Solution for boson-diboson elastic scattering at zero energy in the shape-independent model

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We derive an exact analytic expression for the boson-diboson elastic scattering phase shift in the shape-independent model for positive two-body scattering lengths when the total energy vanishes. A three-body hard-core potential depending upon a hyperradial cutoff parameter R_0 is introduced to obtain a finite result. The exact result is compared with adiabatic hyperspherical calculations of the phase shift, and a similar functional dependence on the cutoff parameter is found. The cutoff parameter plays the role of a renormalization constant in that it renormalizes the wave function at vanishing hyperradius.

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I. INTRODUCTION

The properties of homogeneous dilute Bose condensates depend primarily upon the two-body S-wave scattering length a. This is seen most directly in the expansion [1] of the energy density in powers of $\sqrt{na^3}$, where n is the particle density and where the coefficients of terms of order $\sqrt{na^3}$ and $\sqrt{na^3}\ln(\sqrt{na^3})$ are universal constants. The coefficients of the next-order term—namely, the term na^3—depend upon details of two- and three-body interactions not germane to the two-body scattering length a. Such details are relevant to properties that depend upon the particle interactions when all three particles are close together. This region can be treated with high accuracy using the hyperspherical adiabatic basis set and the hyperspherical close coupling (HCC) method [2,3]. When the spatial extent of the region where the two- and three-body potentials are important is small compared with the scattering length a these details can be incorporated in a single parameter identified as a renormalization constant Λ_* [4–6]. Once the renormalization constant is set, all other observables can be computed unambiguously.

The renormalization constant is set by fitting a low-energy three-body observable to a measured or computed value. This computed value is usually determined numerically—i.e., by solving the three-body Schrödinger equation with realistic two-body potentials at some level of approximation—e.g., by the hyperspherical close coupling method. Explicit three-body interactions can also be included in the HCC basis, if needed [3].

Because the renormalization constant is fundamental to the shape independent representation it is desirable to know the functional form of the observable quantities used to set the renormalization constant as exactly as possible. In this paper we give an exact closed-form solution of the three-body Schrödinger equation for the special case of three identical bosons in the shape-independent model when $a>0$ and the total energy E of the three-body system vanishes. The exact solution involves a renormalization constant—namely, a fixed hyper-radius R_0; thus, this constant can be related exactly to one observable—namely, the elastic scattering phase shift at zero energy.

We find that the dependence of the elastic scattering phase shift upon R_0 is identical to the form obtained by Efimov in a $1/R^2$ model potential analysis [7]. The exact expression is used to compute parameters of Efimov's model at zero energy. Exact solutions for this phase computed using effective field theory (EFT) [6] obtain a form that is similar to that of Ref. [7]. More importantly, Ref. [6] extends Efimov's model to include true molecular effects expected in realistic physical situations. In this way they show how the shape-independent model is fundamental to the theory of three-boson interactions.

The computations of Ref. [6] employ a renormalization constant Λ_* conjugate to a distance $R_* \equiv 1/\Lambda_*$ in atomic units, which are used throughout this report. We show that R_* and R_0 are proportional up to terms of the order 10^{-3} and find the proportionality constant.

While investigating the renormalization constant is an important motivation for the present work, exact solutions for three interacting species, even if only for special cases, are intrinsically interesting since they are limiting cases of general solutions. Such limiting cases can indicate mathematical properties of more general solutions. The $E=0$ solutions are at the energy boundary where the $L=0$ scattering matrix changes from a 1×1 matrix to an infinite-dimensional matrix owing to the opening of the breakup channels. Exact solutions near $E=0$ are therefore of particular significance for tests of theory, generally. In addition, the special solution for $E=0$ is the first term of an expansion in powers of Ea^2. Such expansions are asymptotic, but can be systematically developed once the $E=0$ solutions are available. For these reasons, the special solution at $E=0$ is presented in detail in this report.

The analytic expressions for the zero-energy phase shifts reported in this paper employ hyperspherical coordinates and integral representations of the exact S-wave solutions [8]. The general method is reviewed in Sec. II. The basic equations are solved in Sec. III. The solutions are used in Sec. IV to obtain the elastic scattering phase shift at zero energy. In

that section we present an identity that is used to check the accuracy of our solutions. The phase shift is also compared with those obtained in the one-channel hyperspherical close coupling and the adiabatic hyperspherical approximations. Bound properties of these phase shifts are used to compare these results with the exact solution. Section V summarizes the investigations reported here.

II. REVIEW OF THE STURMIAN METHOD

In the shape-independent model all two-particle interactions are replaced by boundary conditions such that the wave function in the force-free region corresponds to an s wave with the correct scattering length a [9]. This model is also called the zero-range potential (ZRP) model. Since the free-particle Schrödinger equation is separable in a large number of coordinate systems, exact solutions are readily obtained by separation of variables. In this case the wave function is a product of functions of the coordinate variables. For three or more particles, however, the boundary conditions are not separable in any known coordinate system. This means that acceptable solutions must be obtained by integrating the separable solutions over the separation constants [10]. The generally complex integration contour and the amplitude of the product functions must then be chosen to satisfy the boundary conditions.

There are no general methods to find the integration contours nor to completely determine the amplitudes of the product functions. Every case appears different. The main accomplishment of the present work is that both the contours and those amplitudes that satisfy physical and mathematical conditions are determined uniquely. This allows us to compute analytic expressions for the phase shifts in terms standard Γ functions and the roots of simple transcendental equations.

In the hyperspherical Sturmian representation the coordinates of three particles are denoted by one length coordinate, the hyperradius R, and a set of five angles denoted collectively by the five-dimensional unit vector $\hat{\boldsymbol{R}}$. The five angles are taken to be three Euler angles specifying the orientation of the triangle with the three particles at the vertices and two additional angles. The set given by Fedorov and Jensen [11] is used here, although, because only S waves are considered, the three Euler angles factor out and can be ignored. Then it is supposed that $\hat{\boldsymbol{R}}$ represents the direction specified by the two remaining angles. If r_i, $i=1,2,3$ is the relative coordinate of any two particles and $\sqrt{3}s_i/2$ is the coordinate of the third particle relative to midpoint $r_i/2$, then we set $r_i=R\sin\alpha_i$ and $s_i=R\cos\alpha_i$. Any two of the angles α_i can be used to determine $\hat{\boldsymbol{R}}$, although it is convenient to employ all three even though one is redundent.

