

$$ V_K^{K'}=f_K f_{K'} \mathcal{W}_K^{K'}\ , \tag{30} $$

where

$$ \mathcal{W}_K^{K'}(r)=C_K^N C_{K'}^N \frac{1}{r^3}\int_0^r dr_{ij} r_{ij}^2 \left(1-\frac{r_{ij}^2}{r^2}\right)^{(D-5)/2} P_K^{(D-5)/2,1/2}\left(2\frac{r_{ij}^2}{r^2}-1\right) P_{K'}^{(D-5)/2,1/2}\left(2\frac{r_{ij}^2}{r^2}-1\right) \times\{V_0 r_0 \delta(r_{ij}-r_0)-V_1 r_1 \delta(r_{ij}-r_1)\} \tag{31} $$

and where $0\le r_{ij}\le r$. Using $\int_0^r f(x)\delta(x-x_0)dx=f(x_0)$ for $0\le x\le r$, and letting $x=r_{ij}/r$, we obtain

$$ \mathcal{W}_K^{K'}=C_K^N C_{K'}^N \frac{1}{r^3}\sum_{n=0,1}(-1)^n \epsilon\left(\frac{r_n}{r}\right) V_n r_n^3 \left(1-\frac{r_n^2}{r^2}\right)^{\alpha} \times P_K^{\alpha,1/2}\left(2\frac{r_n^2}{r^2}-1\right) P_{K'}^{\alpha,1/2}\left(2\frac{r_n^2}{r^2}-1\right)\ , \tag{32} $$

where

$$ \epsilon(x)=\begin{cases}1, & x<1\\ 0, & x\ge 1\end{cases} \tag{33} $$

and

$$ \alpha=\frac{D-5}{2}=\frac{3A}{2}-4,\quad x=\frac{r_n}{r}\ . \tag{34} $$

Thus, in this case, the potential matrix becomes

$$ V_K^{K'}(x)=f_K f_{K'} C_K^N C_{K'}^N \times\sum_{n=0,1}(-1)^n \epsilon(x) V_n x^3 \times(1-x^2)^{\alpha} P_K^{\alpha,1/2}(2x^2-1) \times P_{K'}^{\alpha,1/2}(2x^2-1)\ . \tag{35} $$

Consequently, the potential matrix can be written in the form

$$ V_K^{K'}(r)=\sum_{n=0,1}(-1)^n V_n \mathcal{V}_K\left(\frac{r_n}{r}\right)\mathcal{V}_{K'}\left(\frac{r_n}{r}\right)\ , \tag{36} $$

where

$$ \mathcal{V}_K(x)=f_K C_K^N x^{3/2}(1-x^2)^{\alpha/2} P_K^{\alpha,1/2}(2x^2-1)\ . \tag{37} $$

Now let us consider three atoms of ^{4}He ($A=3$) with the one and two δ-shell potentials. In the case of one attractive δ-shell potential, the potential matrix becomes Eq. (38), consisting of a product of a function of K times a function of K'. (This "separability" will become very important in the following work.)

$$ V_K^{K'}=-V_1 \mathcal{V}_K\left(\frac{r_1}{r}\right)\mathcal{V}_{K'}\left(\frac{r_1}{r}\right)\ , \tag{38} $$

where

$$ \mathcal{V}_K(x_1)=f_K C_K^2 x_1^{3/2}(1-x_1^2)^{1/4} P_K^{1/2,1/2}(2x_1^2-1) \tag{39} $$

and

$$ f_K=\left\{1+\frac{\frac{4}{\sqrt{3}}\sin\left[\frac{2\pi}{3}(K+1)\right]}{K+1}\right\}^{1/2}\ , \qquad C_K^2=\frac{2(K+1)!}{\Gamma\left(K+\frac{3}{2}\right)}\ . \tag{40} $$

Using the Jacobi polynomial

$$ P_K^{1/2,1/2}(\cos\phi)=\frac{2(K+\frac{1}{2})!}{\sqrt{\pi}(K+1)!}\frac{\sin(K+1)\phi}{\sin\phi}\ , $$

where $\cos\phi=2x_1^2-1$, and similarly for $P_{K'}^{1/2,1/2}$, the potential matrix becomes

$$V_K^{K'} = -V_1 \frac{4}{\pi} \frac{1}{\rho\sqrt{1-(1/\rho^2)}} \sin(K+1)\phi \sin(K'+1)\phi$$
$$\times \left[\left\{ 1 + \frac{\frac{4}{\sqrt{3}} \sin\left[\frac{2\pi}{3}(K+1)\right]}{K+1} \right\} \left\{ 1 + \frac{\frac{4}{\sqrt{3}} \sin\left[\frac{2\pi}{3}(K'+1)\right]}{K'+1} \right\} \right]^{1/2} , \tag{41}$$

with the use of the notation

$$\rho = \frac{1}{x_1} = \frac{r}{r_1} , \quad 2x_1^2 - 1 = \cos\phi . \tag{42}$$

Similarly, for the case of the two δ-shell potential the potential matrix $V_K^{K'}$ becomes

$$V_K^{K'} = \frac{4}{\pi} \left\{ V_0 \frac{1}{\rho\sqrt{1-(1/\rho^2)}} \sin(K+1)\phi \sin(K'+1)\phi - V_1 \frac{1}{\rho_1\sqrt{1-(1/\rho_1^2)}} \sin(K+1)\theta \sin(K'+1)\theta \right\}$$
$$\times \left[\left\{ 1 + \frac{\frac{4}{\sqrt{3}} \sin\left[\frac{2\pi}{3}(K+1)\right]}{K+1} \right\} \left\{ 1 + \frac{\frac{4}{\sqrt{3}} \sin\left[\frac{2\pi}{3}(K'+1)\right]}{K'+1} \right\} \right]^{1/2} , \tag{43}$$

with

$$x_0 = \frac{r_0}{r} , \quad x_1 = \frac{r_1}{r} , \quad \rho = \frac{1}{x_0} , \quad \rho_1 = \frac{1}{x_1} , \tag{44}$$

and

$$2x_0^2 - 1 = \cos\phi , \quad 2x_1^2 - 1 = \cos\theta . \tag{45}$$

IV. DIAGONALIZATION OF THE MATRIX

A technique for the diagonalization of the set of coupled equations of the type given by Eq. (16) was proposed and used by several workers, and is referred to as the extreme adiabatic approximation (EAA) [19,20,29]; in addition, there exists an improved adiabatic approximation, the uncoupled adiabatic approximation (UAA). See, for example, DCF [18], Larsen and Zhen [38], and FJKL [20].

Using the first approach [24], we try to decouple our differential equations by first writing Eq. (16) in a vector and matrix form

$$\frac{d^2\boldsymbol{\phi}}{d\rho^2} + [q^2\mathbf{I} - \mathbf{M}(\rho)]\boldsymbol{\phi} = 0 , \tag{46}$$

where ϕ is a vector and $\mathbf{M}(\rho)$ is the sum of the centrifugal term and the potential matrix. Its matrix elements take the form of

$$M_K^{K'}(\rho) = \frac{4(K+1)^2 - \frac{1}{4}}{\rho^2} \delta_K^{K'} + \frac{m}{\hbar^2} \mathbf{V}_K^{K'}(\rho) . \tag{47}$$

At this point, $\mathbf{M}(\rho)$ is diagonalized by a similarity transformation using the matrix $\mathbf{U}(\rho)$. Using the EAA, where we set

$$\mathbf{U}'(\rho) = 0 , \quad \mathbf{U}''(\rho) = 0 , \tag{48}$$

we can then obtain a set of uncoupled equations

$$\tilde{\boldsymbol{\phi}}'' + [q^2\mathbf{I} - \Lambda(\rho)]\tilde{\boldsymbol{\phi}} = 0 , \tag{49}$$

where

$$\boldsymbol{\phi} = \mathbf{U}\tilde{\boldsymbol{\phi}}, \Lambda(\rho) = \mathbf{U}^T\mathbf{M}(\rho)\mathbf{U} . \tag{50}$$

What we have here are uncoupled equations with a matrix $\Lambda(\rho)$ which is a diagonal set of eigenpotentials.

Dropping the tilde on ϕ, and writing the λ for the lowest eigenpotential, we can write

$$\frac{d^2\phi}{d\rho^2} - \frac{m|E|}{\hbar^2}\phi - \lambda\phi = 0 ,$$

where now ϕ is a normal wave function.

GLP [29] obtained the eigenpotentials by obtaining the solutions of transcendental equations—in the case of a separable potential obtained from a binary δ-function potential, in one dimension. We use the same trick in the case of our one and two δ-shell potentials (see Appendix A).

Proceeding in this way, we find for the one δ-shell potential the following sum rule:

$$1 = \beta \sum_i \frac{f_i^2}{h_i - \lambda} , \tag{51}$$

where

$$f_i = \left[1 + \frac{4}{\sqrt{3}} \frac{\sin\frac{2}{3}\pi i}{i} \right]^{1/2} \sin i\phi ,$$

$$\beta = \frac{4mr_1^2}{\pi\hbar^2} \frac{V_1}{\rho\sqrt{1-(1/\rho^2)}} , \tag{52}$$

and for two δ-shell potential case

$$\left[1-\sum_i \frac{\beta f_i^2}{h_i-\lambda}\right]\left[1+\sum_i \frac{\alpha g_i^2}{h_i-\lambda}\right]=-\alpha\beta\left[\sum_i \frac{f_i g_i}{h_i-\lambda}\right]^2 , \tag{53}$$

where

$$f_i=\left[1+\frac{4}{\sqrt{3}}\frac{\sin\frac{2}{3}\pi i}{i}\right]^{1/2}\sin i\theta ,$$

$$g_i=\left[1+\frac{4}{\sqrt{3}}\frac{\sin\frac{2}{3}\pi i}{i}\right]^{1/2}\sin i\phi ,$$

and

$$\alpha=\frac{4mr_0^2}{\pi\hbar^2}\frac{V_0}{\rho\sqrt{1-(1/\rho^2)}} ,\ \beta=\frac{4mr_0^2}{\pi\hbar^2}\frac{V_1}{\rho_1\sqrt{1-(1/\rho_1^2)}} . \tag{54}$$

We are now able to solve for the eigenpotential λ (which can be written as a sum of the centrifugal term and an effective potential) numerically and also analytically.

