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Hyperspherical harmonics in one dimension: Adiabatic effective potentials for three particles with δ -function interactions

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We investigate the adiabatic eigenfunctions and eigenvalues (and therefore the effective potentials) associated with the hyperspherical harmonic expansion of the wave function for three particles on a line subject to δ -function interactions. Because of the special separability of the potential matrix elements, we obtain the effective potentials as the solutions of a transcendental equation and we also obtain the eigenfunctions in closed form. We demonstrate that the long-range (large hyper-radius ρ) behavior of the effective potentials is qualitatively different from the long-range behavior of the potential matrix elements.

I. INTRODUCTION

The standard method of solving the quantummechanical two-body problem involves expanding the wave function into a series of partial waves, using spherical harmonics as basis functions. For central potentials, one then obtains an infinite set of uncoupled ordinary differential equations in a single radial variable r. These can then be solved for the bound-state energies and scattering phase shifts. These quantities provide a complete description of the two-particle scattering, and also enable one to calculate the contribution of two-body collision effects to equilibrium and nonequilibrium properties of gases.

For the three-body problem, the analogue of the partial-wave series is an expansion of the wave function using hyperspherical harmonics as basis functions.¹ Again, there is a single radial coordinate, ρ , which is a measure of the overall size of the three-body system, and again Schrödinger's equation reduces to a set of ordinary differential equations in this radial coordinate. The principal difference is that these equations are now coupled via the potential terms, and so their solution is a much more complex procedure than in the two-body case.

Nevertheless, the hyperspherical harmonic (HH) method has been used extensively and with considerable success in the study of bound-state problems. We mention just a few investigators whose work we have found especially close to our own: Fabre de la Ripelle and Ballot² in nuclear physics; Fano, Macek, and Lin³ in atomic physics. There have also been limited applications to

scattering problems and rearrangement collisions.

Our involvement in hyperspherical harmonics arises from our interest in statistical mechanics. For dilute fluids, the corrections to equilibrium properties due to three-body collision processes are contained in the third virial coefficient, or the third cluster coefficient in the fugacity expansion for the pressure. The connection between this quantity and the HH formulation of three-body scattering has been worked out in detail for both threedimensional⁴ and two-dimensional⁵ systems, with twobody bound states excluded, but so far there have only been calculations for certain limiting cases. Progress in doing more extensive calculations has been severely limited by the numerical complexity of solving the coupled differential-equation system. In practice, one works with a finite set of equations, which is then increased to demonstrate convergence. This leads to problems in both numerical stability of solutions, and in computer time and storage capacity. Thus some systematic approximation procedure is desirable.

A key approximation which has been found to be very useful in atomic and nuclear physics (see previous references) is the so-called adiabatic approximation (AA), and various modifications of it. Essentially, one expands the wave function in terms of new basis functions which are eigenfunctions of the angular plus interaction-potential part of the Hamiltonian (written in hyperspherical coordinates, as functions of ρ and angles). The expansion coefficients then satisfy a set of coupled differential equations in ρ only. This is exact, but by neglecting the coupling

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terms entirely (that is, the off-diagonal elements), one obtains a set of uncoupled differential equations in the variable ρ , which have the form of two-body Schrödinger equations, but with an effective potential replacing the original potentials.

The AA results in a considerable simplification of the problem. The calculation can now be performed in two separate steps, the first being a matrix diagonalization in order to find the effective potentials, point by point, and the second being the solution of the modified radial equation with this effective potential. In the case of atomic physics, this approach gives qualitative understanding of several-electron processes, in a way which is difficult to obtain otherwise. Nevertheless, questions still remain regarding the extent of its validity, and the implications of its shortcomings, as well as the nature of the convergence as the size of the truncated set of equations is increased.

Thus it is very desirable to investigate the validity of the method within the context of an exactly soluble system. Unfortunately, for the quantum-mechanical threebody problem there are no realistic cases for which the exact solutions are known. Thus we have to restrict ourselves to the somewhat artificial situation of three particles on a straight line. For the case of equal-mass particles interacting via equal-strength δ -function potentials, both the bound-state and scattering solutions are known exactly.^{6,7} Also, the thermodynamics of a onedimensional gas with repulsive δ -function interactions has been worked out.⁸

There is no problem in adapting the HH method to one dimension,⁹ and it also turns out that in the present case one can proceed analytically a long way towards constructing the effective potentials. This enables us to investigate a number of interesting points, which may otherwise have been obscured in a purely numerical calculation. Particularly, we investigate the large- ρ behavior of the effective potential, and also the way in which the solutions change as we increase the number of differential equations in the truncated set. We can also write analytical, closed-form, expressions for the elements of the adiabatic basis. This is important both in itself, and as a tool for the further exploration of the solutions of the transformed coupled (nonapproximated) set of equations.

A word should be said about statistics. A complete set of unsymmetrized harmonics for our model is the set of exponentials $(2\pi)^{-1/2} \exp(iKe)$ with $K = 0, \pm 1, \pm 2, \ldots$ From this we can construct symmetrized combinations (cosines and sines) which transform as Γ_1 and $\overline{\Gamma}_1$ (symmetric and antisymmetric one-dimensional representations) and also select pairs, of either exponentials or sines and cosines, which transform as members of the twodimensional representation Γ_2 . We have done this. (See also the independent work of Perez et al.¹⁰) However, for our purpose, which is to study three identical spinless particles described by fully symmetric wave functions (Γ_1) which include the lowest harmonic, K=0, we can equivalently and much more simply use the unsymmetrized set of exponentials subject to the condition $K \equiv 0 \pmod{6}$. This makes much more apparent the product structure of the matrix elements and leads to the same sum rules as the more formal procedure.