In these coordinates, the arbitrary mass parameter μ in the definition of R,

$$\mu R^2 = m r_i^2 + m s_i^2,$$

where m is the reduced mass of any pair of particles, is set equal to m. For simplicity, it is supposed that all lengths are scaled so that $\mu=1$.

The angular functions are taken to be

$$S(\nu,\hat{\boldsymbol{R}}) = \sum_{i=1}^{3} \frac{\sin\nu(\pi/2-\alpha_i)}{\sin\alpha_i\cos\alpha_i}. \tag{1}$$

These functions are simply solutions to the angular part of the three-particle Schrödinger equation in hyperspherical coordinates. In Ref. [8] they have been interpreted as Sturmian eigenfunctions in the sense that they satisfy the ZRP boundary conditions at specific values of $R/a=\rho(\nu)/a$—i.e., the Sturmian eigenvalues:

$$\frac{\rho(\nu)}{a} = \frac{\nu\cos(\nu\pi/2) - (8/\sqrt{3})\sin(\nu\pi/6)}{\sin(\nu\pi/2)}. \tag{2}$$

The radial function is $R^{-2}K_\nu(\mathcal{K}R)$, where $K_\nu(\mathcal{K}R)$ is the modified Bessel function with $\mathcal{K}=\sqrt{-2E}$. The product $S(\nu,\hat{\boldsymbol{R}})R^{-2}K_\nu(\mathcal{K}R)$ is thereby a solution of the three-particle Schrödinger equation with $E=-2\mathcal{K}^2$.

The product solution satisfies the Schrödinger equation but does not satisfy the zero-range boundary conditions at $r_i=0$, $i=1,2,3$. In order to satisfy those conditions a general solution of the form

$$\psi(\boldsymbol{R}) = R^{-2}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} A(\nu)S(\nu,\hat{\boldsymbol{R}})K_\nu(\mathcal{K}R)\nu d\nu, \tag{3}$$

where $0<c<1$ is a positive constant, is used. The expression has the form of a Kontorovich-Lebedev transform [12], a feature that has been used previously [8], but plays no role in the present application.

The expression in Eq. (3) is a solution only if the integral converges, $A(\nu)$ has no singularities on the strip $0<\mathrm{Re}(\nu)\leqslant 2$, and $A(\nu)$ satisfies the three-term reccurence relations [8]

$$[\nu+1+b(\nu+1)]A(\nu+1) + [\nu-1+b(\nu-1)]A(\nu-1) = \frac{2\nu}{\mathcal{K}a}A(\nu), \tag{4}$$

where

$$b(\nu) = -\frac{8}{\sqrt{3}}\frac{\sin\nu\pi/6}{\cos\nu\pi/2}. \tag{5}$$

The absence of singularities in $A(\nu)$ on the strip $0<\mathrm{Re}(\nu)\leqslant 2$ is required in order to shift the contour ± 1 unit in the derivation of Eq. (4).

For the special case that $\mathcal{K}\to 0$ the Bessel function becomes $\frac{1}{2}\Gamma(\nu)(\frac{1}{2}\mathcal{K}R)^{-\nu}$ and Eq. (4) becomes a Barnes-type integral representation

$$\psi(\boldsymbol{R}) = R^{-2}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} C(\nu)\Gamma(\nu)(R/a)^{-\nu}S(\nu,\hat{\boldsymbol{R}})d\nu. \tag{6}$$

The amplitude $A(\nu)$ becomes

$$C(\nu) = \lim_{\mathcal{K}\to 0} A(\nu)\frac{1}{2}\left(\frac{\mathcal{K}a}{2}\right)^{-\nu}\nu, \tag{7}$$

where $C(\nu)$ satisfies the two-term recurrence relation

$$C(\nu-1)=\frac{\nu-1}{\nu-1+b(\nu-1)}C(\nu), \tag{8}$$

which is solved in closed form in the next section. Note that for the special case $\mathcal{K}=0$ the contour is only shifted by +1 unit in the derivation of the two-term recurrence relation. In this case one can take $c=0^+$ and there must be no singularities of $[\nu+b(\nu)]C(\nu)$ on the smaller strip $0<\mathrm{Re}(\nu)\leqslant 1$.

III. COMPUTATION OF EXPANSION COEFFICIENTS

If the quantity $b(\nu)$ in Eq. (8) were a constant, then the two-term recurrence relation would be trivially solved in terms of the ratio of Γ functions—namely, $C(\nu)\to\Gamma(\nu+b)/\Gamma(\nu)$. The quantity $b(\nu)$ is, however, not a constant, but is a periodic function with period 6—i.e., $b(\nu+6)=b(\nu)$.

When $b(\nu)$ is a periodic function with period k it is useful to generalize the definition of the Γ function according to

$$\Gamma_k(\nu+1,b)=[\nu+b(\nu)]\Gamma_k(\nu,b). \tag{9}$$

The properties of this periodic Γ function are discussed in the Appendix. There it is shown that the periodic Γ function can be written as a product of ordinary Γ functions [see Eq. (A5)].

In terms of this new function $C(\nu)$ is simply

$$C^{(1)}(\nu)=\frac{\Gamma_6(\nu,b)}{\Gamma(\nu)}, \tag{10}$$

aside from a multiplicative periodic function with period 1. The periodic function must be chosen so that ψ of Eq. (3) satisfies physical boundary conditions and $C(\nu)$ has no singularities on the strip $0<\nu\leqslant 1$.

It is readily apparent from Eq. (5) that $C^{(1)}(\nu)$ has essential singularities where $\cos\nu\pi/2$ vanishes. The singularities of $C^{(1)}(\nu)$ are illustrated in Fig. 1(a). In this figure the function is plotted at values of ν slightly shifted into the complex plane. This smooths out the poles; however, essential singularities still appear.