Appendix B contains an outline of the procedures used in the numerical calculations. We can also find the eigenpotential analytically by carrying out analytically the summation in the sum rule given by Eq. (51), thereby obtaining Eq. (C5). In Eq. (C5) we rescaled r by dividing by r_1, as in (42), in a manner which will be described in the following section for the one δ-shell potential (see Appendix C, Sec. 1). The more complicated two δ-shell case is also shown in Appendix C, Sec. 1.

As we shall see later, the lowest eigenpotential in the EAA diverges negatively as $\rho(=r/r_0)$ goes to d $(=r_1/r_0)$. We will also check the eigenpotential when ρ is near d using the uncoupled adiabatic approximation which, as shown by BFL [19], gives us an upper bound on the ground state energy. The UAA retains the diagonal elements of $\mathbf{U}''(\rho)$ while the diagonal elements of $\mathbf{U}^{\mathrm{T}}\mathbf{U}'$ are zero automatically due to normalization of the eigenvectors forming $\mathbf{U}$.

Since

$$\left[\mathbf{U}^T\frac{d\mathbf{U}}{d\rho}\right]_{KK}=0 ,\ \left[\mathbf{U}^T\frac{d^2\mathbf{U}}{d\rho^2}\right]_{KK}=-\sum_l\left[\frac{d\mathbf{U}_{lK}}{d\rho}\right]^2, \tag{55}$$

we obtain

$$\tilde{\phi}_K''+q^2\tilde{\phi}_K+\left\{-\sum_l\left[\frac{d\mathbf{U}_{lK}}{d\rho}\right]^2-\Lambda_K(\rho)\right\}\tilde{\phi}_K=0 . \tag{56}$$

As we can see, the difference between EAA and UAA is the sum of the squares of $d\mathbf{U}_{lK}/d\rho$ which involves the derivative of the eigenvectors of $\mathbf{M}(\rho)$, i.e.,

$$\lambda_K(\rho)_{\mathrm{UAA}}=\lambda_K(\rho)_{\mathrm{EAA}}+\sum_l\left[\frac{d\mathbf{U}_{lK}}{d\rho}\right]^2 . \tag{57}$$

The $\mathbf{U}_{lK}$ is the Kth normalized eigenvector. The eigenvector corresponding to the lowest eigenvalue will be the same as $[\chi_n]$ in Eq. (C15), i.e.,

$$[\chi_n]=\frac{\chi_n}{\left[\sum_n|\chi_n|^2\right]^{1/2}} . \tag{58}$$

In our one δ-shell case in Eq. (C17) (see Appendix C, Sec. 2) it is given by

$$\chi_n=\frac{V_1 m r_1^2}{\hbar^2\pi}\frac{\rho}{\sqrt{1-(1/\rho^2)}}\frac{\left[1+\frac{4}{\sqrt{3}}\frac{\sin\frac{2}{3}\pi n}{n}\right]^{1/2}\sin n\phi}{n^2+s^2} . \tag{59}$$

We need to find $\sum_n\{d[\chi_n(\rho)]/d\rho\}^2$ in order to obtain λ_{UAA}.

V. RESULTS

We determined the parameters of the one and two δ-shell potentials, in Eqs. (1) and (2), in the manner described in previous sections. We used the Mason-Rice 1 potential for two ^{4}He atoms to determine the binary δ-shell potential parameters which we then used in our three-helium-atom cluster calculations. The resulting values are shown in Table I. Through this procedure we obtained a mean square radius a of 16.89 Å for the two-body bound state using the Mason-Rice 1 potential. We then used this value of a for both (the one and two) δ-shell potential cases.

We proceeded to solve the Schrödinger equation (15) of a three-^{4}He-atom cluster, by using the HH expansion method and the two types of binary δ-shell potentials in order to obtain the coupled equations in Eq. (16). We then decoupled the equations using the adiabatic approximation, specifically, the EAA. We diagonalized the matrix $\mathbf{M}_K^{K'}$ in Eq. (47). We then rescaled Eq. (16) to a dimensionless form in which the dimensionless distance, which we call the hyperradius ρ, is obtained by dividing r by the parameter r_1 as defined in Eq. (42) for the case of the one δ-shell potential. The corresponding hyperradius ρ, for the case of the two δ-shell potential, is obtained by dividing r by the parameter r_0 as in Eq. (44). This rescaling proved convenient in our calculations.

We succeeded in obtaining the lowest eigenpotentials both numerically and analytically. The numerical approach proved to require very extensive computation. For example, the numerical work in Eq. (B8), which includes summation over the index n in Eqs. (B9) and (B10) for the one δ-shell potential case, involved a summation over n up to around 131 000 to make the result agree with the analytical calculation to an accuracy of 10^{-5} at each point of ρ. In other words, we needed a lot of harmonics to carry out the numerical work. Fortunately, an analytical approach allowed a summation over n to infinity and permitted us to find the eigenpotential as the solution of a transcendental equation, with an enormous saving of time. It also gave us the possibility of obtaining

TABLE I. Values of parameters for the binary potentials.

Parameter	One δ shell	Two δ shell
V_0 (K)		3.525
V_1 (K)	0.393	3.335
r_0 (Å)		2.756
r_1 (Å)	6.537	3.135
$d(=r_1/r_0)$		1.1375

analytical results for the eigenpotential in critical regions.

In the single attractive δ-shell potential case, the lowest eigenpotential includes only the centrifugal term for $0<\rho\leq 1$; for $\rho \geq 1$, the attractive δ-shell part contributes. We found a singularity in the eigenpotential at $\rho=1$. Past the singularity the eigenpotential increases as ρ increases, and asymptotically ($\rho \rightarrow \infty$) the eigenpotential converges to a negative constant value (see Fig. 1). For the two δ-shell potentials we found the same behavior as in the case of the one δ-shell potential for the region $0<\rho\leq 1$ because there is no effect of the presence of the δ shells in this region. Past this point the eigenpotential feels the repulsive δ-shell part so that the curve increases up to $\rho=d(\equiv r_1/r_0)$, which is the position where the attractive δ-shell potential starts to contribute. At this point we again found an attractive singularity at $\rho=d$. Beyond $\rho=d$ the eigenpotential increases asymptotically, approaching a negative constant value (see Fig. 2).

A. Singular behaviors of the eigenpotentials

We investigated the singular behavior of the eigenpotential starting with the one δ-shell potential case at point $\rho=1+\epsilon$, when ϵ is small. Analytical calculations using Eq. (C5), which includes the variables ρ and ϕ, allowed us to determine the behavior of the eigenpotential; in this case we rescaled by r_1 as shown previously in Eq. (42).

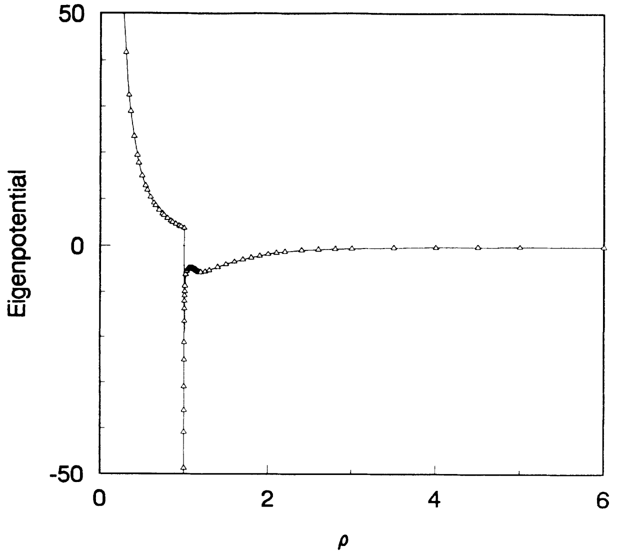

FIG. 1. The eigenpotential of three atoms of ^{4}He using the one δ-shell potential.

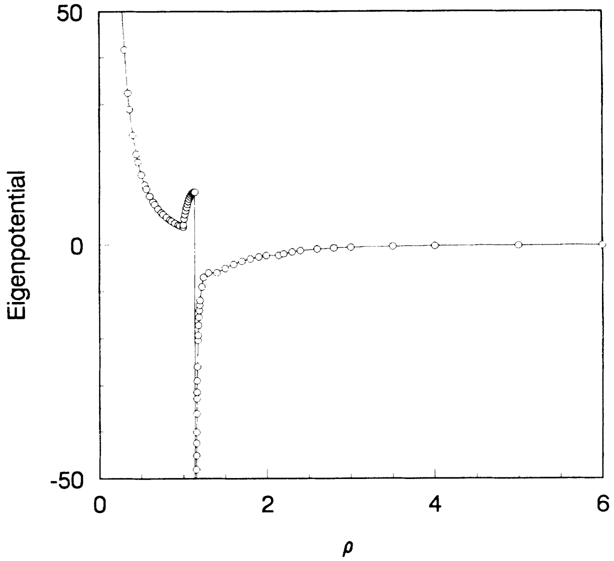

FIG. 2. The eigenpotential of three atoms of ^{4}He using the two δ-shell potential.