II. THE HYPERSPHERICAL HARMONIC METHOD

We consider a system of three identical particles moving in one dimension and interacting via two-body potentials $V(|x_i - x_j|)$, x_1, x_2, x_3 being the Cartesian coordinates of the particles. The center-of-mass coordinate Rand the Jacobi coordinates ξ, η are defined by

$$R = \left(\frac{1}{3}\right)^{1/2} (x_1 + x_2 + x_3) ,$$

$$\xi = \left(\frac{2}{3}\right)^{1/2} \left[\frac{x_1 + x_2}{2} - x_3\right] ,$$

$$\eta = \left(\frac{1}{2}\right)^{1/2} (x_1 - x_2) .$$
(2.1)

We now introduce the "hyperspherical" coordinates ρ, θ which for the present case are simply plane polar coordinates,

$$\eta = \rho \cos\theta, \ \xi = \rho \sin\theta, \ 0 \le \theta \le 2\pi \ . \tag{2.2}$$

Then Schrödinger's equation for the three particles, with center-of-mass motion removed, is

$$-\frac{\hbar^2}{2m} \left[\frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \theta^2} \right] \psi(\rho, \theta) + V(\rho, \theta) \psi(\rho, \theta)$$
$$= E \psi(\rho, \theta) , \quad (2.3)$$

where

$$V(\rho,\theta) = V(\sqrt{2}\rho \mid \cos\theta \mid) + V[\sqrt{2}\rho \mid \cos(\theta - 2\pi/3) \mid]$$

+ $V(\sqrt{2}\rho \mid \cos(\theta + 2\pi/3 \mid)).$ (2.4)

The hyperspherical harmonic (or K-harmonic) expansion of the wave function takes the form

$$\psi(\rho,\theta) = \sum_{K=-\infty}^{\infty} \rho^{-1/2} \phi_K(\rho) \frac{e^{iK\theta}}{\sqrt{(2\pi)}} , \qquad (2.5)$$

and inserting this in (2.3) leads to the infinite set of coupled ordinary differential equations

$$-\frac{\hbar^2}{2m} \left[\frac{d^2}{d\rho^2} - \frac{K^2 - \frac{1}{4}}{\rho^2} \right] \phi_K(\rho) + \sum_{K'} V_{KK'}(\rho) \phi_{K'}(\rho) = E \phi_K(\rho) , \quad (2.6)$$

where

$$V_{KK'}(\rho) = \frac{1}{2\pi} \int_0^\infty e^{i(K'-K)\theta} V(\rho,\theta) d\theta . \qquad (2.7)$$

The procedure now is to truncate the set (2.6) at some value K_{max} and solve the resulting finite set. This should then be repeated with increasing K_{max} until the numerical values, for the particular bound-state energies or scattering quantities that we are interested in, have converged.

However, in this paper we do not wish to solve the truncated set exactly, but rather to investigate an approximation method, the adiabatic approximation, which uncouples the equations of the set, and reduces the problem to that of solving a single differential equation.

We start by writing (2.6) in the form

$$\frac{d^2 \Phi}{d\rho^2} + \frac{2mE}{\hbar^2} \Phi - \mathbf{M} \Phi = \mathbf{0} , \qquad (2.8)$$

where Φ is a vector with components ϕ_K and **M** is the square matrix with elements

$$M_{KK'}(\rho) = \frac{K^2 - \frac{1}{4}}{\rho^2} \delta_{KK'} + \frac{2m}{\hbar^2} V_{KK'}(\rho) . \qquad (2.9)$$

 ${\bf M}$ is Hermitian, and so can be diagonalized by a unitary matrix ${\bf U}.$ Let

$$\mathbf{U}^{\dagger}\mathbf{M}\mathbf{U} = \mathbf{\Lambda} , \qquad (2.10)$$

where $\mathbf{U}^{\dagger}\mathbf{U} = \mathbf{I}$ and $\mathbf{\Lambda} = \mathbf{\Lambda}(\rho)$ is a diagonal matrix. Also define $\widetilde{\mathbf{\Phi}}$ by

$$\widetilde{\boldsymbol{\Phi}} = \boldsymbol{U}^{\dagger} \boldsymbol{\Phi} . \qquad (2.11)$$

Then, multiplying (2.8) on the left by U^{\dagger} , we find

$$\frac{d^2 \widetilde{\Phi}}{d\rho^2} + \frac{2mE}{\hbar^2} \widetilde{\Phi} - \Lambda \widetilde{\Phi} + \mathbf{U}^{\dagger} \frac{d^2 \mathbf{U}}{d\rho^2} \widetilde{\Phi} + 2\mathbf{U}^{\dagger} \frac{d\mathbf{U}}{d\rho} \frac{d\widetilde{\Phi}}{d\rho} = \mathbf{0} .$$
(2.12)

The AA (also called the extreme adiabatic approximation) consists of neglecting all the ρ derivatives of U; that is, we assume that U is a slowly varying function of ρ . Thus

$$\frac{d\tilde{\Phi}}{d\rho^2} + \frac{2mE}{\hbar^2}\tilde{\Phi} - \Lambda\tilde{\Phi} = 0. \qquad (2.13)$$

A is a diagonal matrix whose elements Λ_K can be labeled by the quantum number K according to the requirement that

$$\Lambda_K \to \frac{K^2 - \frac{1}{4}}{\rho^2}, \quad V \to 0 \;. \tag{2.14}$$

Thus in the AA we have to solve the set of uncoupled equations

$$\frac{d^2 \widetilde{\phi}_K}{d\rho^2} + \frac{2mE}{\hbar^2} \widetilde{\phi}_K - \left[\Delta_K + \frac{K^2 - \frac{1}{4}}{\rho^2} \right] \widetilde{\phi}_K = 0 , \quad (2.15)$$

where

$$\Delta_K \equiv \Lambda_K - \frac{K^2 - \frac{1}{4}}{\rho^2} .$$
 (2.16)

Note that (2.15) is formally equivalent to the radial Scrhödinger equation for two particles in two dimensions interacting via the potential Δ_K .

The above formulates the AA in terms of matrix diagonalization. An alternative, but entirely equivalent, treatment is given in Appendix A.

III. δ -FUNCTION INTERACTION

We now apply the above scheme to a particularly simple case: three identical particles on a straight line interacting via equal-strength δ functions. This system can be solved exactly,^{6,7} and the motivation behind our treatment is to find how well the HH method, with the AA, reproduces these exact solutions.

The two-body potential is

$$V(|x_{i}-x_{j}|) = g\delta(x_{i}-x_{j}), \qquad (3.1)$$

where g is the strength of the interaction. Transforming to hyperspherical coordinates gives, for the sum of the three binary potentials [see (2.1)],

$$V(\rho,\theta) = \frac{g}{\sqrt{2\rho}} \left[\delta(|\cos\theta|) + \delta(|\cos(\theta - 2\pi/3)|) + \delta(|\cos(\theta + 2\pi/3)|) \right].$$
(3.2)

Note that although the δ -function potential is highly singular, nevertheless $V(\rho, \theta)$ is a smooth, differentiable function of ρ ; the discontinuities are entirely in θ . Thus we expect the AA to be valid for this potential.