It is necessary to eliminate these singularities by multiplying by a periodic function. As the periodic function we use a product of Γ functions similar to those that are used to construct $\Gamma_6(\nu,b)$. If the argument ν is replaced by a constant p, the resulting function is periodic and has singularities similar to those of $\Gamma_6(\nu,b)$. The function, thus obtained, is called $N_6(p,b(\nu))$:

$$N_6(p,b(\nu))=\Gamma(p/6)^{-6}\prod_{i=0}^{5}\Gamma\left(\frac{p+b(\nu+i)}{6}\right), \tag{11}$$

where the function has been normalized to unity as $\nu\to\pm i\infty$. With the choice $p=3$ the ratio $\Gamma_6(\nu,b)/N_6(3,b(\nu))$ has no essential singularities on the interval $-2<\nu\leqslant 2$; thus, we take for the coefficient

$$C^{(2)}(\nu)=\frac{\Gamma_6(\nu,b)}{\Gamma(\nu)N_6(3,b(\nu))}. \tag{12}$$

This coefficient now has no essential singularities on the strip $0<\mathrm{Re}(\nu)\leqslant 2$; however, it does have an infinite number of poles on the real ν axis. This is illustrated in Fig. 1(b), where $C^{(2)}(\nu)$ slightly shifted away from the real axis is plotted. The smoothed-out poles are still evident. On the strip $0<\nu\leqslant 2$ these poles are at $\nu=\nu_j-m$ where ν_j is a root of the equation $\nu+b(\nu)=0$ and m is a positive or negative integer.

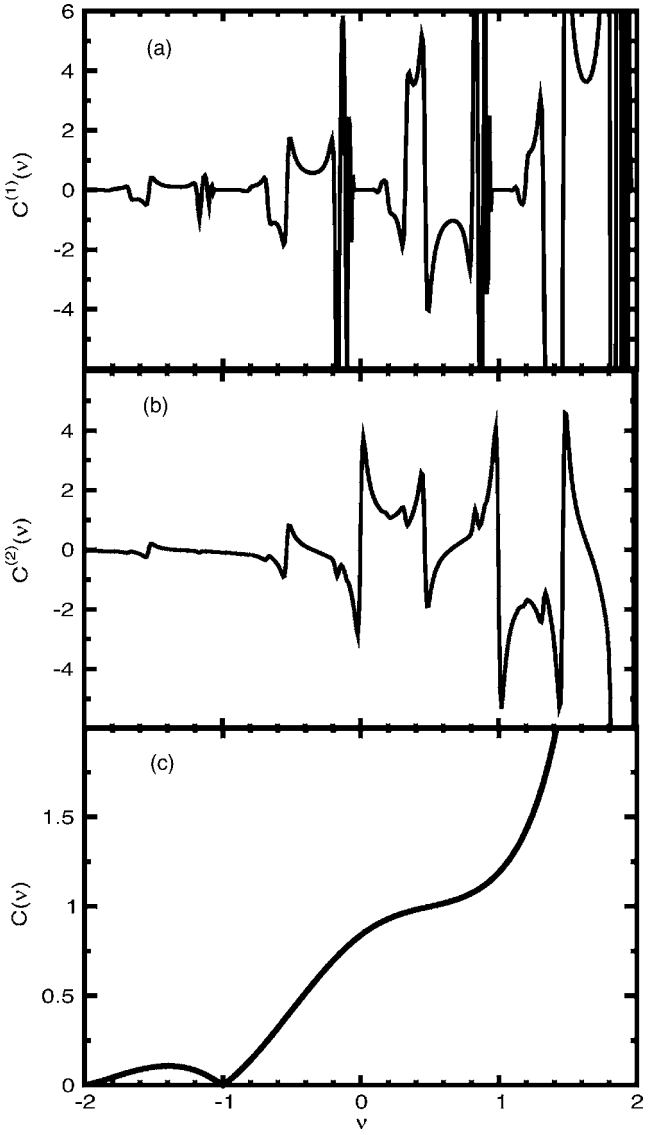

FIG. 1. Plots of (a) $C^{(1)}(\nu)$ and (b) $C^{(2)}(\nu)$ vs $\mathrm{Re}(\nu)$ for $\nu=\mathrm{Re}(\nu)+0.1i$ showing the singularities of these two coefficients. The coefficient $C(\nu)$ on the real axis (c) is seen to be smooth on the interval $-2\leqslant\nu<2$ with a pole at $\nu=2$.

The roots ν_j come in pairs since both ν_j and $-\nu_j$ are roots. Those with positive real parts are labeled ν_j, $j=1,\ldots$. There is also one pair of purely imaginary roots at $\nu=\pm it_0$ where $t_0=1.006\,237\,825\ldots$. It is convenient to define the root $\nu_0=+it_0$. Now the poles of $C^{(2)}(\nu)$ on the positive real axis and at ν_0 can be eliminated by multiplying by the periodic function $\Pi_{j=0}^{\infty}\sin\pi(\nu-\nu_j)$, but the coefficient thus obtained does not give a convergent integral along the imaginary axis owing to the exponential divergence of $\sin\pi(\nu-\nu_j)$ as $\nu\to\pm i\infty$. This divergence can be remedied by multiplying by yet another periodic function $\Pi_{j=1}^{\infty}1/\sin\pi(\nu-d_j)$, with appropriately chosen d_j.