For s very large, where $s=\frac{1}{4}\sqrt{4|\lambda|\rho^2-1}$, i.e., ρ near 1, Eq. (C5) reduces to

$$1=\frac{V_1 m r_1^2}{4s\hbar^2}\left[\frac{1}{\sqrt{2\epsilon}}+\frac{7}{8}\sqrt{2\epsilon}+\cdots\right] \times\left(1-e^{-4\sqrt{2\epsilon}[1-(5/12)\epsilon+\cdots]s}\right) . \tag{60}$$

Multiplying Eq. (60) by $4\sqrt{2\epsilon}s$, we obtain

$$4\sqrt{2\epsilon}s=\frac{V_1 m r_1^2}{\hbar^2}\left[1+\frac{7}{4}\epsilon+\cdots\right] \times\left(1-e^{-4\sqrt{2\epsilon}[1-(5/12)\epsilon+\cdots]s}\right) . \tag{61}$$

We now let $4\sqrt{2\epsilon}s=x_c+\Delta+\Delta^2\cdots$ assuming Δ to be a function of ϵ, and small. We choose x_c to be the zeroth order solution of Eq. (61); Eq. (61) can then be converted to the following form by letting $\epsilon \rightarrow 0$:

$$x_c=\frac{V_1 m r_1^2}{\hbar^2}\left(1-e^{-x_c}\right) , \tag{62}$$

where x_c is a constant. The eigenpotential obtained from just x_c agrees with the exact analytical value to within 0.02% in the region where ϵ is very small ($\epsilon<10^{-4}$). Now we add the first order correction to x_c by including the Δ term, which is the term proportional to ϵ, obtaining

$$x_e+\Delta=\frac{V_1 m r_1^2}{\hbar^2}\left[1+\frac{7}{4}\epsilon\right]\left(1-e^{-(x_c+\Delta)}\right) . \tag{63}$$

Thus we find for the one δ-shell potential case, neglecting higher order terms of Δ (or ϵ), the following expression:

$$\Delta=\frac{\dfrac{V_1 m r_1^2}{\hbar^2}\dfrac{7}{4}\left(1-e^{-x_c}\right)}{\left[1-\dfrac{V_1 m r_1^2}{\hbar^2}e^{-x_c}\right]}\epsilon . \tag{64}$$

As mentioned before, when ϵ is small, the first order correction in Δ (and therefore in ϵ) for the eigenpotential is very small compared with the constant term, x_c, for the case of the one δ-shell potential, as well as for the case of the two δ-shell potential. When we solve for s in Eq. (61), the eigenpotential $|\lambda|$ is found to have the following form:

$$|\lambda|=\frac{x_c^2}{8\epsilon}+\left[\frac{\Delta x_c}{4\epsilon}+0.25-\frac{x_c^2}{4}\right]+O(\epsilon)+\cdots \; . \tag{65}$$

The dominant term in Eq. (65) is therefore

$$\lambda=-\frac{x_c^2}{8(\rho-1)} \; . \tag{66}$$

Similarly, for the two δ-shell potential case, at the points $\rho=d+\epsilon$, when ϵ is small, analytical calculations using Eq. (C7) (which include the variables ρ,ρ_1, ϕ, and θ) also allow us to determine the behavior of the eigenpotential. In this case we rescaled r by r_0 and made the definition $\rho_1=\rho/d$, where $d=r_1/r_0$, as shown previously in Eq. (44).

Assuming that s is very large, the eigenpotential, evaluated with x_c from the zeroth order approximation (ϵ is very small), agrees with the exact analytical values to within 0.25% for this two δ-shell potential case. The eigenpotential $|\lambda|$ in the two δ-shell case is

$$|\lambda|=\frac{x_c^2}{8d\epsilon}+\left[\frac{\Delta x_c}{4d\epsilon}+\frac{0.25}{d^2}-\frac{x_c^2}{4d^2}\right]+O(\epsilon)+\cdots \; . \tag{67}$$

The dominant term in Eq. (67) is therefore

$$\lambda=-\frac{x_c^2}{8d(\rho-d)} \; . \tag{68}$$

As we can see from Eqs. (66) and (68), the eigenpotentials behave like a Coulomb potential, i.e., they go as $1/x$ when we make a shift of $x=\rho-d$ for the two δ-shell potential case, and a shift of $x=\rho-1$ for the one δ-shell potential case.

Since, as we see above, the eigenpotential diverges as $1/x$ when using the EAA approach, we consider it important to investigate the behavior of the eigenpotential using the UAA approach since it yields an upper bound for the binding energy. To check the UAA at a point ρ which had a very large negative value for the eigenpotential using the EAA, we first had to calculate the eigenvector χ_n. The latter is given in explicit form in (C17) and the equations leading up to it, which result from the use of $\mathbf{M}(\rho)$. In order to obtain the UAA eigenpotential we then had to calculate the square of the derivative of the normalized eigenvector $[\chi_n(\rho)]$ given in Eq. (C15), which became

$$\sum_{n=1}^{\infty}\left[\frac{d[\chi_n(\rho)]}{d\rho}\right]^2 \propto \frac{1}{\epsilon^2} \tag{69}$$

as shown in Eq. (C30) (see Appendix C, Sec. 2) where ϵ is defined by $\rho=1+\epsilon$ and is very small.

From this we concluded that near the attractive δ threshold, whereas the EAA eigenpotentials behave as $\lambda \propto -a/x$ in both the one and two δ-shell cases (when we make the shifts with $x=\rho-1$ and $x=\rho-d$ near $\rho\to 1$ and $\rho\to d$), in the case of the UAA the eigenpotential is seen to behave as $\lambda \propto -(a/x)+(b/x^2)$ where a and b are positive constants [see Eqs. (57) and (69)]. We see that the eigenpotential is strongly positive near $x=0$.

Thus we see that the attractive (negative) singularity—given by the EAA—is overwhelmed by the repulsive (positive) singularity of the UAA. It is strongly suggested, by our calculations of the UAA eigenpotential near the threshold of the attractive δ shell, that the UAA eigenpotential is everywhere positive, which implies a zero binding energy. The difference between the binding energies from the UAA and the EAA will then be equal to the magnitude of the EAA result, so that the error can be quite large.

We note that usually—i.e., for more conventional binary potentials—the difference between the UAA and the EAA, for the binding energies, is small.

B. Nonsingular behavior with the repulsive δ shell

One can observe from the behavior of the eigenpotential at $\rho=1$ (at the position of repulsive δ shell) in the two δ-shell potential case that there is no singularity in the eigenpotential, a situation very different from the attractive δ-shell case, as can be seen from Fig. 2. As we shall show in Appendix C, Sec. 1, the eigenpotential λ is positive in this case. The lowest value s does not lead to a divergence in λ at $\rho=1$; rather one obtains $s=1$ which, therefore, gives a finite value for the eigenpotential at $\rho=1$ of $\lambda=3.75$.

C. Asymptotic behavior of the eigenpotentials

For both the one and the two δ-shell potentials the eigenpotentials converge to a negative constant value as $\rho\to\infty$. It has been shown that the behavior of such eigenpotentials at large ρ represents an asymptotic situation corresponding to a two-body bound state and a free particle [49]. In our one δ-shell potential case, as $\rho\to\infty$, (51) can be transformed into

$$x_s-\frac{\pi V_1 m r_0^2}{4\hbar^2}\frac{\rho^2}{\rho_1}\left(1-e^{-4x_s/\pi\rho_1}\right)=0 \; , \tag{70}$$

where $s=\frac{1}{4}\sqrt{4|\lambda|\rho^2-1}$ and $x_s=\pi s$ and $\lambda=-(4s^2+0.25)/\rho^2$. Solving Eq. (70) for λ (or x_s), we found that the eigenpotential at $\rho\to\infty$ has the value $\lambda=-0.11992$ asymptotically for the one δ-shell potential case. This value corresponds to the binary energy -0.034 K of two ^{4}He atoms using the Mason-Rice 1 potential.

However, the asymptotic behavior of the eigenpotential is considerably more complicated in the two δ-shell potential case because here it is difficult to convert Eq. (C7) into a simpler form like that of Eq. (70), as $\rho\to\infty$. In this case we obtain the convergent eigenpotential λ_{conv} using an asymptotic extrapolation of the form

$$\lambda_{\text{conv}}=\lambda_\rho+C\frac{\ln\rho}{\rho} \; . \tag{71}$$

Using values of the eigenpotential at $\rho=40$, $\rho=41$,

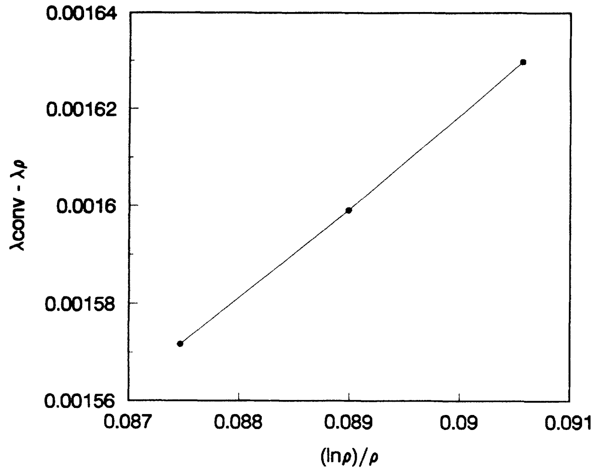

FIG. 3. The linear relation for the extrapolation of the convergent eigenpotential.

$\rho=42$, and $\rho=43$, we obtained a value of 0.0180 for the coefficient C in Eq. (71).

Using the above results we obtained an extrapolated value $\lambda_{\text{conv}}=-0.0202$. This dimensionless value of λ_{conv} corresponds to a value of -0.032 K, slightly different from the value of -0.034 K, the value of the two-body bound state obtained with the Mason-Rice 1 potential. Figure 3 shows the linear dependence of the eigenpotential with respect to the variable $(\ln\rho)/\rho$.

D. Behavior of the eigenpotentials when considering only the attractive δ-shell part of the two δ-shell potential

It is interesting to see how the repulsive δ-shell potential affects the eigenpotential in the region $\rho>d$ for the two δ-shell potential case. The eigenpotential, in the region where $\rho>d$, is important because this is the region where the eigenpotential is affected by both δ shells, whereas the information contained in the eigenpotential for a hyperradius ρ less than d must be ignored, as we shall see, when determining the wave functions.