It is a straightforward calculations to show that the potential matrix elements (2.7) are

$$V_{KK'}(\rho) = \begin{cases} \frac{1}{\pi} \frac{3g}{\sqrt{2}\rho} e^{i(K'-K)\pi/2}, & K-K' \equiv 0 \pmod{6} \\ 0, & \text{otherwise} \end{cases}.$$
(3.3)

Note that the nonzero elements of $V_{KK'}(\rho)$ are precisely equal to three time the matrix elements of $V(|x_1-x_2|)$ and are proportional to ρ^{-1} . Also, $V_{KK'}(\rho)$ vanishes unless $K \equiv K' \pmod{6}$, this property being, in fact, a consequence of the invariance of $V(\rho, \theta)$ under permutation of the particles, and so not peculiar to the δ -function interaction. Thus the complete set of equations (2.6) is divided into six distinct subsets, corresponding to $K \equiv n \pmod{6}$, $n=0,1,\ldots,5$. The equations within each subset are coupled, but there is no coupling to a member of any other subset. This means that each of the six subsets of equations can be treated entirely separately. Thus, in the following, we assume that $K = K' \pmod{6}$.

The AA involves diagonalizing the matrix

$$M_{KK'}(\rho) = \frac{K^2 - \frac{1}{4}}{\rho^2} \delta_{KK'} + \frac{c}{\rho} e^{-iK\pi/2} e^{iK'\pi/2} , \qquad (3.4)$$

where $c = (2m/\hbar^2)(3g/\pi\sqrt{2})$. In general, one would expect to have to do this numerically. But in the present case, because the potential term in (3.4) is separable, one can proceed analytically.

Consider first the more general problem of finding the eigenvalues and eigenvectors of an $N \times N$ matrix **H** with elements

$$H_{ii} = h_i \delta_{ii} + \lambda f_i g_i , \qquad (3.5)$$

where h_i , f_i , g_i , and λ are arbitrary. We thus wish to find χ_i and ϵ such that

$$\sum_{i} H_{ij} \chi_j = \epsilon \chi_i . \tag{3.6}$$

Substituting (3.5) into (3.6) leads to

$$\chi_i = \frac{\lambda f_i}{\epsilon - h_i} \sum_j g_j \chi_j .$$
(3.7)

Multiplying each side by g_i and summing over *i* gives, upon cancelling the common factor $\sum_i g_i \chi_i$,

$$1 = \lambda \sum_{i} \frac{f_{i}g_{i}}{\epsilon - h_{i}} .$$
(3.8)

This is a polynomial in ϵ , the roots of which are eigenvalues of **H**.¹¹ Equation (3.7) shows that the corresponding (unnormalized) eigenvectors have components

$$\chi_i = \lambda \frac{f_i}{\epsilon - h_i} . \tag{3.9}$$

Applying this to the present case, we find that **M** has eigenvalues Λ_K satisfying

$$1 = \frac{c}{\rho} \sum_{K'} \frac{1}{\Lambda_K - \frac{K'^2 - \frac{1}{4}}{\rho^2}}$$
 (3.10)

In terms of the effective potential Δ_K defined by (2.16), (3.10) is

$$1 = \frac{c}{\rho} \sum_{K'} \frac{1}{\Delta_K + \frac{K^2 - K'^2}{\rho^2}}$$
 (3.11)

The (unnormalized) eigenvector corresponding to Δ_K has components

$$\chi_{K'}^{(K)} = \frac{c}{\rho} \frac{e^{-iK'\pi/2}}{\Delta_K + \frac{K^2 - {K'}^2}{\rho^2}} .$$
(3.12)

Comparison with (2.10) shows that the columns of U are the normalized eigenvectors; that is,

$$U_{K'K} = \chi_{K'}^{(K)} / \sum_{K'} |\chi_{K'}^{(K)}|^2 .$$
(3.13)

The procedure now is to solve (3.11) for Δ_K and substitute in (3.12) to get $\chi^{(K)}$. Equation (3.11) holds when K, K' take either a finite or infinite range of values. In the latter case, we can do the sum explicitly, as will now be shown. We restrict ourselves to the case where $K \equiv 0 \pmod{6}$; other cases can be treated similarly.

Let

$$K' = 6k'$$
, (3.14)

$$z^{2} = (\rho/6)^{2} \left[\Delta_{K} + \frac{K^{2}}{\rho^{2}} \right].$$
 (3.15)

Then (3.11) becomes

$$1 = \frac{\rho c}{36} \sum_{k'=-\infty}^{\infty} \frac{1}{z^2 - k'^2} . \tag{3.16}$$

The standard result¹²

$$\sum_{k=-\infty}^{\infty} \frac{1}{z^2 - k^2} = \frac{\pi}{z} \cot(\pi z), \quad z \neq 0, \pm 1, \dots$$
(3.17)

applied to (3.16) gives

$$\pi z \tan(\pi z) = (\pi/6)^2 \rho c$$
 (3.18)

Once this has been solved for z, Δ_K is found from

$$\Delta_K = [z^2 - (K/6)^2](6/\rho)^2 . \tag{3.19}$$

Equation (3.18) defines z as a multivalued function of ρ . Its solutions are given by the intersections of the curves

$$y = \pi z \tan(\pi z) \tag{3.20}$$

and

$$y = (\pi/6)^2 \rho c$$
 (3.21)

This is illustrated in Fig. 1. To determine the appropriate branch, we first note that (see Appendix B)

$$\Delta_{K} \sim \begin{cases} c/\rho, \ \rho \to 0, \ K = 0\\ 2c/\rho, \ \rho \to 0, \ K \neq 0 \end{cases}$$
(3.22)

Thus from (3.15) we have

$$z \to K/6, \ \rho \to 0$$
, (3.23)

and this establishes that, for a given $K \neq 0$, we must choose the solution of (3.18) satisfying

$$\frac{K\pi}{6} - \frac{\pi}{2} < \pi z < \frac{K\pi}{6} + \frac{\pi}{2}$$
 (3.24)

For K=0 and c > 0, the range is $0 < \pi z < \pi/2$. Finally, for K=0 and c < 0 we must proceed somewhat differently. In Fig. 1 there is no intersection for this case, the reason being that z as defined by (3.18) is imaginary. It is clear that in this case (3.15) and (3.18) must be replaced by

$$\zeta^2 = -(\rho/6)^2 \Delta_0 \tag{3.25}$$

and

$$\pi \zeta \tanh(\pi \zeta) = -(\pi/6)^2 \rho c$$
 (3.26)

The equations $y = \pi \zeta \tanh(\pi \zeta)$ and $y = -(\pi/6)^2 \rho c$ have a real point of intersection.