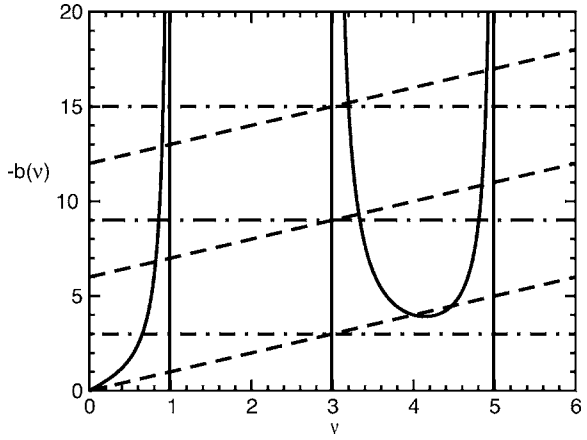

FIG. 2. Plot of $-b(\nu)$ (solid lines) and the functions $f_n(\nu)=6n+3$ (dot-dashed lines) and $g_n(\nu)=\nu+6n$ (dashed lines), $n=0,1,2,\ldots$, vs ν on the interval $0<\nu<6$. The curves $f_n(\nu)$, $n\geqslant 1$, intersect with $-b(\nu)$ at d_j and the curves $g_n(\nu)$ intersect at ν_j. The curve $g_0(\nu)=\nu$ intersects at two real points and at the imaginary points $\pm it_0$. The curve $f_0(\nu)=3$ intersects at one real point on the interval $0<\nu<1$, but at two imaginary points on the interval $3<\mathrm{Re}(\nu)<5$.

In order that this final $C(\nu)$ not have poles at d_j it is necessary that $\sin\pi(\nu-d_j)$ vanish only at the points where $N_6(3,b(\nu))$ has poles—i.e., where $3+b(\nu)=-6n$. Thus the d_j are solutions of the equation

$$3+b(d_j)=-6n, \tag{13}$$

where n is a positive integer. For later reference it is useful to note that Eq. (13) can be written as a cubic equation in the quantity $x=e^{i\pi\nu/3}$:

$$(x^3+1)+\frac{8i}{3\sqrt{3}(1+2n)}(x^2-x)=0. \tag{14}$$

Because the product of the three roots of Eq. (14) must equal the constant term—i.e., unity—it follows that the sum of the three d_j's for a given n must sum up to $6q$ where q is an integer. This property is used later to simplify the elastic scattering phase shift.

Since only one of the complex roots of $\nu+b(\nu)=0$ is taken, the roots ν_j and d_j are matched one for one, as illustrated in Fig. 2 where the function $-b(\nu)$ is plotted on the interval $0\leqslant\nu\leqslant 6$. Also plotted are the constant lines $f(\nu)=6n+3$, $n=0,1,2\ldots$, which intersect with $b(\nu)$ at $\nu=d_j$, and the sloping lines $f(\nu)=6n+\nu$, which intersect with $b(\nu)$ at $\nu=\nu_j$. This figure shows that the first root ν_0 of $\nu+b(\nu)=0$ is complex, while two roots of $3+b(\nu)=0$ are complex. For sufficiently large n it is apparent that there is a root d_j for each ν_j and that $d_j\to\nu_j$ as $n\to\infty$. The one-for-one matching of the roots means that $\lim_{\nu\to\pm i\infty}P(\nu)=1$, as is required to obtain a convergent integral.

The removal of the poles is accomplished by the choice of ν_j and d_j in the periodic function $P(\nu)$ given by

$$P(\nu)=\prod_{j=0}^{\infty}\frac{\sin\pi(\nu-\nu_j)}{\sin\pi(\nu-d_j)}. \tag{15}$$

The resulting $C(\nu)$,

$$C(\nu)=\frac{\Gamma_6(\nu,b)}{\Gamma(\nu)N_6(3,b(\nu))}P(\nu), \tag{16}$$

is a smooth function of ν on the real axis for $-2<\nu<2$ as shown in Fig. 1(c). It is also analytic on the strip $0<\mathrm{Re}\,\nu<2$ and has poles on the boundary of this region at $\nu=-\nu_0=-it_0$ and $\nu=2$. The poles at complex ν play an important role in selecting the renormalization constant, as will be shown in the next sections.

IV. PHASE SHIFT

A. Evaluation of the wave function at large R

The final suitable expression for $C(\nu)$ is used in the Barnes-type integral representation of Eq. (6) to write an exact solution of the three-body Schrödinger equation at zero energy—namely,

$$\psi=\frac{1}{R^2}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}C(\nu)\Gamma(\nu)S(\nu,\hat{\boldsymbol{R}})R^{-\nu}d\nu. \tag{17}$$

The integral may be evaluated for large R by the method of stationary phase. For this purpose we consider just one term in the Sturmian function and represent it generically as $\sin\nu(\pi/2-\alpha)/(\sin\alpha\cos\alpha)$.

At large R only large values of ν contribute significantly. For large, purely imaginary, ν the coefficient $C(\nu)$ becomes

$$\lim_{\nu\to\pm i\infty}C(\nu)=\exp\left[\pm i\pi\sum_{j=0}^{\infty}(\nu_j-d_j)\right]. \tag{18}$$

Since the sum over d_j is an even integer, the sum over d_j could be omitted. Because ν_j approaches d_j rapidly as j becomes large, this term is retained in the calculations. The term with $\nu_0=it_0$ gives the magnitude of $C(\nu)$, namely $\exp(\mp\pi t_0)$. The remaining phase on the right hand side of Eq. (18) is defined as δ_∞:

$$\delta_\infty=-\pi\lim_{m\to\infty}\sum_{j=1}^{6m-1}(\nu_j-d_j)+\pi d_0. \tag{19}$$

The actual calculations of δ_∞ stop at finite values of $6m$ of the order of 10^4.

The stationary phase evaluation is now easily carried out. Since there are two points of stationary phase, one for positive values of $-i\nu$ and one for negative values, we find that

$$\psi\to-\frac{e^{-r/a}}{2ir}\left(e^{\pi t_0}\frac{e^{i(\delta_\infty+s/a)}}{s}-e^{-\pi t_0}\frac{e^{-i(\delta_\infty+s/a)}}{s}\right), \tag{20}$$

where we have used $R\cos\alpha=s$ and $R\sin\alpha=r$.

Note that this wave function represents a diboson bound state with energy $-1/2a^2$ and a third particle moving freely with respect to the diboson at an energy of $1/2a^2$ so that the total energy is indeed equal to zero. Even so, it is apparent

that the function ψ does not have the correct asymptotic form to describe elastic scattering; however, the correct form can always be obtained by combining the function and its complex conjugate. This will be done after the behavior at small R is extracted.