Let us now consider only the attractive δ-shell potential part of the two δ-shell potential case; setting $V_0=0$ in Eq. (C7), we then obtain Eq. (C5) of the one δ-shell potential case. We now calculate the eigenpotential λ using the parameters which are shown in Table I. The comparisons of the eigenpotentials between the case where we consider only the attractive δ-shell potential part, in the two δ-shell potential case, and the case where both the attractive and the repulsive δ-shell parts are included in the two δ-shell potential case, are shown in Fig. 4.

From that figure we can see that the eigenpotential obtained when considering only the attractive δ-shell part is lower than the one obtained by considering both the attractive and the repulsive δ-shell parts, as $\rho\rightarrow\infty$; on the other hand, they have the same behaviors, similar to the Coulomb potential, in that they are proportional to $1/(\rho-d)$ at $\rho=d+\epsilon$, when ϵ is small.

The asymptotic convergent value of the eigenpotential is obtained in the same way for the case of the two δ-shell potential when the repulsive δ-shell part is ignored, as for the one δ-shell potential case. The eigenpotential now becomes $\lambda=-1.18748$, giving rise to an asymptotic value for the eigenpotential of -1.89 K, very far from the two-body value.

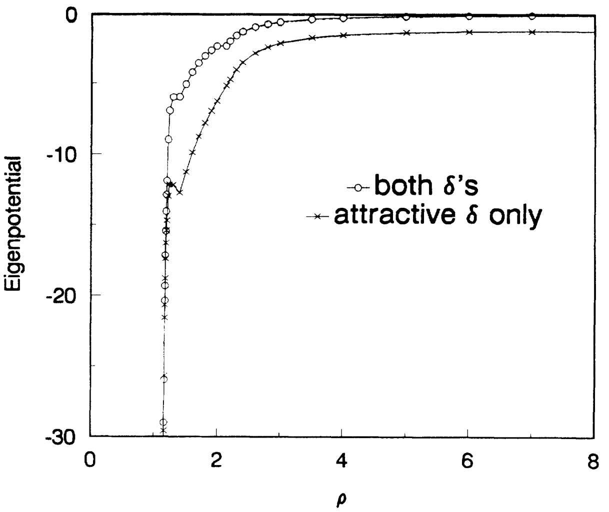

FIG. 4. The eigenpotential, considering only the attractive δ-shell potential part where $\rho>1.1375$.

VI. BINDING ENERGY

To find the wave function and the binding energy of a three-body bound state, we have to integrate the lowest uncoupled differential equation in (49) with the lowest eigenpotential; the results for the eigenpotentials are shown in Figs. 1 and 2. As we shall see, we do not include the eigenpotential inside $\rho\leq 1$ and $\rho\leq d$, in the one δ-shell potential case and the two δ-shell potential case, respectively. Hence the wave functions start at zero when we integrate Eq. (49) starting at the position at which there are singularities, i.e., $\rho=1$ for one δ, and $\rho=d$ for the two δ-shell case. We use Milne numerical integration [48] for this work; this method requires information about the wave function at two starting points.

As was shown before, the behavior of the eigenpotential at $\rho=1+\epsilon$ has the form $\lambda=-\alpha/(\rho-1)$ where $\alpha=x_c^2/8$ for the one δ-shell potential [Eq. (66)], and the form $\lambda=-\alpha/(\rho-d)$ where $\alpha=x_c^2/(8d)$ for the two δ-shell potential [Eq. (68)]. The values for x_c and α for our model potentials are given in Table II.

To learn how to handle such potentials we solve the Schrödinger equation with a Coulomb potential for the region $\rho>1$, since our eigenpotential for the case of one δ-shell behaves like a Coulomb potential in the region around $\rho=1$. We show how we deal with the divergence of the eigenpotential around $\rho=1$ in order to get the binding energy.

Loudon [39], Haines and Roberts [40], Andrews [41], and Hammer and Weber [42] tried to solve the problem of a one-dimensional hydrogen atom using a Coulomb potential. Andrews [43] concluded that for the one-dimensional hydrogen atom the Coulomb singularity acts as an impenetrable barrier, so that all wave functions

TABLE II. Parameters characterizing the eigenpotentials near their singularity.

Parameter	One δ shell	Two δ shell
x_c	0.693	2.479
α	0.060	0.675

must vanish as $x \to 0$, where $x=0$ is the position of the singularity, and therefore there is no physical connection between the regions on the left $(x<0)$ and right $(x>0)$ sides with the potential $|x|^{-1}$.

To confirm such ideas and get the binding energy with a radial Coulomb potential, we can use two different approaches. The first is to ignore the region interior to the location of the singular point as in Andrew's argument; the second is to consider a cutoff potential and to solve for the binding energy as the cutoff potential gets deeper and deeper as in Loudon's approach.

The radial equation for our system, for the region of $0<\rho\le 1$, is

$$\left\{-\frac{d^2}{d\rho^2}+\frac{3.75}{\rho^2}+k^2\right\}u(\rho)=0\ , \tag{72}$$

where

$$k=\left[\frac{mr_1^2}{\hbar^2}|E_0|\right]^{1/2} \tag{73}$$

and only the centrifugal term appears.

Using a cutoff potential (as in Fig. 5) for the region of $1<\rho\le 1+\rho_c$, where ρ_c, the cutoff position, is very small, we then obtain

$$\left\{-\frac{d^2}{d\rho^2}-k^2q^2\right\}u(\rho)=0\ , \tag{74}$$

where

$$q^2=\frac{|V_0|}{|E_0|}-1\ . \tag{75}$$

Finally, for the region $\rho>1+\rho_c$, and using the Coulomb potential, we find

$$\left\{-\frac{d^2}{d\rho^2}+\left[-\frac{\alpha}{\rho-1}+k^2\right]\right\}u(\rho)=0\ , \tag{76}$$

where

$$\alpha=\frac{x_c^2}{8}\ . \tag{77}$$

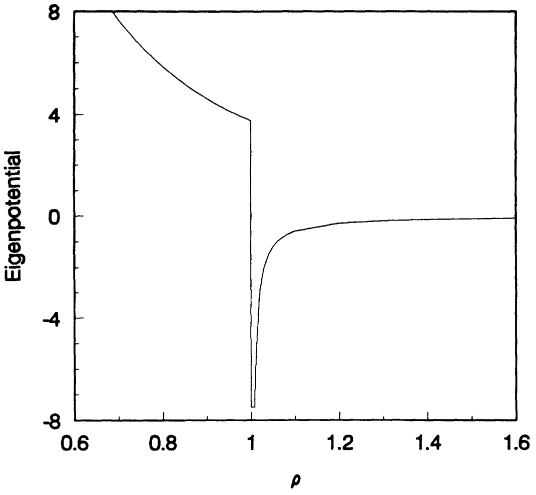

FIG. 5. The cutoff potential.

From this it follows, letting $x=k\rho$ and $z=\rho-1$, that $y_{\rm I}(x)$,$y_{\rm II}(x)$, and $y_{\rm III}(z)$, the solutions in the three different regions, are given by

$$y_{\rm I}(x)=A\sqrt{x}I_2(x)\ , \tag{78}$$

$$y_{\rm II}(x)=B_1\cos qx+B_2\sin qx\ , \tag{79}$$

$$y_{\rm III}(z)=C_1\mathcal{M}_{\alpha/2k,1/2}(2kz)+C_2\mathcal{W}_{\alpha/2k,1/2}(2kz)\ , \tag{80}$$

where A,B_1,B_2,C_1, and C_2 are the coefficients, and $I_2(x)$ is the modified Bessel function [44] which is related to the Bessel function by

$$I_2(x)=-J_2(ix)\ ,$$

and where the Whittaker functions $\mathcal{M}_{\alpha/2k,1/2}(2kz)$ and $\mathcal{W}_{\alpha/2k,1/2}(2kz)$ are confluent hypergeometric functions [45–47]. The condition for having a bound state is that the coefficient C_1 must be zero, so that $y_{\rm III}(z)=0$ as $z\to\infty$.

Now using the boundary conditions

$$y_{\rm I}(x)=y_{\rm II}(x)\ ,\ y_{\rm I}'(x)=y_{\rm II}'(x)\ ,$$

at $\rho=1$, and

$$y_{\rm II}(x)=y_{\rm III}(z),\ y_{\rm II}'(x)=y_{\rm III}'(z)\ ,$$

at $\rho=r_1$, where $r_1=1+\rho_c$, we obtain

$$\left\{\left[B_2q-\frac{B_1}{\rho_c}(1-k\rho_c)\right]\cos qkr_1-\left[B_1q+\frac{B_2}{\rho_c}(1-k\rho_c)\right]\sin dkr_1\right\}U\left[1-\frac{\alpha}{2k}\ ,\ 2,\ 2k\rho_c\right]$$
$$=(B_1\cos qkr_1+B_2\sin qkr_1)U'\left[1-\frac{\alpha}{2k}\ ,\ 2,\ 2k\rho_c\right]\ , \tag{81}$$

where

$$B_1 = 8\sqrt{k}\,I_2(k)\cos qk - \frac{4}{q}\left\{\frac{I_2(k)}{\sqrt{k}} + 2\sqrt{k}\,I_2'(k)\right\}\sin qk \ ,$$
$$B_2 = 8\sqrt{k}\,I_2(k)\sin qk + \frac{4}{q}\left\{\frac{I_2(k)}{\sqrt{k}} + 2\sqrt{k}\,I_2'(k)\right\}\cos qk \ . \quad (82)$$

As $\rho_c \to 0$, we find that the binding energy converges to a finite value. This procedure gives the same result, as shown below, as that obtained by forcing the wave function to be zero at $\rho = 1$. Following that method, the bound-state wave function has the form

$$y(z) = z e^{-ikz}{}_1F_1\left[1 - \frac{\alpha}{2k}, 2; 2kz\right] \quad (83)$$

and is the well behaved solution of the differential equation Eq. (76) at $z=0$ $(z=\rho-1)$, where the potential diverges, while the second solution diverges as $z \to 0$. A solution which satisfies the correct conditions at infinity is obtained only when $1-(\alpha/2k)$ is zero or a negative integer. Then ${}_1F_1$ reduces to a polynomial. Otherwise it diverges as $z \to \infty$ exponentially (e^z). Therefore the lowest energy is satisfied by

$$1 - \frac{\alpha}{2k} = 0 \quad (84)$$

so that the binding energy is seen to be

$$|E_0| = \frac{\alpha^2}{4}\frac{\hbar^2}{m r_1^2} \ . \quad (85)$$

This value in Eq. (85) is exactly the same as that obtained when you let $\rho_c \to 0$ in Eq. (81).