FIG. 1. Plot of $y = \pi z \tan \pi z$ as a function of z, together with the lines $y = (\pi/6)^2 \rho c$, for the cases $\rho = 10$, $c = \pm 1$. The intersections determine the adiabatic effective potentials Δ_K via Eq. (3.19).

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FIG. 2. Adiabatic effective potentials Δ_K , derived from an infinite set of coupled equations, as functions of the hyperradius ρ for the repulsive case c = 1.

IV. THE EFFECTIVE POTENTIAL Δ_K

We now wish to look in detail at the effective potential Δ_K derived in Sec. III. For an infinite set of equations, Δ_K is determined by (3.18) and (3.19). One way of finding z is to write (3.18), using (3.24), as

$$z = \frac{K}{6} + \frac{1}{\pi} \arctan\left[\frac{\pi\rho c}{36}\frac{1}{z}\right]$$
(4.1)

and iterate, starting with z = K/6 (or z small for the case K = 0). Δ_K is then given by (3.19). For the exceptional case $\Delta_0(c < 0)$, (3.25) and (3.26) can be written as

$$\sqrt{-\Delta_0} = -\frac{\pi c}{6} / \tanh\left[\frac{\pi \rho}{6} \sqrt{-\Delta_0}\right],$$
 (4.2)

which can again be solved by iteration.

The results of some of these calculations are shown in Figs. 2 and 3, where we plot Δ_K against ρ for K=0, 6,



FIG. 3. Adiabatic effective potentials Δ_K , derived from an infinite set of coupled equations, as functions of the hyperradius ρ for the attractive case c = -1.

and 12, and $c = \pm 1$. (There is no loss in generality in taking these values for c, since any other value simply rescales Δ_K and ρ as Δ_K/c^2 and $\rho | c |$. Also, we do not need to consider negative values of K, since using the symmetric basis would lead to the use of only nonnegative indices. Formally, we can verify that $\Delta_{-K} = \Delta_K$.)

A word should be said about the curve crossings in Fig. 3. These are, of course, crossings of the effective potentials, Δ_K ; the adiabatic eigenvalues Λ_K , which are related to Δ_K by (2.16), exhibit no such crossings. This is evident graphically, or it can be proved using the equations defining Δ_K given above.

A. Analysis of the results

The most striking feature of these graphs is the behavior of Δ_0 (c = -1) for large ρ , and this will be discussed below. Let us start with the other curves, which go to zero for large ρ . The original potential matrix element was

$$\frac{2m}{\hbar^2} V_{KK'}(\rho) = \frac{c}{\rho} e^{-iK\pi/2} e^{iK'\pi/2} , \qquad (4.3)$$

and so behaved as ρ^{-1} for both small and large ρ . The limiting behavior of the effective potential Δ_K is studied in Appendix B. We find that for small ρ the behavior is still ρ^{-1} [see (B2)], but for large ρ , Δ_k falls off as ρ^{-2} [always excepting the case Δ_0 (c < 0)]; the leading terms are given explicitly in (B9) and (B10). Thus there has been a remodeling of the tail of the potential, with the original ρ^{-1} tail becoming a much more manageable ρ^{-2} . One finds a similar remodeling of the tail for three particles in two dimensions, where the basic ρ^{-2} behavior of the matrix elements is changed to a $(\rho^2 \ln \rho)^{-1}$ behavior for large ρ .¹³

The general situation regarding long-range behavior is as follows. A system of three particles subject to shortrange binary potentials can have significant interaction even for large values of ρ , since for particular values of the angles specific particles can be close together. (For example, ρ and r_{13} can be large and r_{12} small, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ being the distance between particles *i* and *j*.) Matrix elements which involve weighted integrals over the angles, and therefore the configurations of the three particles, will have long-range tails (which behave as ρ^{-d} where *d* is the dimension). The actual long-range interaction, in the AA given by the adiabatic potential, can have a behavior which is analytically distinct from that of the matrix elements.

The results given above are associated with three particles asymptotically free at large distances (with a wave function equal to a function of ρ times the appropriate adiabatic eigenfunction). The scattering of these particles from each other will then be *qualitatively* affected by changes in the tail. This is especially evident in the threshold behavior of the phase shifts as a function of the energy. For the one-dimensional case, a ρ^{-1} tail gives a phase shift which diverges for small values of the wave number q as $q^{-1} \ln q$, whereas a ρ^{-2} tail gives a constant. This ρ^{-2} tail dominates the low-energy scattering and the

AA gives phase shifts of $-3\pi/2$ and $3\pi/2$ for the repulsive and attractive cases, respectively. A comparison with the work of McGuire and Dodd⁶ leads us to believe these threshold values to be correct.

We now turn to the attractive case with K=0. The potential Δ_0 (c < 0) shows quite exceptional behavior in that it does not go to zero as $\rho \rightarrow \infty$, but rather to $-\pi^2 c^2/36$, and also the approach to this limit is exponential, rather than powerlike. [See Appendix B and especially (B19).] Now, $-\pi^2 c^2/36$ is precisely the energy of the two-body bound state for the δ -function potential $g\delta(|x_1-x_2|)$.

To understand this, let us again suppose that ρ and r_{13} are large and that r_{12} is small. We can verify that, to leading order in an expansion in ρ^{-1} and therefore asymptotically correct, the derivatives in ρ in (2.3) give us the kinetic energy associated with the relative motion of particle 3 and the center of mass of particles 1 and 2. Still referring to (2.3), the derivative term in θ , divided by ρ^2 and again to leading order, gives us the relative kinetic energy between 1 and 2. Since the binary potentials are short ranged we see that for small values of r_{12} the functional equation for the adiabatic eigenfunction [Eq. (A9)] is simply the two-body Schrödinger equation. If the two-body Hamiltonian admits a two-body bound state in its spectrum, that negative eigenvalue will appear as the asymptotic behavior of one of our effective potentials. The corresponding AA wave function (amplitude times eigenfunction) then either represents a solution which at large ρ describes one particle (free) and a two-body bound state or, if the potential depth and masses of the particles permit it, a three-body bound state. In Sec. V, below, we shall show that one further aspect of Δ_0 (c < 0) is its prediction of a single three-body bound state.