B. Wave function at small R

The Barnes-type integral can be evaluated exactly by closing the integration contour around the circle at infinity in the left half plane, where $\Gamma_6(\nu,b)$ is small except at its poles. In this case one obtains a sum over terms in ascending powers of R and at small R the dominant term comes from the pole at $\nu=-it_0$. The contribution from this pole is

$$\psi \approx (R/a)^{it_0-2}\,\mathrm{Res}[C(-it_0)]\Gamma(-it_0)S(-it_0,\hat{\boldsymbol{R}})$$
$$= e^{i\Delta(R)}(R/a)^{-2}|\mathrm{Res}[C(-it_0)]\Gamma(-it_0)|S(-it_0,\hat{\boldsymbol{R}}), \quad (21)$$

where $\mathrm{Res}[C(-it_0)]$ denotes the residue of $C(\nu)$ at $\nu=-it_0$, $\Delta(R)$ is the phase

$$\Delta(R) = \delta_0 + t_0 \ln(R/a), \quad (22)$$

and δ_0 is the phase of $\mathrm{Res}[C(-it_0)]\Gamma(-it_0)$.

The function $R^2\psi$ has a divergent phase at the origin, consistent with the Thomas effect [13,14]. To use the ZRP model for predictive purposes it is necessary to renormalize the function to remove this divergence.

The renormalization is accomplished by noting that the complex conjugate function ψ^* is also a solution, so that a linear combination of ψ and ψ^* which vanishes as some small value of $R=R_0$ can be formed. The value of R_0 is not known *a priori* and must be chosen by some criteria such that the ZRP model is physically realistic. One choice will be discussed below.

Since $iS(-it_0,\hat{\boldsymbol{R}})$ is real, the function that vanishes at R_0 is

$$\Psi = \frac{1}{2}(e^{-i\Delta(R_0)}\psi + e^{i\Delta(R_0)}\psi^*). \quad (23)$$

The asymptotic form of Ψ gives the phase shift at $E=0$—namely,

$$\delta = \delta_\infty - \Delta(R_0) + \arctan\frac{e^{-2\pi t_0}\sin 2\Delta(R_0)}{1+e^{-2\pi t_0}\cos 2\Delta(R_0)}. \quad (24)$$

Equation (24) together with Eqs. (18) and (22) represents a completely analytic result for the elastic scattering phase shift at zero energy.

The renormalization constant R_0 is identified as the radius of a hard-core three-body potential since the wave function vanishes on the hypersurface $R=R_0$. The value of R_0 is chosen so that the renormalized phase matches a measured phase or the phase computed using realistic two-body potentials. Once this constant is chosen other physical quantities can be computed in the low-energy region using the ZRP model.

The renormalization is seen to affect the phase shift by subtracting a term that diverges as $R_0\to 0$ and adding a small term that oscillates with R_0. The effect of this small term is shown in Fig. 3(a) where $\delta(R_0)+t_0\ln(R_0/a)$ is plotted versus R_0/a. The phase is nearly constant except for a small oscillation with amplitude $e^{-2\pi t_0}\approx 1.8\times 10^{-3}$. Figure 3(b) shows the small oscillation on a finer scale.

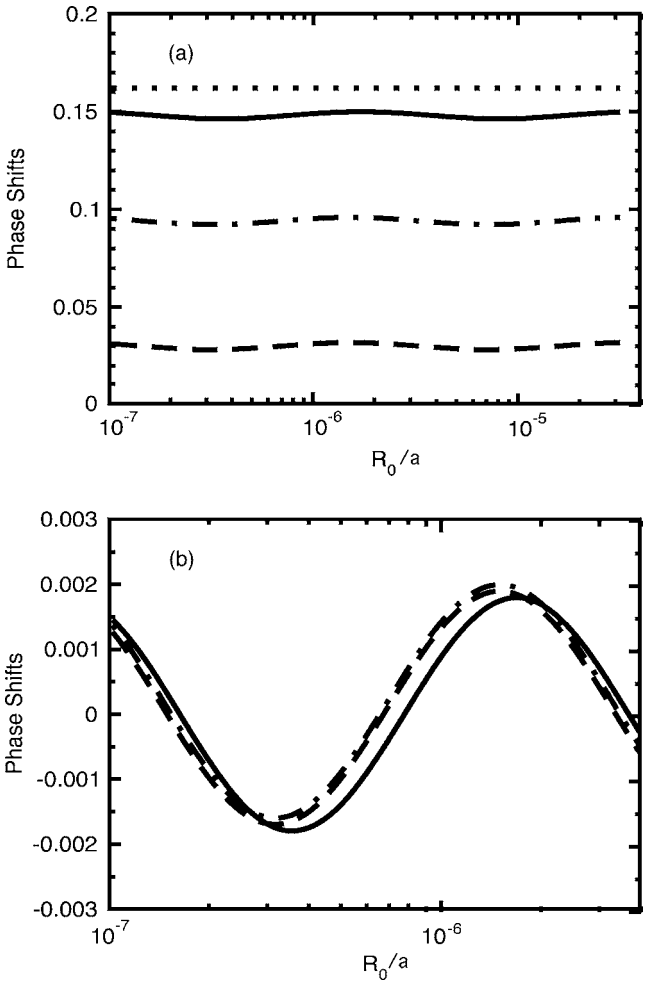

FIG. 3. Plot of the phase shifts $\delta+t_0\log(R_0/a)$ vs R_0/a. (a) The solid curve is the exact result, the dashed curve is the one-channel close-coupling result, and the dot-dashed curve is the adiabatic phase. The adiabatic phase in the WKB approximation is shown as the dotted curve. In (b) the curves are shown on a finer scale and moved to a common zero to compare the small oscillations in different approximations.

If this small oscillation is ignored, then extracting the term $t_0\ln(R_0/a)$ gives an elastic scattering phase that is essentially equal to $\delta_\infty-\delta_0$. In general, however, the small oscillation should not be ignored and the elastic scattering phase is taken to be $\delta(R_0)$ of Eq. (24) with R_0 chosen so that the phase matches an experimental value at precisely zero energy.