Consequently, we can conclude that the inside wave function for $\rho < 1$ plays no role in determining the wave function for $\rho > 1$. Thus, in our calculations using the δ-shell potentials, the integration of differential equations using the eigenpotential should ignore the region $\rho \le 1$. The important region begins at the point where the eigenpotential is proportional to $1/(\rho-1)$ in the case of one δ-shell potential, and $1/(\rho-d)$ in the case of the two δ-shell potential, both cases starting at the hyperradius of the eigenpotential divergence. Using this information we can now apply the Milne step numerical integration method to calculate the values of the binding energy for the eigenpotentials.

Because the eigenpotentials converge to negative constants asymptotically, due to the existence of a two-body bound state [49] and a free particle as the asymptotic state of the wave function for energies higher than that of the two-body binding energy, we lift the eigenpotential up to the x axis (i.e., we subtract out the asymptotic negative constants) when integrating, using Milne's method, in our numerical program. Subtracting the asymptotic values of the eigenpotentials which correspond to the value of the two-body bound state (−0.034 K), we then obtain the binding energy of the three-body bound state relative to the two-body bound state plus a free particle. We note that, in the two δ-shell potential case, a subtracted asymptotic value of −0.032 K corresponds quite closely to the two-body bound-state value of −0.034 K. In the one δ-shell case, the asymptotic value of −0.034 K which we obtain for the eigenpotential corresponds exactly to the two-body binding energy. The binding energies relative to the 2+1 configuration are then −0.149 K for the one δ-shell potential case and −1.024 K for the two δ-shell potential.

To the above values we now add the asymptotic values that we subtracted, so as to obtain the three-body binding energy which can be compared to the three free particle system. In this way we obtain a binding energy of −0.183 K for the one δ-shell potential case and −1.056 K for the two δ-shell potential case.

Of course, when we ignore the repulsive δ part of the eigenpotentials in the two δ-shell case, the binding energy becomes bigger than when both the δ-shell potentials are properly taken into account (see Fig. 4). Therefore, in this case, when subtracting out the asymptotic value of −1.89 K, we are not surprised to obtain an huge value of −4.83 K. The subtracted asymptotic value clearly does not come even close to the binding energy of the two-body bound state plus one free particle.

By comparison, the binding energies of a trimer of ^{4}He have been obtained by others using various potential models and different methods. Bruch and McGee [11] obtained a binding energy for the ^{4}He trimer in the range of −0.05 to −0.2 K, using variational calculations and various pair potentials: namely, the MDD-1 (Morse dipole-dipole), MDD-2, FDD-1 (Frost-Musulin-V_{DD}), and Lennard-Jones 6-12 potential with different parameters. Nakaichi, Akaishi, and Tanaka [6] obtained energies of the ^{4}He trimer in the range from −0.08 to −0.2 K using various potentials, which included Smith-Thakkar, MDD-2, Beck, Lennard-Jones and exponential-spline-Morse-spline-van der Waals (ESMMSV) through the method of amalgamation of two-body correlations into the multiple-scattering process (ATMS). Later again Nakaichi, Lim, Akaishi, and Tanaka [8] obtained −0.087 K using a realistic He-He potential and the Faddeev-UPE (unitary pole expansion) method. Nakaichi-Maeda and Lim [7] obtained a trimer energy of −0.092 K using HFDHE2 and Fadeev-Yakubovsky (FY) theory. PZPWH calculated the trimer energy as −0.117 K using a HFDHE2 potential and the Green's function Monte Carlo (GFMC) method in a study of droplets of ^{4}He. Cornelius and Glöckle [10]

TABLE III. Calculated values of the three-body energy.

Potential	Method	Energy (K)
One δ shell	HHEM	−0.183
Two δ shell	HHEM	−1.056
Smith-Thakkar	ATMS	−0.180
Lennard-Jones	ATMS	−0.082
MDD-2	ATMS	−0.105
MDD-2	Faddeev-UPE	−0.087
ESMMSV	ATMS	−0.079
HFDHE2	GFMC	−0.117
HFDHE2	FY	−0.092
HFDHE2	Faddeev	−0.110
Yamaguchi	Separable app.	−0.123

found a trimer energy of -0.11 K using the HFDHE2 potential and a Faddeev scheme. Recently Loucks and Levinger [9] obtained a timer energy of -0.123 K using a Yamaguchi potential and a separable approximation. In Table III, we compare our results with those of other investigators for the binding energies of three-^{4}He-atom clusters—obtained using different methods and potentials.

VII. DISCUSSION AND CONCLUSIONS

In our work we have calculated the binding energy of a three-^{4}He-atom cluster. In this calculation we used hyperspherical harmonic expansions and binary δ-shell potentials in two separate cases, the first with a single δ-shell potential and the second with two δ-shell potentials. Using the hyperspherical harmonics formalism, we obtained an infinite set of coupled differential equations. To decouple the equations, we used the adiabatic approximation and obtained the eigenpotential numerically and analytically; the analytical work became possible because the δ-function potential yielded a separable product for the potential matrix.

We found that there are singularities in the eigenpotentials at the position of the threshold of influence of the attractive δ-shell potential for each δ-shell case. The wave function for the hyperradius ρ less than the critical value plays no role in determining the wave function for ρ further out when we calculate the binding energy; in each case the wave function is forced to go to zero at the attractive singularity. On the other hand it turned out that there is no singularity in the eigenpotential at the position of the repulsive δ shell. Thus we find that while the attractive delta can contribute amply to the wave function (though, by forcing the wave function to go to zero, is also mimics a repulsive interaction), the only role of the repulsive δ-shell part, in the case of the two δ-shell potential, is to lift the eigenpotential for values of ρ larger than the critical ρ (the location of the attractive singularity).

Doing the calculation for the three-^{4}He-cluster, we obtained a binding energy of -0.183 K using the one δ-shell potential, and binding energies of -1.056 K using the two δ-shell potential. We observe that the binding energy of -0.183 K using the one δ-shell potential falls within the range of -0.05 to -0.21 K obtained by other theoretical workers, in contrast to the result obtained for the two δ-shell potential case.

The result is better when the binary potential has no repulsive part (i.e., the one δ-shell potential case) since we see that when we take two δ shells—the first one of which is repulsive—the region which contains the repulsive part is ignored when solving for the wave function generated by the eigenpotential: this behavior may be characterized as a pathology of the δ-function potentials. While the EAA and the UAA still give us a lower bound and an upper bound for the binding energy, the difference between these bounds is very large and our method loses its usefulness. To the pathology associated with the three-body problem in three dimensions—with zero range infinite potentials located at the origin in binary potentials—we can now add the case of the attractive δ-shells.

Moreover, our work suggests that the realization of our goal—the calculation of the binding energies of molecular clusters—must rely on using not only a more realistic potential but also the hyperspherical techniques that we have used successfully in nuclear physics. We anticipate that the study of the binding energies of these clusters, as a function of the number of particles, will lead to an understanding of the "preferred" bound states, characterized by the so-called "magic numbers," found experimentally.

APPENDIX A: DIAGONALIZATION OF THE MATRIX

For the case of the one δ-shell potential—for $\rho > 1$—we consider a matrix H with elements

$$H_{ij}=h_i\delta_{ij}-\beta f_i f_j \ , \tag{A1}$$

where we have let $i=K+1$ in Eq. (47), and where h_i represents the centrifugal term and the second term represents the potential matrix resulting from the attractive δ-shell potential. H satisfies the equation

$$\sum_j H_{ij}\chi_j=\lambda\chi_i \ . \tag{A2}$$

Substituting Eq. (A1) into Eq. (A2) gives

$$\chi_i=\frac{\beta f_i}{h_i-\lambda}\sum_j f_j\chi_j \ . \tag{A3}$$

After multiplying both sides of f_i, summing over i, and dividing by the factor $\sum_i f_i\chi_i$, Eq. (A3) gives us a sum rule which can be used to determine the eigenvalue λ:

$$1=\beta\sum_i \frac{f_i^2}{h_i-\lambda} \ . \tag{A4}$$

Equation (A3) shows that the corresponding unnormalized eigenvector has components

$$\chi_i=\frac{\beta f_i}{h_i-\lambda} \ . \tag{A5}$$

Similarly, in the case of the two δ-shell potential, for $\rho > 1$, the general matrix H has elements of the form

$$H_{ij}=h_i\delta_{ij}+\alpha g_i g_j-\beta f_i f_j \ , \tag{A6}$$

where we again have let $i=K+1$ in Eq. (47), and where h_i represents the centrifugal term while the second term represents the potential matrix resulting from the repulsive δ shell and the negative (third) term stands for the potential matrix which results from the attractive δ-shell potential. Since H satisfies Eq. (A2), substituting Eq. (A6) into Eq. (A2) gives

$$\chi_i=\left[\frac{\beta f_i}{h_i-\lambda}\right]\sum_j f_j\chi_j-\left[\frac{\alpha g_i}{h_i-\lambda}\right]\sum_j g_j\chi_j \ . \tag{A7}$$