Before leaving these matters, we should emphasize that, preceding us, much thought has been devoted to the behavior of this adiabatic potential by investigators centered about Fano.³ The initial investigations of asymptotic bound-state situations was directed around the lines of Macek and Lin.³ Our model is useful due to its simplicity and to the possibility of writing down exact expressions, for example, for the adiabatic eigenfunctions for all ρ (see Appendixes), and expansions for the effective potentials. We have, of course, also obtained a wealth of numerical data.

B. Convergence

It is of interest to study the way in which Δ_K obtained from 2N + 1 equations [which we denote by $\Delta_K(N)$] approaches Δ_K obtained from the infinite set [denoted by $\Delta_K(\infty)$], as N increases. This is a question of great practical importance in more complex cases, where $\Delta_K(\infty)$ is not known exactly, and one can only calculate $\Delta_K(N)$ for increasing values of N.

We restrict our discussion to Δ_0 . Figure 4 shows Δ_0 for the repulsive case (c = +1) and N=0, 1, and 10. On the scale used $\Delta_0(\infty)$ is indistinguishable from $\Delta_0(10)$. It is seen that $\Delta_0(N)$ approaches $\Delta_0(\infty)$ quite smoothly and quickly. The asymptotic approach to the limit is well described by

$$\Delta_0(N) = \Delta_0(\infty) + \alpha/N , \qquad (4.4)$$

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FIG. 4. Adiabatic effective potentials $\Delta_0(N)$, derived from (2N+1) coupled equations, as functions of the hyperradius ρ for the repulsive case c = 1. On the scale of the graph, $\Delta_0(\infty)$ is indistinguishable from $\Delta_0(10)$.

where α depends on ρ but is almost independent of N for $N > N_0$. In the repulsive case, $N_0 \simeq 8$ gives a good fit.

For the attractive case, the situation is rather different. Figure 5 shows $\Delta_0(N)$ for c = -1 and N=0, 1, 10, 100, and ∞ . The approach to $\Delta_0(\infty)$ is now much slower, and the rate depends strongly on ρ , being quite rapid for small ρ and very slow for large ρ . In fact, there is a noncommutivity between the limits $\rho \rightarrow \infty$ and $N \rightarrow \infty$, as is clear from (B3) and (B19). Thus one cannot hope to get the tail of $\Delta_0(c < 0)$ by straightforward solution of a finite set of



FIG. 5. Adiabatic effective potentials $\Delta_0(N)$, derived from (2N+1) coupled equations, as functions of the hyperradius ρ for the attractive case c = -1.

equations, even for very large N. Again, the approach to the limit can be fitted to a relation of the type (4.4), but N_0 is now much larger, and also depends on ρ in such a way that $N_0 \rightarrow \infty$ as $\rho \rightarrow \infty$.

For the two-dimensional case,¹³ the overall picture is very similar, except that a much larger number of harmonics (several hundred) is required to attain convergence in the asymptotic region, even in the repulsive case. Also, the number of harmonics increases steadily as ρ is increased.

V. THREE-BODY BOUND STATE

Three attractive delta-function bosons have one bound state at the energy

$$E = -\frac{\hbar^2}{2m} \frac{\pi^2 c^2}{9} .$$
 (5.1)

We now investigate how closely the HH method approximates this value.

The simplest approximation is to take only the K=0 equation from (2.6), and neglect its coupling to the others entirely. This gives the equation

$$\frac{d^2\phi_0}{d\rho^2} + \frac{2mE}{\hbar^2}\phi_0 - \left[\frac{c}{\rho} - \frac{1}{4\rho^2}\right]\phi_0 = 0.$$
 (5.2)

This is related to Whittaker's equation, and it is readily shown that it has bounded solutions for energies

$$E_n = -\frac{1}{(2n+1)^2} \frac{\hbar^2 c^2}{2m}, \quad n = 0, 1, 2, \dots$$
 (5.3)

with the corresponding wave functions

$$\phi_0^{(n)} = e^{-z/2} z^{1/2} L_n(z) , \qquad (5.4)$$

where $z = 2\rho |c|/(2n+1)$ and $L_n(z)$ is the *n*th-order Laguerre polynomial. The lowest energy level of the series,

$$E_0 = -\frac{\hbar^2 c^2}{2m} , \qquad (5.5)$$

reproduces the exact energy level (5.1) to within 10%. (This was already pointed out by Amado and Coelho.⁹) The value (5.5) is reasonable, given that it is a first approximation, but there is also the problem of the remaining infinite sequence of spurious energy levels.

The next approximation would be to consider three coupled equations (K,K'=-6,0,6) from (2.6). In the AA, this gives the effective potential

$$\Delta_0 = \frac{c}{\rho} + \frac{18}{\rho^2} - \left[\frac{18^2}{\rho^4} + \frac{c^2}{\rho^2}\right]^{1/2}.$$
(5.6)

Treating this as a perturbation on c/ρ , and employing first-order perturbation theory, gives the lowest energy level as

$$E_0 = -1.028 \frac{\hbar^2 c^2}{2m} . \tag{5.7}$$

This is an improvement on (5.5), but there still remains the problem of the infinite number of energy levels, arising from the ρ^{-1} behavior of Δ_0 as $\rho \rightarrow \infty$. As shown in Appendix B, this long-range behavior of Δ_0 persists for any finite number of coupled equations [see (B3)], so the problem of the spurious energy levels remains.

But when we consider the infinite set of coupled equations the situation changes. Δ_0 now approaches its asymptotic limit exponentially, as shown by (B19). This is a crucial change of behavior, and a numerical investigation now confirms that there is now only one bound state.¹⁴ A first-order perturbation calculation employing the small- ρ series obtained from (3.26),

$$\Delta_{0} = \frac{c}{\rho} - \frac{\pi^{2}c^{2}}{108} + \frac{\pi^{4}c^{3}}{14\,580}\rho - \frac{\pi^{6}c^{4}}{2\,755\,620}\rho^{2} + O(\rho^{3}) ,$$

$$\rho \to 0$$
(5.8)

gives

$$E_B = -1.099 \frac{\hbar^2 c^2}{2m} , \qquad (5.9)$$

which is within 0.22% of the exact value (5.1).