A similar form for the elastic scattering phase shift was obtained by Efimov in a model that considers a wave incident at small R on an attractive $(-t_0^2-1/4)/(2R^2)$ hyperradial effective potential. This potential is cut off at $R\approx a\sqrt{t_0^2+1/4}$ after which it becomes a constant equal to the energy eigenvalue $-1/(2a^2)$ of the two-body dimer. The wave at the origin is reflected with amplitude s_{11} and transmitted with amplitude s_{12}. The logarithmic derivative of the wave at R_0 is a parameter of the model. This model connects with our exact result if we set

$$s_{11} = e^{-2\pi t_0} e^{-i2\delta_0},$$

$$s_{12} = \sqrt{1 - e^{-4\pi t_0}} e^{i\delta_\infty - i\delta_0}, \tag{25}$$

and introduce the renormalizing phase θ:

$$\theta = -t_0 \ln(R/a) + \pi/2, \tag{26}$$

where the factor of $\pi/2$ emerges because the logarithmic derivative in our model becomes infinite, corresponding to a wave that vanishes at R_0. Of course we could use alternative boundary conditions at R_0; however, $\Psi(R_0, \hat{\mathbf{R}}) = 0$ is chosen because the adiabatic hyperradial potential always has a hard-core $1/R^2$ barrier equal to $(4-1/4)/(2R^2)$ for any realistic two-body or three-body interaction which is less singular than $1/r^2$ at the origin [18]. For such hard cores, the low-energy wave function sensibly vanishes as R^2 near $R \approx 0$. In any event, the form we obtain agrees exactly with the form given in Ref. [7].

The phase shift at zero energy has also been computed exactly using effective field theory [4,6]. The phase shift is found to be $\delta = t_0 \log(a\Lambda_*) + 1.94$, where Λ_* is a renormalization constant in momentum space. To connect with our result one need only note that a conjugate renormalization constant with dimensions of length is obviously $R_* = 1/\Lambda_*$ up to a dimensionless multiplicative constant. This has the same form as our result if small terms of order $e^{-2\pi t_0} \approx 1.8 \times 10^{-3}$ are neglected.

C. Checks

Because the zero-energy solutions that we have found are unusual in that they are exact solutions of a nontrivial three-body problem that can be used to explore the renomalization consants, it is useful to check the results as throughly as possible. We have done this by verifying that a simple Wronskian relation is satisfied by our solution and by comparing the exact phase with approximate calculations that provide bounds on the exact values.

1. Hyperspherical Wronskian relation

Wronskian relations are standard properties of solutions to one-dimensional second-order differential equations and have long been used to relate properties of wave functions at small distances to asymptotic properties and, e.g., are familiar in the context of the Jost function formulation of collisions and spectra [16]. Their use with multiparticle systems is less familiar; thus, a brief derivation for any number N of particles [17] is given and applied to the exact wave function of Eq. (6) with Eq. (16).

Multiparticle Wronskian relations are most readily formulated in hyperspherical coordinates, since these coordinates employ one coordinate R with dimensions of length. All other coordinates called hyperangles $\hat{\mathbf{R}}$ are dimensionless and are defined on finite intervals. More importantly, the Schrödinger equation has no cross derivatives involving R and the hyperangles. In these coordinates the free-particle Hamiltonian is the sum of a hyperradial kinetic energy operator T_R and an angular part $H_{\hat{R}}$, equal to the generalized angular momentum operator divided by $2R^2$, so that [17]

$$H = T_R + H_{\hat{R}} \tag{27}$$

and all derivatives with respect to R are confined to T_R in the coordinate representation of H.

If $R^{-(3N-4)/2}\phi_1$ and $R^{-(3N-4)/2}\phi_2$ are two solutions of the Schrödinger equation for the same total energy E, then the multiparticle Wronskian relation is

$$W(\psi_1, \psi_2) = \int \left(\frac{\partial \phi_1}{\partial R} \phi_2 - \phi_1 \frac{\partial \phi_2}{\partial R} \right) d\hat{\mathbf{R}} = \text{const}, \tag{28}$$

where we have used that

$$\int \phi_1 H_{\hat{R}} \phi_2 d\hat{\mathbf{R}} = \int \phi_2 H_{\hat{R}} \phi_1 d\hat{\mathbf{R}}. \tag{29}$$

In the present case, the Wronskian is evaluated with the function $R^{5/2}\psi$ of Eq. (6) and the linearly independent function $R^{5/2}\psi^*$ at large and small values of R. At large R use of $R^{5/2}\psi$ and $R^{5/1}\psi^*$ from Eq. (20) in Eq. (28) gives the simple result

$$W = i\frac{3}{2} \sinh 2\pi t_0 = i3 \sinh \pi t_0 \cosh \pi t_0. \tag{30}$$

Alternatively, evaluation of W at small R using Eq. (22) gives

$$W = 2it_0 |\text{Res}[C(-it_0)]\Gamma(-it_0)|^2 \int |S(it_0, \hat{\mathbf{R}})|^2 d\hat{\mathbf{R}}, \tag{31}$$

where $\text{Res}[C(-it_0)]$ may be written explicitly as

$$\text{Res}[C(-it_0)] = \frac{\Gamma_6(1-it_0, b)}{N_6(3, -it_0)\Gamma(-it_0)} \cdot \frac{1}{\left. \frac{d[\nu + b(\nu)]}{d\nu} \right|_{\nu=-it_0}}. \tag{32}$$

The integral over angular coordinates has been evaluated by Kartavtsev [15] in another context. In our notation his result is

$$\int |S(it_0, \hat{\mathbf{R}})|^2 d\hat{\mathbf{R}} = -3i \sinh \pi t_0 \left. \frac{d[\nu + b(\nu)]}{2\nu d\nu} \right|_{\nu=-it_0}. \tag{33}$$

Using Eqs. (30) and (31) in Eq. (31) gives a second, completely analytic expression for W—namely,

$$W = -\frac{i3 \sinh \pi t_0}{\left. \frac{d[\nu + b(\nu)]}{d\nu} \right|_{\nu=it_0}} \left| \frac{\Gamma_6(1-it_0, b) P(-it_0)}{N_6(3, b(-it_0))} \right|^2. \tag{34}$$

The Wronskian relation requires that these two values be identical; indeed, it should be possible to transform Eq. (34) into the simple expression of Eq. (30). We have not been able to do this, but numerical evaluation of both expressions shows that they are identical to ten significant figures, which

is near the limit of accuracy of the calculations. Thus, the exact solution given by Eq. (6) is in accordance with the multiparticle Wronskian relation.