After multiplying both sides by f_i (or g_i), summing over i, and dividing by the factor $\sum_i f_i\chi_i$ (or $\sum_i g_i\chi_i$), Eq. (A7) gives

$$1=\beta\sum_i \frac{f_i^2}{h_i-\lambda}-\alpha\sum_i \frac{f_i g_i}{h_i-\lambda}\frac{\left[\sum_j g_j\chi_j\right]}{\left[\sum_i f_i\chi_i\right]} \ ,$$

and

$$1=\beta\sum_i \frac{f_i g_i}{h_i-\lambda}\,\frac{\left[\sum_j f_j\chi_j\right]}{\left[\sum_i g_i\chi_i\right]}-\alpha\sum_i\frac{g_i^2}{h_i-\lambda}\ . \tag{A8}$$

Canceling the common factor,

$$\frac{\sum_j g_j\chi_j}{\sum_i f_i\chi_i}$$

in (A8) gives us, again, a sum rule:

$$\left[1-\sum_i\frac{\beta f_i^2}{h_i-\lambda}\right]\left[1+\sum_i\frac{\alpha g_i^2}{h_i-\lambda}\right]=-\alpha\beta\left[\sum_i\frac{f_ig_i}{h_i-\lambda}\right]^2 . \tag{A9}$$

APPENDIX B: NUMERICAL CALCULATION

When we let $h_i=C_i/\rho^2$ and $\lambda=(C_n/\rho^2)+\Delta_n$, in the case of the one δ-shell potential, Eq. (51) has the form

$$\Delta_n=f(\Delta_n)\ , \tag{B1}$$

where

$$f(\Delta_n)=\frac{-\beta f_n^2}{1-\beta l_1}\ , \tag{B2}$$

with

$$\beta=\frac{4mr_1^2}{\pi\hbar^2}\,\frac{V_1}{\rho\sqrt{1-(1/\rho^2)}}\ ,$$

$$l_1=\sum_{i\neq n}{}'\frac{f_i^2}{\dfrac{C_i-C_n}{\rho^2}-\Delta_n}\ , \tag{B3}$$

and

$$f_n^2=\left[1+\frac{4}{\sqrt{3}}\,\frac{\sin\frac{2}{3}\pi n}{n}\right](\sin n\phi)^2\ , \tag{B4}$$

with f_i in Eq. (B3) given by Eq. (52).

Defining

$$g(\Delta_n)=f(\Delta_n)-\Delta_n \tag{B5}$$

and using the Newton-Raphson method [50], we obtain

$$\Delta_{n+1}=\Delta_n-\frac{g(\Delta_n)}{g'(\Delta_n)}\ , \tag{B6}$$

where

$$g(\Delta_n)=G-\Delta_n,\ g'(\Delta_n)=P-1\ , \tag{B7}$$

which leads to

$$\Delta_{n+1}=\frac{G-\Delta_nP}{1-P}\ , \tag{B8}$$

where

$$G=\frac{-\beta f_n^2}{1-\beta l_1}\ , \tag{B9}$$

and

$$P=-\frac{\beta^2f_n^2l_2}{(l-\beta l_1)^2}\ . \tag{B10}$$

In Eqs. (B9) and (B10), l_1 is given by (B3) and l_2 by

$$l_2=\sum_{i\neq n}{}'\frac{f_i^2}{\left[\dfrac{C_i-C_n}{\rho^2}-\Delta_n\right]^2}\ , \tag{B11}$$

f_n^2 is given by

$$f_n^2=\left[1+\frac{4}{\sqrt{3}}\,\frac{\sin\frac{2}{3}\pi n}{n}\right](\sin n\phi)^2\ . \tag{B12}$$

Similarly, in the case of the two δ-shell potential, Eq. (53) has the same form as (B1) where

$$f(\Delta_n)=\frac{-\beta f_n^2(1+\alpha m_1)+\alpha g_n^2(1-\beta l_1)+2\alpha\beta f_ng_nfg_1}{(1+\alpha m_1)(1-\beta l_1)+\alpha\beta(fg_1)^2}\ , \tag{B13}$$

with

$$\alpha=\frac{4mr_0^2}{\pi\hbar^2}\,\frac{V_0}{\rho\sqrt{1-(1/\rho^2)}}\ ,$$

$$\beta=\frac{4mr_0^2}{\pi\hbar^2}\,\frac{V_1}{\rho_1\sqrt{1-(1/\rho_1^2)}}\ ,$$

$$l_1=\sum_{i\neq n}{}'\frac{f_i^2}{\dfrac{C_i-C_n}{\rho^2}-\Delta_n}\ ,$$

$$m_1=\sum_{i\neq n}{}'\frac{g_i^2}{\dfrac{C_i-C_n}{\rho^2}-\Delta_n}\ , \tag{B14}$$

$$fg_1=\sum_{i\neq n}{}'\frac{f_ig_i}{\dfrac{C_i-C_n}{\rho^2}-\Delta_n}\ ,$$

$$f_n^2=\left[1+\frac{4}{\sqrt{3}}\,\frac{\sin\frac{2}{3}\pi n}{n}\right](\sin n\theta)^2\ ,$$

$$g_n^2=\left[1+\frac{4}{\sqrt{3}}\,\frac{\sin\frac{2}{3}\pi n}{n}\right](\sin n\phi)^2\ ,$$

and where f_i and g_i are given by Eq. (54).

Using the Newton-Raphson method again, we obtain the same Eq. (B8) as in the one δ-shell potential case, but with

$$G=\frac{-\beta f_n^2(1+\alpha m_1)+\alpha g_n^2(1-\beta l_1)+2\alpha\beta f_ng_nfg_1}{(1+\alpha m_1)(1-\beta l_1)+\alpha\beta(fg_1)^2} \tag{B15}$$

$$P=[\alpha\beta(-f_n^2m_2-g_n^2l_2+2f_ng_nfg_2)\{(1+\alpha m_1)(1-\beta l_1)+\alpha\beta(fg_1)^2\}-\{\alpha g_n^2(1-\beta l_1)-\beta f_n^2(1+\alpha m_1)+2\alpha\beta f_ng_nfg_1\}$$
$$\times\{\alpha g_2(1-\beta l_1)-\beta h_2(1+\alpha m_1)+2\alpha\beta fg_1fg_2\}]/[(1+\alpha m_1)(1-\beta l_1)+\alpha\beta(fg_1)^2]^2\ , \tag{B16}$$

where

$$l_2=\sum_{i\neq n}{}'\frac{f_i^2}{\left[\dfrac{C_i-C_n}{\rho^2}-\Delta_n\right]^2}\ ,$$
$$m_2=\sum_{i\neq n}{}'\frac{g_i^2}{\left[\dfrac{C_i-C_n}{\rho^2}-\Delta_n\right]^2}\ , \tag{B17}$$
$$fg_2=\sum_{i\neq n}{}'\frac{f_ig_i}{\left[\dfrac{C_i-C_n}{\rho^2}-\Delta_n\right]^2}\ .$$

APPENDIX C: ANALYTICAL CALCULATION

1. The EAA eigenpotential

Consider the case of the one δ-shell potential. Equation (51) tells us that

$$1=\frac{V_1mr_1^2}{\hbar^2}\frac{4}{\pi}\frac{\rho}{\sqrt{1-(1/\rho^2)}}\times\sum_{n=1}^{\infty}\frac{\left[1+\dfrac{4}{\sqrt{3}}\dfrac{\sin\frac{2\pi}{3}n}{n}\right](\sin n\phi)^2}{\left[4n^2-\dfrac{1}{4}\right]-\lambda\rho^2}\ , \tag{C1}$$

where λ is negative for $\rho>1$. Using the relation $\sin^2n\phi=\frac{1}{2}(1-\cos2n\phi)$ and letting $s=\frac{1}{4}\sqrt{4\rho^2|\lambda|-1}$, we get

$$1=\frac{V_1mr_1^2}{2\hbar^2\pi}\frac{\rho}{\sqrt{1-(1/\rho^2)}}\times\sum_{n=1}^{\infty}\frac{\left[1+\dfrac{4}{3}\dfrac{\sin\frac{2\pi}{3}n}{n}\right](1-\cos2n\phi)}{n^2+s^2}\ . \tag{C2}$$

Multiplying the terms in parentheses in the sum of Eq. (C2) and using the following identity [51]:

$$\sum_{n=1}^{\infty}\frac{\cos nx}{n^2+s^2}=\frac{1}{2s^2}-\frac{\pi}{2}\frac{\cos[s\{(2n+1)\pi-x\}]}{s\sin s\pi} \tag{C3}$$

as well as

$$\int_0^b d\lambda\sum_{n=1}^{\infty}\frac{\cos n\lambda}{n^2+s^2}=\sum_{n=1}^{\infty}\frac{\sin nb}{n(n^2-s^2)}\ ,$$

and

$$\sin A\cos B=\tfrac{1}{2}\{\sin(A-B)+\sin(A+B)\}\ ,$$

and also,

$$2n\pi\leq x\leq(2n+2)\pi\ , \tag{C4}$$

Equation (C2) then becomes

$$1=\frac{V_1mr_1^2}{2\pi\hbar^2}\frac{\rho}{\sqrt{1-(1/\rho^2)}}\left[\frac{\pi}{2s}\{\coth\pi s(1-\cosh2\phi s)+\sinh2\phi_s\}+\frac{2\pi}{\sqrt{3}s^2}(1-\cosh2\phi s)\left[\coth\pi s\sinh\frac{2\pi}{3}s-\cosh\frac{2\pi}{3}s\right]\right] \tag{C5}$$

with the following conditions on the angle ϕ:

$$0\leq2\phi\leq2\pi\ ,$$
$$0\leq\frac{2\pi}{3}+2\phi\leq2\pi\ , \tag{C6}$$
$$0\leq\frac{2\pi}{3}-2\phi\leq2\pi\ .$$

As we increase the hyperradius ρ to find the eigenpotential λ at each ρ, and since ϕ is a function of ρ as shown in (42), we have to apply the sum rule—given by Eq. (C5)—while satisfying the inequality conditions (C6).