VI. CONCLUSION

This paper is the first step in a comprehensive investigation of the HH approach to the three-body problem in the context of an exactly soluble model. We have shown that, using the AA, many steps which normally have to be done numerically can be done analytically, and that it is a simple matter to calculate effective potentials, $\Delta_K(\rho)$. This enables us to investigate convergence as a function of the number of coupled equations used, and to analyze closely the behavior of $\Delta_K(\rho)$ as a function of ρ .

The most significant feature is the behavior of $\Delta_K(\rho)$ as $\rho \rightarrow \infty$. Whereas the original potential matrix elements $V_{KK'}(\rho)$ have a ρ^{-1} behavior, in $\Delta_K(\rho)$ this is modified to ρ^{-2} , thus giving rise to a qualitatively different threshold behavior for the scattering three-body phase shifts. An exception is $\Delta_0(\rho)$ for the attractive case, where a ρ^{-1} behavior is retained for a finite number of equations, but is changed completely (tending exponentially to the two-body bound-state energy) for an infinite number of equations. This exponential decay gives the correct result of only one three-body bound state (however, see Ref. 14), and also gives the binding energy to within 0.22%.

Thus we see that the HH method with the AA works well for the calculation of three-body bound states, and this is in line with the results of other investigators. We also think that in our results for the adiabatic potentials and the adiabatic basis lie the correct starting points for a fruitful investigation of the scattering and rearrangement properties of the system, using configuration-space methods. We propose to develop these topics in the future.

Also for future publication is the investigation of the terms neglected in going from (2.12) to (2.13). These include the diagonal elements of the matrix $\mathbf{U}^{\dagger}d^{2}\mathbf{U}/d\rho^{2}$, which give a correction to the AA, and the off-diagonal elements of the terms involving $d\mathbf{U}/d\rho$ and $d^{2}\mathbf{U}/d\rho^{2}$, which couple the adiabatic channels. Preliminary results indicate that these will not drastically modify the behavior we have found using the AA.

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APPENDIX A: ALTERNATIVE FORMULATION OF ADIABATIC APPROXIMATION

The Schrödinger equation (2.3) can be written

$$\left[-\frac{\partial^2}{\partial\rho^2} + H_{\rho} - \frac{2mE}{\hbar^2}\right]\phi(\rho,\theta) = 0 , \qquad (A1)$$

where $\phi(\rho, \theta) = \rho^{1/2} \psi(\rho, \theta)$ and H_{ρ} is the operator

$$H_{\rho} = -\frac{1}{\rho^2} \left[\frac{\partial^2}{\partial \theta^2} + \frac{1}{4} \right] + \frac{2m}{\hbar^2} V(\rho, \theta) . \tag{A2}$$

We now seek solutions of the eigenvalue-eigenfunction equation

$$H_{\rho}B_{K}(\rho,\theta) = \Lambda_{K}(\rho)B_{K}(\rho,\theta) , \qquad (A3)$$

where the label K has been assigned by the requirement that $\Lambda_K \rightarrow (K^2 - \frac{1}{4})/\rho^2$ as $V(\rho, \theta) \rightarrow 0$. Expanding $B_K(\rho, \theta)$ in HH as

$$B_{K}(\rho,\theta) = \sum_{K''} U_{K''K}(\rho) \frac{e^{iK''\theta}}{\sqrt{(2\pi)}} , \qquad (A4)$$

allows (A3) to be put in the form

$$\sum_{K''} \left[\frac{K^2 - \frac{1}{4}}{\rho^2} \delta_{K'K''} + \frac{2m}{\hbar^2} V_{K'K''} \right] U_{K''K} = \Lambda_K U_{K'K} .$$
(A5)

Comparison with (2.10) shows that Λ_K is the total effective potential and that $U_{KK'}$ are just the elements of **U**. It then follows from (2.5) and (2.11) that

$$\phi(\rho,\theta) = \sum_{K} \widetilde{\phi}_{K}(\rho) B_{K}(\rho,\theta) . \qquad (A6)$$

That is, the ϕ_K are the coefficients for the expansion of the wave function in terms of the basis functions $B_K(\rho, \theta)$. Substituting (A6) into (A1), multiplying by $B_{K'}(\rho, \theta)$, integrating over θ and making use of the orthonormality relation

$$\int_0^{2\pi} B_K(\rho,\theta) B_{K'}(\rho,\theta) d\theta = \delta_{KK'} , \qquad (A7)$$

gives

$$\frac{d^{2}\widetilde{\phi}_{K'}}{d\rho^{2}} + \left[\frac{2mE}{\hbar^{2}} - \Lambda_{K'}\right]\widetilde{\phi}_{K'} + \sum_{K} \left[\left[B_{K'}, \frac{\partial^{2}B_{K}}{\partial\rho^{2}} \right] \widetilde{\phi}_{K} + 2 \left[B_{K'}, \frac{\partial B_{K}}{\partial\rho} \right] \frac{\partial\widetilde{\phi}_{K}}{\partial\rho} = 0,$$
(A8)

where the brackets (,) denote an integral over θ . Neglecting the ρ derivatives of B_K again leads to the AA, (2.15).

We thus see that for the AA we can either solve the differential equation (A3) or diagonalize the matrix \mathbf{M} given by (2.9).