2. Comparison with adiabatic and one-channel phases

A second check on our exact solution is to compare it with other, more standard computations. The hyperspherical close coupling method provides such a check. In this case the exact wave function is approximated by an expansion in the hyperspherical adiabatic basis set. It is known that if only one term is employed the resulting approximate phase is a lower bound to the exact phase shift [18,19].

The adiabatic potential energy curves $U_j(R)$ are easily computed from the single Sturmian eigenvalue $\rho(\nu)$ of Eq. (2). The adiabatic and Sturmian eigenvalues are related according to

$$U_j(R) = \frac{\nu_j^2(R) - 1/4}{2R^2}, \tag{35}$$

where $\nu_j(R)$ is a solution of the equation

$$\rho(\nu) = R. \tag{36}$$

Because $\rho(\nu)$ is a cot-like function, it has an infinite number of branches for $-\infty < \nu^2 < \infty$; thus, there are an infinite number of roots ν_j of Eq. (36). The root $\nu_0(R)$ is equal to $\nu_0 = it_0$ in the limit $R \to 0$ and becomes equal to $\nu_0(R) = iR/a$ in the limit that $R \to \infty$. The $1/R^2$ singularity at the origin is consistent with the Thomas effect, while the large-R limit ensures that this channel corresponds to elastic scattering from the bound diboson state.

The one-channel HCC method requires the second derivative diagonal term $Q_{0,0}$ which adds to the adiabatic potential $U_0(R)$. Analytic expressions for $Q_{0,0}(R)$ are given in Refs. [15]. The one-channel close-coupling (HCC) phase has been computed using the potential $U_0(R)$ and the diagonal nonadiabatic derivative matrix $Q_{0,0}(R)$ for the lowest adiabatic state.

To obtain finite phases it is necessary to replace $U_0(R)$ by a hard-core hyperradial potential for $R < R_0$ to regularize the solution. The one-channel HCC equation is then solved numerically to obtain the phase shift $\delta^{(1)}(R_0/a)$. The resulting phase varies with R_0/a as $-t_0 \ln(R_0/a)$. The dashed line in Fig. 3 shows $\delta^{(1)} + t_0 \ln(R_0/a)$ vs R_0/a. As expected it lies below the exact phase.

The one-channel HCC phase shows the same oscillation with R_0 seen in the exact phase. This slight oscillation, shown on a finer scale in Fig. 3(b), allows us to find approximate values for δ_∞ and δ_0. The phase $\delta_0^{(1)}$ is found by fitting the small oscillations to the expression $\arctan[e^{-2\pi t_0} \sin 2\Delta^{(1)}(R_0)]/[1 + e^{-2\pi t_0} \cos 2\Delta^{(1)}(R_0)]$, where $\Delta^{(1)} \times (R_0/a) = \delta_0^{(1)} + t_0 \ln(R_0/a)$. The phase $\delta_\infty^{(1)}$ is then found by computing $\delta_\infty^{(1)} = \delta^{(1)} + \Delta^{(1)}(R_0/a)$. These values are shown in Table I, together with the exact results.

The adiabatic phase—i.e., the phase obtained when the diagonal derivative matrix element $Q_{0,0}(R)$ is omitted in the one-channel HCC equation—is shown as the dot-dashed curve in Fig. 3. Spruch [20] has shown that this approximate phase is an upper bound to the exact phase when the two-body interactions are given by well-behaved local potentials. It is apparent that the adiabatic phase in the present case is not an upper bound to the exact phase. This does not contradict the bound theorem, since our two-body potentials are replaced by ZRP boundary conditions and an explicit infinite three-body potential at small R has been introduced.

TABLE I. Computed phases δ_∞ and δ_0 in three approximations compared with the exact values.

Approximation	δ_∞	δ_0	$\delta_\infty - \delta_0$
Exact	1.736	1.588	0.148
One-channel HCC	1.734	1.703	0.031
Adiabatic	1.795	1.702	0.093
EFT [6]	1.75		
WKB adiabatic			0.1623

The WKB adiabatic phase plus $t_0 \ln(R_0/a)$ is also shown in Fig. 3 since the small oscillatory term is absent in this approximation. Remarkably, this phase is quite close to $\delta_\infty - \delta_0$. Since there is no explanation for this good agreement, it must be regarded as accidental.

Using the fitting procedure described above we have extracted the two phases $\delta_\infty^{(\mathrm{ad})}$ and $\delta_0^{(\mathrm{ad})}$ given in Table I. It appears that δ_∞ is bounded by the two approximate phases, as would be the case for well-behaved two-body potentials, where δ_0 vanishes because both the regular and irregular functions are real near $R \approx 0$ and the factors $\exp(\pm \pi t_0)$ are replaced by ± 1 at large R.

As a further check on the phase we note that the lower bound is variational, but the upper bound is not. This means that the error in the lower bound is quadratic in the error in ψ, but that the error in the upper bound is linear in the error in ψ. If the error in the lower bound for δ_∞ is Δ^2, then the error in the upper bound should be of order 2Δ. It follows that, to first approximation, the difference between the adiabatic and one-channel HCC results for δ_∞ is of the order of $2\Delta = 0.061$ while the error in the one-channel HCC is of the order of $\Delta^2 \approx 0.001$. These error estimates are in qualitative agreement with the entries in Table I; i.e., the variational lower bound is much closer to the exact result than is the nonvariational upper bound.