Similarly, for the two δ-shell potential Eq. (53) can be put in the form (C7) by letting $s=\frac{1}{4}\sqrt{4\rho^2|\lambda|-1}$,

$$1+V_0\gamma\xi_1\left[\frac{1}{2s}\left\{\frac{(1-\cosh 2\phi_s)}{\tanh\pi s}+\sinh 2\phi s\right\}+\frac{2}{\sqrt{3}s^2}(1-\cosh 2\phi s)\left[\frac{\sinh\frac{2\pi}{3}s}{\tanh\pi s}-\cosh\frac{2\pi}{3}s\right]\right]$$

$$-V_1\gamma\xi_2\frac{\rho}{\rho_1}\left[\frac{1}{2s}\left\{\frac{(1-\cosh 2\theta s)}{\tanh\pi s}+\sinh 2\theta s\right\}+\frac{2}{\sqrt{3}s^2}(1-\cosh 2\theta s)\left[\frac{\sinh\frac{2\pi}{3}s}{\tanh\pi s}-\cosh\frac{2\pi}{3}s\right]\right]$$

$$-V_0V_1\gamma^2\xi_1\xi_2\frac{\rho}{\rho_1}\left[\frac{1}{2s}\left\{\frac{(1-\cosh 2\phi s)}{\tanh\pi s}+\sinh 2\phi s\right\}+\frac{2}{\sqrt{3}s^2}(1-\cosh 2\phi s)\left[\frac{\sinh\frac{2\pi}{3}s}{\tanh\pi s}-\cosh\frac{2\pi}{3}s\right]\right]$$

$$\times\left[\frac{2}{\sqrt{3}s^2}(1-\cosh 2\theta s)\left[\frac{\sinh\frac{2\pi}{3}s}{\tanh\pi s}-\cosh\frac{2\pi}{3}s\right]\right.$$

$$\left.+\frac{1}{2s}\left\{\frac{(1-\cosh 2\theta s)}{\tanh\pi s}+\sinh 2\theta s\right\}\right]$$

$$=4V_0V_1\gamma^2\xi_1\xi_2\frac{\rho}{\rho_1}\left[\frac{1}{2s}\sinh\theta_s\left[\cosh\phi s-\frac{\sinh\phi s}{\tanh\pi s}\right]+\frac{2}{\sqrt{3}s^2}\sinh\phi s\sinh\theta s\left[\cosh\frac{2\pi}{3}s-\frac{\sinh\frac{2\pi}{3}s}{\tanh\pi s}\right]\right]^2, \tag{C7}$$

where

$$\gamma=\frac{mr_0^2}{2\hbar^2}, \tag{C8}$$

and

$$\xi_1=\frac{\rho}{\sqrt{1-(1/\rho^2)}},\quad \xi_2=\frac{\rho}{\sqrt{1-(1/\rho_1^2)}}, \tag{C9}$$

with the following conditions:

$$0\le 2\phi\le 2\pi,\quad 0\le 2\theta\le 2\pi,$$

$$0\le\frac{2\pi}{3}+2\phi\le 2\pi,\quad 0\le\frac{2\pi}{3}+2\theta\le 2\pi, \tag{C10}$$

$$0\le\frac{2\pi}{3}-2\phi\le 2\pi,\quad 0\le\frac{2\pi}{3}-2\theta\le 2\pi.$$

As ρ increases, again we have to apply the sum rule, Eq. (C3), while satisfying the inequality conditions (C10) on ϕ and θ, in Eq. (C7).

When we consider ρ lying in the region $1<\rho\le d$ for the case of the two δ-shell potential, we have only the repulsive δ shell so that the eigenpotential λ is positive. Equation (C7) then becomes

$$1=-\frac{V_0mr_0^2}{\hbar^2}\frac{4}{\pi}\frac{\rho}{\sqrt{1-(1/\rho^2)}}\times\sum_{n=1}^{\infty}\frac{\left[1+\frac{4}{\sqrt{3}}\frac{\sin\frac{2\pi}{3}n}{n}\right]\sin n\phi^2}{(4n^2-\frac{1}{4})-|\lambda|\rho^2}.$$

Letting $s=\frac{1}{4}\sqrt{4\rho^2|\lambda|+1}$, we obtain

$$1=-\frac{V_0mr_0^2}{2\hbar^2\pi}\frac{\rho}{\sqrt{1-(1/\rho^2)}}\times\sum_{n=1}^{\infty}\frac{\left[1+\frac{4}{\sqrt{3}}\frac{\sin\frac{2\pi}{3}n}{n}\right](1-\cos 2n\phi)}{n^2-s^2}. \tag{C12}$$

Using the following relation:

$$\sum_{n=1}^{\infty}\frac{1}{n^2-s^2}=\frac{1}{2s^2}-\frac{\pi}{2s}\cot\pi s, \tag{C13}$$

in Eq. (C12), we then obtain

$$1=-\frac{V_0mr_0^2}{2\hbar^2}\frac{\rho}{\sqrt{1-(1/\rho^2)}}\left[\frac{1}{2s}\left\{\frac{(1-\cos 2\phi s)}{\tan\pi s}-\sin 2\phi s\right\}+\frac{2}{\sqrt{3}s^2}(1-\cos 2\phi s)\left[\frac{\sin\frac{2\pi}{3}s}{\tan\pi s}-\cos\frac{2\pi}{3}s\right]\right]. \tag{C14}$$

2. The UAA eigenpotential

In the UAA approximation for one δ-shell potential, considering only the region near the critical ρ, we need to calculate the term $\sum_n\{d[\chi_n(\rho)]/d\rho\}^2$, where $[\chi_n]$ is the normalized eigenvector:

$$[\chi_n]=\frac{\chi_n}{\left[\sum_n |\chi_n|^2\right]^{1/2}} \; . \tag{C15}$$

The unnormalized eigenvector χ_n [see Eq. (A5)] is

$$\chi_n=\frac{4V_1mr_1^2}{\hbar^2\pi}\,\frac{1}{\rho\sqrt{1-(1/\rho^2)}}\,\frac{\left[1+\frac{4}{\sqrt{3}}\frac{\sin\frac{2}{3}\pi n}{n}\right]^{1/2}\sin n\phi}{\frac{\left[4n^2-\frac{1}{4}\right]}{\rho^2}+|\lambda|} \tag{C16}$$

or

$$\chi_n=\frac{V_1mr_1^2}{\hbar^2\pi}\,\frac{\rho}{\sqrt{1-(1/\rho^2)}}\,\frac{\left[1+\frac{4}{\sqrt{3}}\frac{\sin\frac{2}{3}\pi n}{n}\right]^{1/2}\sin n\phi}{n^2+s^2} \; , \tag{C17}$$

where $s=\frac{1}{4}\sqrt{4\rho^2|\lambda|-1}$.

The derivative term of χ_n is

$$\frac{d\chi_n}{d\rho}=\frac{V_1mr_1^2}{\hbar^2\pi}\left[1+\frac{4}{\sqrt{3}}\frac{\sin\frac{2}{3}\pi n}{n}\right]^{1/2}\left[\left\{\frac{1}{\left[1-\frac{1}{\rho^2}\right]^{1/2}}-\frac{1}{\rho^2\left[1-\frac{1}{\rho^2}\right]^{3/2}}\right\}\right.$$
$$\left.\times\frac{\sin n\phi}{n^2+s^2}+\frac{2n}{\rho\left[1-\frac{1}{\rho^2}\right]}\frac{\cos n\phi}{n^2+s^2}-\frac{|\lambda|}{2}\frac{\rho^2}{\left[1-\frac{1}{\rho^2}\right]^2}\frac{\sin n\phi}{n^2+s^2}\right] \; , \tag{C18}$$

where $\phi=\cos^{-1}[(2/p^2)-1]$ and we have used the chain rule, $dg/d\rho=(dg/d\phi)(d\phi/d\rho)$, where $g(\phi)=\sin n\phi$.

Assuming that s is very big near $\rho=1$, the square of the derivative of χ_n becomes

$$\left[\frac{d\chi_n}{d\rho}\right]^2=\left[\frac{V_1mr_1^2}{\hbar^2}\right]^2\frac{1}{4\pi}\left[\frac{1}{2s^3}\frac{1}{\left[1-\frac{1}{\rho^2}\right]^3}\left[1-\frac{2}{\rho^2}\right]^2\{1-(1+2\phi s)e^{-2\phi s}\}\right.$$
$$\left.+\frac{2}{s}\frac{1}{\rho^2\left[1-\frac{1}{\rho^2}\right]^2}\{1+(1-2\phi s)e^{-2\phi s}\}+\frac{4}{s}\frac{\phi}{\rho}\frac{\left[1-\frac{2}{\rho^2}\right]}{\left[1-\frac{1}{\rho^2}\right]^{5/2}}e^{-2\phi s}\right] \; . \tag{C19}$$