To demonstrate the first approach, we again consider the δ -function interaction. Equation (A3) is

$$\left[-\frac{1}{\rho^2}\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{4}\right) + \frac{2m}{\hbar^2}V(\rho,\theta)\right]B_K(\rho,\theta)$$
$$= \Lambda_K B_K(\rho,\theta) . \quad (A9)$$

where

$$\frac{2m}{\hbar^2}V(\rho,\theta) = \frac{\pi}{3}\frac{c}{\rho}\sum_{\mu=0}^5\delta(\theta-\theta_\mu), \qquad (A10)$$

and $\theta_{\mu} = (2\mu + 1)\pi/6$. For $\theta \neq \theta_{\mu}$, (A10) is simply

$$\frac{\partial^2}{\partial \theta^2} + q_K^2 \left| B_K(\rho, \theta) = 0 \right|, \qquad (A11)$$

where

$$q_{K} = (\frac{1}{4} + \rho^{2} \Lambda_{K})^{1/2} = \rho (\Delta_{K} + K^{2} / \rho^{2})^{1/2} .$$
 (A12)

The solutions in the six sectors are then connected by the boundary conditions,

$$B_K(\rho,\theta_\mu-) = B_K(\rho,\theta_\mu+) , \qquad (A13)$$

$$\frac{\partial B_K}{\partial \theta}\Big|_{\theta_{\mu}+} - \frac{\partial B_K}{\partial \theta}\Big|_{\theta_{\mu}-} = \frac{\pi}{3}\rho c B_K(\rho,\theta_{\mu}) .$$
(A14)

This second condition follows upon integrating (A9) with respect to θ over a small interval including θ_{μ} .

To be precise, we look for the completely symmetric solution; that is, we seek a solution in the sector $|\theta| < \pi/6$ and require that it be repeated in the othe five sectors. The above considerations, together with the invariance of the differential equation and boundary conditions under $\theta \rightarrow -\theta$, restrict B_K to have the general form

$$B_{K}(\rho,\theta) = A_{K}(\rho) \cos \left[q_{K} \left[\theta - \frac{m\pi}{3} \right] \right], \qquad (A15)$$

where *m* is an integer determined by $|\theta - m\pi/3| < \pi/6$. The boundary condition (A13) is satisfied, and (A14) leads to

$$q_K \tan\left[\frac{\pi}{6}q_K\right] = \frac{\pi\rho c}{6} , \qquad (A16)$$

which is precisely the relation determining the effective potential found previously by the matrix-diagonalization method. [In (3.18), $z=q_K/6$.] It only remains to show that $K \equiv 0 \pmod{6}$, and this follows from the requirement that, as $c \rightarrow 0$, (A15) tends to the free-particle solution

$$B_{K}^{(0)}(\rho,\theta) = A_{K}^{(0)}(\rho)\cos(K\theta) .$$
 (A17)

(Note $q_K \rightarrow K$ as $\Delta_K \rightarrow 0.$)

 $B_K(\rho,\theta)$ satisfies the orthonormality condition (A7). For K' = K this determines $A_K(\rho)$. We find

$$\int_{0}^{2\pi} [B_{K}(\rho,\theta)]^{2} d\theta = 12 [A_{K}(\rho)]^{2} \int_{0}^{\pi/6} \cos^{2}(q_{K}\theta) d\theta ,$$
(A18)

leading to

$$A_K(\rho) = \left[\pi + \frac{3}{q_K} \sin\left(\frac{\pi}{3}q_K\right)\right]^{-1/2}, \qquad (A19)$$

which, upon use of (3.18), can be written

$$A_{K}(\rho) = \left\{ \pi + \left(\frac{\pi \rho c}{36} \right) / \left[\left(\frac{q_{K}}{6} \right)^{2} + \left(\frac{\pi \rho c}{36} \right)^{2} \right] \right\}^{-1/2}.$$
(A20)

For the case K=0, c<0, it is convenient to rewrite the above equations as

$$B_0(\rho,\theta) = A_0(\rho) \cosh\left[\overline{q}_0\left(\theta - \frac{m\pi}{3}\right)\right], \qquad (A21)$$

where

$$A_0(\rho) = \left\{ \pi - \left[\frac{\pi \rho c}{36} \right] / \left[\left[\frac{\overline{q}_0}{6} \right]^2 - \left[\frac{\pi \rho c}{36} \right]^2 \right] \right\}^{-1/2},$$
(A22)

and \overline{q}_0 satisfies

$$\overline{q}_0 \tanh\left(\frac{\pi \overline{q}_0}{6}\right) = -\frac{\pi \rho c}{6} . \tag{A23}$$

We can also construct $B_K(\rho, \theta)$ using the matrix approach. Inserting (3.13) into (A4), and restricting the sum to be over K'' = 6n, leads to

$$B_{K}(\rho,\theta) = \frac{1}{M_{K}(\rho)} \frac{1}{\sqrt{(2\pi)}} \frac{\rho c}{36} \sum_{n=-\infty}^{\infty} \frac{(-1)^{n} \cos(6n\theta)}{z^{2} - n^{2}} ,$$
(A24)

where

$$[M_{K}(\rho)]^{2} = \sum_{K'} |\chi_{K'}^{(K)}(\rho)|^{2}$$
$$= \frac{c^{2}\rho^{2}}{(36)^{2}} \sum_{n=-\infty}^{\infty} \frac{1}{(z^{2}-n^{2})^{2}}, \qquad (A25)$$

and $z = (\rho/6)\Delta_K + K^2/\rho^2)^{1/2}$. The above sums can be done using¹²

$$\sum_{k=-\infty}^{\infty} (-1)^k \frac{\cos(kx)}{z^2 - k^2} = \pi \frac{\cos[z(2m\pi - x)]}{z \sin z\pi} , \quad (A26)$$

where $(2m-1)\pi < x < (2m+1)\pi$ and

$$\sum_{k=-\infty}^{\infty} \frac{1}{(z^2 - k^2)^2} = \frac{\pi}{2z^2} \left[\frac{\cos(\pi z)}{z} + \pi \operatorname{cosec}^2(\pi z) \right],$$
(A27)

which can be obtained by differentiating (3.17) with respect to z. We find

$$B_{K}(\rho,\theta) = \frac{1}{M_{K}(\rho)} \frac{\pi}{\sqrt{(2\pi)}} \frac{\rho c}{36} \frac{\cos[z(2m\pi - 6\theta)]}{z\sin(\pi z)} ,$$
(A28)

and

$$M_{K}(\rho) = \frac{\rho c}{36} \frac{1}{z} \left[\frac{18}{\rho c} + \frac{\pi^{2}}{2} \operatorname{cosec}^{2}(\pi z) \right]^{1/2}.$$
 (A29)

Inserting (A29) in (A28) leads to our previous results, (A15) and (A19).

Thus we have demonstrated that the δ -function case can be solved by either the differential-equation approach, based on (A3), or the matrix approach, based on (A5). In more complex cases, the usual approach would be via (A5), using a matrix of finite dimension.