It must be emphasized that the proportionality constants in the error estimates are not known. In addition, there is no rigorous basis for using these estimates with δ_∞ rather than $\delta(R_0)$. For this reason the phase comparison check is only reliable for verifying that $\delta^{(1)}(R_0)$ is a lower bound to the exact phase. Even here it is understood that the bounds are on the absolute phase, whereas the computed and exact phases have been extracted from the asymptotic function and are therefore known only modulo π. It is important, however, to note that the small oscillations are present in the exact result and both one-channel approximations as shown in Fig. 3. They are possibly a general feature of phase shifts for potentials with sufficiently strong $-1/R^2$ singularities as suggested by Efimov's analysis [7].

Our renormalization constant R_0 has a direct physical interpretation as the radius of a hard-core three-body potential. In the work of Refs. [4–6] a similar, but not necessarily identical, renormalization constant emerges. In that work accurate results are obtained by numerical solutions of integral equations and are, in principle, exact in the sense that physical quantities can be computed as accurately as desired given sufficient computational resources.

As discussed in Sec. IV B, the constant Λ_* of Ref. [4] is a momentum and is therefore conjugate to a length R_*. It appears that our R_0 is proportional to R_* up to terms of the order of $e^{-2\pi}\approx 1.8\times 10^{-3}$. If the small oscillatory terms are ignored, one finds $R_*=6.0R_0$, but owing to the small oscillatory term that appears in our exact phase, the renormalization constants may not be exactly proportional. Even so, the functional dependences of the phases on R_* and R_0 are very nearly identical even though the phases are obtained using completely different, essentially exact, methods. The main differences, besides the methods used, are that our results are limited to zero energy but the elastic scattering phase is given in closed form so that an additional small oscillatory term is identified.

With the interpretation of the phase shift given by Eq. (27) and the relation between R_* and R_0 it is possible to extract a phase δ_∞ from the effective field theory results given in Ref. 6. The difference in the phases γ_0 given in Eqs. (224) and γ in Eq. (227) of that paper is just our δ_∞. Using the explicit values at zero energy, namely $\gamma_0=1.94$ and $\gamma=0.19$, we obtain the value of $\delta_\infty=1.75$ given as the EFT result in Table I. This number is exact within numerical errors and agrees very well with ours to the precision of the computed values.

The exact solution in the relatively simple analytic form obtained here is specific to the energy $E=0$. At $E\neq 0$ it is always possible to solve the three-term recurrence relation (4) numerically. Then a periodic function such that $A(\nu)\cos \pi\nu/2$ has no singularities on the strip $0<\mathrm{Re}(\nu)\leqslant 2$ must be constructed. Because the interval has length 2 rather than 1, two independent solutions of three-term recurrence relations [8] are employed. A full description of the procedure is beyond the scope of the present report, although the zero-energy solutions provides a useful guide for the steps needed to find solutions at $E\neq 0$.

The zero-energy solutions may also be used to find solutions at nonzero energies in terms of power series in $(Ka)^2$. This is accomplished by setting

$$A(\nu)=K^\nu C(\nu)\tilde{A}(\nu,(Ka)^2), \tag{37}$$

where $\tilde{A}(\nu,(Ka)^2)$ is expanded in a power series in $(Ka)^2$. Again, the details of such calculations are beyond the scope of the present report. The important point here is that the analytic form for the zero-energy solution—namely, $C(\nu)$—plays a central role.

V. SUMMARY

We have obtained an exact solution for the zero-energy wave function of three particles interacting via zero-range potentials with positive scattering length. The solution is given in the form of a Barnes integral which is shown to diverge as R^{it_0} for small R_0. An acceptable solution is found by forming a linear combination that vanishes exactly at $R=R_0$, equivalent to modifying the original system by adding an explicitly three-body hard-core potential. The phase shift for elastic boson diboson scattering at zero energy is obtained and its dependence upon R_0 exhibited explicitly. The constant R_0 is interpreted as a renormalization constant and can be chosen to match observed or computed zero-energy phase shifts. With the chosen value for R_0, other properties of the system can be computed.

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APPENDIX: A PERIODIC Γ FUNCTION

The usual gamma function $\Gamma(\nu)$ is a solution of the defining equation

$$\Gamma(\nu)=(\nu-1)\Gamma(\nu-1).$$

Many generalizations of this function are employed in the mathematical literature [21]; however, the generalization that emerges naturally in the present application does not appear in any standard references.

Our periodic gamma function $\Gamma_n(z,b)$ is defined as a solution of the recurrence relation

$$\Gamma_n(z,b)=[z-1+b(z-1)]\Gamma_n(z-1,b), \tag{A1}$$

where $b(z)$ is a function with period n—i.e., $b(z+n)=b(z)$. To express this function in terms of the usual $\Gamma(z)$ first iterate the recurrence relation n times

$$\begin{aligned}\Gamma_n(z,b)&=[z-1+b(z-1)][z-2+b(z-2)]\cdots\\&\quad\times[z-n+b(z-n)]\Gamma_k(z-n,b)\\&=n^n\prod_{k=0}^{n-1}\left(\frac{z+k+b(z+k)}{n}-1\right)\Gamma_k(z-n,b).\end{aligned} \tag{A2}$$

Using the periodicity of $b(z)$, it is simple to show that the expression

$$\Gamma_n(z,b)=Nn^z\prod_{k=0}^{n-1}\Gamma\left(\frac{z+k+b(z+k)}{n}\right) \tag{A3}$$

satisfies the iterated recurrence relation (A2). The constant N is arbitrary, but comparison with Gauss' multiplication formula [22] for the gamma function, namely,

$$\Gamma(z) = (2\pi)^{(1-n)/2} n^{z-1/2} \prod_{k=0}^{n-1} \Gamma\left(\frac{z+k}{n}\right), \tag{A4}$$

shows that if we take $N=(2\pi)^{(1-n)/2}n^{-1/2}$, then $\Gamma_n(z,b)=\Gamma(z+b)$ when b is a constant or, more generally, when $b(z)$ has period 1. Thus we take the definition of the periodic gamma function $\Gamma_n(z,b)$ as

$$\Gamma_n(z,b) = \frac{n^{z-1/2}}{(2\pi)^{(n-1)/2}} \prod_{k=0}^{n-1} \Gamma\left(\frac{z+k+b(z+k)}{n}\right), \tag{A5}$$

where $b(z)$ has period n.

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