Here use has been made of the relations

$$\sum_{n=1}^{\infty}\frac{\sin\frac{2\pi}{3}n}{n(n^2+s^2)}=-\frac{1}{2}\int_0^1 d\lambda\left[\frac{d}{ds}\sum_{n=1}^{\infty}\frac{\cos\frac{2\pi}{3}n\lambda}{n^2+s^2}\right] , \tag{C20}$$

$$\sum_{n=1}^{\infty}\frac{1}{(n^2+s^2)^2}=-\frac{1}{2s}\frac{d}{ds}\sum_{n=1}^{\infty}\frac{1}{n^2+s^2} , \tag{C21}$$

$$\sum_{n=1}^{\infty}\frac{\sin 2n\phi}{(n^2+s^2)^2}=-\frac{1}{2n}\frac{d}{d\phi}\sum_{n=1}^{\infty}\frac{\cos 2n\phi}{(n^2+s^2)^2} , \tag{C22}$$

$$\sum_{n=1}^{\infty} \frac{\sin\frac{2\pi}{3}n}{n(n^2+s^2)^3} = \frac{2\pi}{3}\int_0^1 d\lambda \sum_{n=1}^{\infty} \frac{\cos\frac{2\pi}{3}n\lambda}{(n^2+s^2)^3} , \tag{C23}$$

$$\sum_{n=1}^{\infty} \frac{\cos 2n\phi}{(n^2+s^2)^2} = -\frac{1}{2s}\frac{d}{ds}\sum_{n=1}^{\infty} \frac{\cos 2n\phi}{(n^2+s^2)} , \tag{C24}$$

$$\sum_{n=1}^{\infty} \frac{\cos 2n\phi}{(n^2+s^2)^3} = \frac{1}{8s^2}\left[\frac{d^2}{ds^2}\sum_{n=1}^{\infty} \frac{\cos 2n\phi}{(n^2+s^2)} - \frac{1}{s}\frac{d}{ds}\sum_{n=1}^{\infty} \frac{\cos 2n\phi}{(n^2+s^2)} \right] , \tag{C25}$$

$$\sum_{n=1}^{\infty} \frac{\cos\frac{2\pi}{3}n\phi}{(n^2+s^2)^4} = -\frac{1}{48s^3}\left[\frac{d^3}{ds^3}\sum_{n=1}^{\infty} \frac{\cos\frac{2\pi}{3}n\phi}{(n^2+s^2)} - \frac{3}{s}\frac{d^2}{ds^2}\sum_{n=1}^{\infty} \frac{\cos\frac{2\pi}{3}n\phi}{(n^2+s^2)} + \frac{3}{s^2}\frac{d}{ds}\sum_{n=1}^{\infty} \frac{\cos\frac{2\pi}{3}n\phi}{(n^2+s^2)} \right] , \tag{C26}$$

and

$$\sin A \cos B = \tfrac{1}{2}\{\sin(A+B)+\sin(A-B)\} . \tag{C27}$$

The square of the denominator in Eq. (C15) becomes

$$\sum_n |\chi_n|^2 = \left[\frac{V_1 m r_1^2}{\hbar^2 \pi} \right]^2 \frac{\rho^2}{2\left[1-\frac{1}{\rho^2}\right]} \sum_n \left\{ \frac{1}{(n^2+s^2)^2} + \frac{4}{\sqrt{3}}\frac{\sin\frac{2\pi}{3}n}{n(n^2+s^2)^2} - \frac{\cos 2n\phi}{(n^2+s^2)^2} - \frac{4}{\sqrt{3}}\frac{\sin\frac{2\pi}{3}n\cos 2n\phi}{n(n^2+s^2)^2} \right\} . \tag{C28}$$

Again, assuming that s is very large near $\rho=1$, Eq. (C28) becomes

$$\sum_n |\chi_n|^2 = \left[\frac{V_1 m r_1^2}{\hbar^2} \right]^2 \frac{\rho^2}{\left[1-\frac{1}{\rho^2}\right]} \frac{1}{8\pi s^3} \times \{1-(1+2\phi s)e^{-2\phi s}\} , \tag{C29}$$

where we have used (C20) and (C27).

Therefore, by dividing Eq. (C19) by Eq. (C29), the square of the derivative of the normalized eigenvector $[\chi_n]$ becomes

$$\sum_{n=1}^{\infty} \left[\frac{d[\chi_n]}{d\rho} \right]^2 \propto \frac{1}{\epsilon^2} \tag{C30}$$

for the region $\rho=1+\epsilon$, where ϵ is small.

---

[1] P. W. Stephens and J. G. King, Phys. Rev. Lett. **51**, 1538 (1983).

[2] I. A. Harris, R. S. Kidwell, and J. A. Northby, Phys. Rev. Lett. **53**, 2390 (1984).

[3] O. Echt, K. Sattler, and E. Recknagel, Phys. Rev. Lett. **47**, 1121 (1981).

[4] Fei Luo, George C. McBane, Geunsik Kim, Clayton F. Giese, and W. Ronald Gentry, J. Chem. Phys. **98**, 3564 (1993).

[5] V. R. Pandharipande, J. G. Zabolitzky, Steven C. Pieper, R. B. Wiringa, and U. Helmbrecht, Phys. Rev. Lett. **50**, 1676 (1983).

[6] S. Nakaichi, Y. Akaishi, and H. Tanaka, Phys. Lett. **68A**, 36 (1978).

[7] S. Nakaichi-Maeda and T. K. Lim, Phys. Rev. A **28**, 692 (1983).

[8] S. Nakaichi, T. K. Lim, Y. Akaishi, and H. Tanaka, Phys. Rev. A **26**, 32 (1982).

[9] Roger Loucks and J. S. Levinger, Ann. Phys. (Leipzig) **7**, 115 (1991).

[10] Th. Cornelius and W. Glöckle, J. Chem. Phys. **85**, 3906 (1986).

[11] L. W. Bruch and Ian J. McGee, J. Chem. Phys. **59**, 409 (1973).

[12] J. M. Blatt, J. N. Lyness, and S. Y. Larsen, Phys. Rev. **131**, 2131 (1963).

[13] V. R. Pandharipande, Steven C. Pieper, and R. B. Wiringa, Phys. Rev. B **34**, 4571 (1986).

[14] R. A. Aziz, V. P. S. Nain, J. S. Carley, W. L. Taylor, and G. T. McConville, J. Chem. Phys. **70**, 4330 (1979).

[15] L. M. Delves, Nucl. Phys. **29**, 268 (1962).

[16] A. M. Badalyan and Yu.A. Simonov, Yad. Fiz. **3**, 1032 (1966) [Sov. J. Nucl. Phys. **3**, 755 (1966)].

[17] Yu. A. Simonov, Yad. Fiz. **3**, 630 (1966) [Sov. J. Nucl. Phys. **3**, 461 (1966)]; **7**, 1210 (1968) [**7**, 722 (1968)].

[18] T. K. Das, H. T. Coelho, and M. Fabre de la Ripelle, Phys. Rev. C **26**, 2281 (1982).

[19] L. L. Ballot, M. Fabre de la Ripelle, and J. S. Levinger, Phys. Rev. C **26**, 2301 (1982).

[20] M. Fabre de la Ripelle, Young-Ju Jee, A. D. Klemm, and S. Y. Larsen, Ann. Phys. (N.Y.) **212**, 195 (1991).

[21] S. Y. Larsen and P. L. Mascheroni, Phys. Rev. A **2**, 1018 (1970).

[22] M. Fabre de la Ripelle, Ann. Phys. (N.Y.) **147**, 281 (1983).

[23] S. Y. Larsen and J. E. Kilpatrick, in *Few Body Systems and Nuclear Forces,* edited by H. Zingl, M. Haftel, and H. Zankel, Lecture Notes in Physics, Vol. 87 (Springer-Verlag, Berlin, 1978), Pt. II, p. 497.

[24] S. Y. Larsen, A. Palma, and M. Berrondo, J. Chem. Phys. **77**, 5816 (1982).

[25] J. B. McGuire, J. Math. Phys. **5**, 622 (1964).

[26] C. N. Yang, Phys. Rev. **168**, 1920 (1968).

[27] C. N. Yang and C. P. Yang, J. Math. Phys. **10**, 1115 (1969).

[28] L. R. Dodd, J. Math. Phys. **11**, 207 (1970).

[29] W. G. Gibson, S. Y. Larsen, and J. Popiel, Phys. Rev. A **35**, 4919 (1987).

[30] James J. Popiel, Ph.D. thesis, Temple University, 1991 (unpublished).

[31] J. J. Popiel and S. Y. Larsen, Few-Body Syst. **15**, 129 (1993).

[32] L. H. Thomas, Phys. Rev. **47**, 903 (1935).

[33] Edward A. Mason and William E. Rice, J. Chem. Phys. **22**, 522 (1954).

[34] C. Poulat, S. Y. Larsen, and O. Novaro, Mol. Phys. **30**, 645 (1975).

[35] Yea-Hwang Uang and C. Stwalley, J. Chem. Phys. **76**, 5069 (1982).

[36] J. E. Kilpatrick, W. E. Keller, and E. F. Hammel, Phys. Rev. **97**, 9 (1955).

[37] M. Fabre de la Ripelle, in *Models and Methods in Few-Body Physics,* edited by L. S. Ferreira, A. C. Fonseca, and L. Streit, Lecture Notes in Physics Vol. 273 (Springer-Verlag, Berlin, 1986), p. 283.

[38] S. Y. Larsen and Jei Zhen, Mol. Phys. **65**, 237 (1988).

[39] R. Loudon, Am. J. Phys. **27**, 649 (1959).

[40] Larry K. Haines and David H. Roberts, Am. J. Phys. **37**, 1145 (1969).

[41] M. Andrews, Am. J. Phys. **34**, 1194 (1966); **44**, 1064 (1976).

[42] C. L. Hammer and T. A. Weber, Am. J. Phys. **56**, 281 (1988).

[43] M. Andrews, Am. J. Phys. **56**, 776 (1988).

[44] *Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972).

[45] L. J. Slater and D. Lit, *Confluent Hypergeometric Functions* (Cambridge University Press, Cambridge, England, 1960).

[46] Herbert Buchholz, *Confluent Hypergeometric Function with Special Emphasis on its Applications* (Springer-Verlag, New York, 1969).

[47] J. B. Seaborn, *Hypergeometric Functions and Their Application* (Springer-Verlag, New York, 1991).

[48] W. E. Milne, Am. Math. Mon. **49**, 96 (1942).

[49] S. Y. Larsen, *Few-Body Methods* (World Scientific, Singapore, 1986), p. 467.

[50] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge University Press, Cambridge, England, 1981).

[51] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, London, 1965).