APPENDIX B: ASYMPTOTIC BEHAVIOR OF $\Delta_K(\rho)$

1. Behavior as $\rho \rightarrow 0$

Consider the case where the AA is applied to 2N + 1 equations with K and K' varying from -6N to 6N. Equation (3.11) can be written

$$1 = \frac{c}{\rho} \left[\frac{\epsilon_K}{\Delta_K} + \sum_{\substack{K' \\ (K' \neq \pm K)}} \frac{1}{\Delta_K + \frac{K^2 - K'^2}{\rho^2}} \right], \quad (B1)$$

where $\epsilon_0 = 1$ and $\epsilon_K = 2$, $K \neq 0$. It then follows that

$$\Delta_K \sim \epsilon_K c / \rho, \ \rho \to 0 . \tag{B2}$$

This conclusion still applies if $N = \infty$, as can be established directly from (3.18) and (3.19) [or (3.25) and (3.26) for the case K = 0, c < 0].

2. Behavior as $\rho \rightarrow \infty$

The behavior of Δ_K is now somewhat more complicated, and we need to consider several cases.

a. 2N + 1 equations, N finite

 Δ_K is determined by (3.11). This expression has singularities at $\Delta_K = -(K^2 - K'^2)/\rho^2$, and since Δ_K is a continuous function of ρ this means that it must be constrained to lie between two adjacent singularities for all ρ . The particular interval can be determined by condition (B2), and the asymptotic form can then be found from (3.11). We find the following special cases:

$$\begin{split} \Delta_{0} & (c < 0) = \frac{(2N+1)c}{\rho} + \frac{12N(N+1)}{\rho^{2}} + O\left[\frac{1}{\rho^{3}}\right], \\ & \rho \to \infty \quad (B3) \\ \Delta_{6N} & (c > 0) = \frac{(2N+1)c}{\rho} - \frac{12N(2N-1)}{\rho^{2}} + O\left[\frac{1}{\rho^{3}}\right], \\ & \rho \to \infty \quad (B4) \end{split}$$

For all other cases,

$$\Delta_{K} = \frac{\alpha_{K}}{\rho^{2}} + O\left[\frac{1}{\rho^{3}}\right], \quad \rho \to \infty$$
(B5)

where a_K is the smallest positive (for c > 0) or negative (for c < 0) solution of

$$\sum_{K'} \frac{1}{\alpha_K + K^2 - {K'}^2} = 0 .$$
 (B6)

b. Infinite set of equations

Except for Δ_0 (c < 0) (to be treated below), we now use (3.18) and (3.19). Again, the singularity structure of (3.18) determines the allowed interval for Δ_K , and this in turn determines the asymptotic behavior. From (3.18) and (3.24), we have

$$\pi z = \frac{K\pi}{6} + \arctan\left[\frac{\pi\rho c}{36z}\right],\tag{B7}$$

and using the expansion

$$\arctan t = \pm \frac{\pi}{2} - \frac{1}{t} + \frac{1}{3t^3} - \cdots, |t| > 1$$
 (B8)

where the plus is for t > 0 and the minus is for t < 0, we arrive at the expansions

$$\Delta_{K} (c > 0) = \frac{6|K|+9}{\rho^{2}} - \frac{72}{\pi^{2}c} (|K|+3)^{2} \frac{1}{\rho^{3}} + O\left[\frac{1}{\rho^{4}}\right],$$

$$\rho \to \infty \quad (B9)$$

$$\Delta_{K} (c < 0) = \frac{-6|K|+9}{\rho^{2}} - \frac{72}{\pi^{2}c} (|K|-3)^{2} \frac{1}{\rho^{3}} + O\left[\frac{1}{\rho^{4}}\right],$$

$$\rho \to \infty, K \neq 0. \quad (B10)$$

c. Infinite set of equations, K = 0, c < 0

Equations (3.25 and (3.26) give)

 $\tanh \pi \zeta = \pi \rho \mid c \mid /36\zeta \;, \tag{B11}$

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where $\zeta = \rho \sqrt{(-\Delta_0)}/6$ is real and non-negative. Thus $0 < \tanh \pi \zeta < 1$ and so from (B11)

$$0 < \pi \rho | c | / 36\zeta < 1$$
, (B12)

which gives

$$\Delta_0 < -\pi^2 c^2 / 36 . \tag{B13}$$

Thus Δ_0 is always bounded above by $-\pi^2 c^2/36$, and, in fact, from (B11) it follows that

$$\Delta_0(c<0) \rightarrow -\pi^2 c^2/36 \text{ as } \rho \rightarrow \infty . \tag{B14}$$

This is to be contrasted with the limiting behavior for a finite set of equations, (B3).

To investigate in more detail the way in which Δ_0 (c < 0) approaches the limit (B14), we write (B11) as

$$\pi \rho \sqrt{(-\Delta_0)} / 6 = \frac{1}{2} \ln \left[\frac{\sqrt{(-\Delta_0)} + \pi |c| / 6}{\sqrt{(-\Delta_0)} - \pi |c| / 6} \right].$$
(B15)

Setting

$$\sqrt{(-\Delta_0)} = \pi |c| / 6 + \epsilon \tag{B16}$$

gives

$$\pi^{2} \rho | c | /36 + \pi \rho \epsilon / 6 = \frac{1}{2} \ln(1 + \pi | c | /3\epsilon) .$$
 (B17)

For ϵ small, we have as a first approximation

$$\pi^2 \rho |c| / 36 \simeq \frac{1}{2} \ln(\pi |c| / 3\epsilon)$$
, (B18)

which leads to

$$\Delta_0(c<0) \sim -\frac{\pi^2 c^2}{36} (1+4e^{-\pi^2 |c|\rho/18} + \cdots), \ \rho \to \infty .$$
(B19)

Thus the approach to the limit is exponential, in contrast to all other cases.

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¹⁴More precisely, a careful numerical treatment, as well as confirming the existence of a bound state with E_B given by (5.9), also reveals a discrete level at $-(\hbar^2 c^2/2m)(\pi^2/36)$ + 0.000 97). Recalling that $-(\hbar^2 c^2/2m)(\pi^2/36)$ is the energy of the two-body bound state, we see that this corresponds to an extremely weakly bound three-body state, and is certainly negligible to the level of accuracy we expect from the AA. Its existence reflects the fact that the AA *is* an approximation, albeit a very good one as far as bound states in this model are concerned.