

# Exact solution for three particles interacting via zero-range potentials

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Exact solutions for three identical bosons interacting via zero-range  $s$ -wave potentials are derived. The solutions are contour integrals over a product of hyperradial Bessel functions times angular functions weighted by a coefficient. The product function is a solution of the free-particle Schrödinger equation and the weight function is chosen to satisfy the zero-range boundary conditions. Scattering matrix elements for boson-dimer elastic scattering, breakup of a dimer into three particles and the time-reversed recombination process are derived. For vanishing total energy  $E$ , these quantities are given as closed-form functions of the two-body  $s$ -wave scattering length  $a$  and a three-body renormalization constant  $R_0$ . The exact results obtained by this method are compared with those obtained using other methods. Differences in the functional dependence on  $R_0$  of the order of 2% are noted. Comparison with the hidden-crossing theory finds similar agreement with the functional dependence upon  $a$  and  $R_0$ .

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## I. INTRODUCTION

There is considerable theoretical evidence that only two-body  $s$ -wave scattering lengths  $a$  and a second parameter, called a renormalization constant  $R_0$ , are adequate to describe the properties of dilute Bose condensates, threshold three-body recombination, and a class of three-body loosely bound states predicted by Efimov [1]. The role of the renormalization constant is extensively discussed in Refs. [2–7]. There it is shown to enter into the description of three-body interactions as a second scale factor independent of  $a$ . The dependence of physical quantities on  $R_0$  is deduced through fits of exact calculations to relatively simple functional forms involving  $\ln(R_0/a)$ . The functional form is found to be universal, up to small corrections. Properties of real systems are found to be insensitive to details of the interactions, leading to the important prediction that properties of Bose condensates are universal in that systems with identical values of  $a$  and  $R_0$  will exhibit similar properties independently of other details of the two-body interactions. This property is called universality [3,4,8] and it is prospectively an important feature of dilute Bose condensates.

Zero-range models where the scattering length is introduced via boundary conditions [9,10] [see Eq. (1) below] are basic to the theory of two-particles that interact via a constant  $s$ -wave scattering length. When such interactions are employed for three or more particles, it is found that solutions exhibit a nonphysical divergence called the Thomas effect [11] when all three particles are close together. To avoid this divergence a cutoff distance  $R_0$  is introduced.

The role of this cutoff is controversial. Following the demonstration by Danilov [10] that the solutions for three

particles interacting via zero-range potentials are not unique, Ref. [6] concludes that solutions with the Thomas-effect divergence are unphysical and must be excluded. The author further asserts that there remains one physically acceptable solution even after the divergent solutions are deleted. This assertion, however, contradicts our previous result [12,13] where we find an analytic solution for the special case of zero energy and positive scattering length. That exact solution describes elastic boson-diboson scattering and exhibits the Thomas effect. If that solution is eliminated, then there are no solutions representing boson-diboson scattering contrary to the assertion of Ref. [6] that a physically acceptable solution exists. We therefore conclude that for zero-range potentials with constant scattering length the renormalization constant  $R_0$  is needed.

This conclusion follows more generally from the hyperspherical close coupling expansion [14] with zero-range potentials [15]. This theory uses a representation in adiabatic eigenfunctions and potential curves and there one finds that the effective potential for the elastic scattering channel always shows the Thomas effect, i.e., an attractive  $-b/R^2$ ,  $b > \frac{1}{4}$  potential, in the limit that the hyperradius  $R$  vanishes. Furthermore, Kartavtsev [16] shows that this channel is coupled to all other channels, thus all solutions generally exhibit the Thomas effect.

Of course, it is understood that the Thomas effect does not appear when realistic two-body potentials are employed. To model two-body interactions with zero-range interactions more realistically, Fedorov and Jensen [7] allow the effective range parameter  $M(k^2) = k \cot \delta$  to be energy dependent. They then show that with a suitable choice of parameters and the replacement of the two-body kinetic energy  $k^2/2m$  by  $U_n(R)$ , where  $U_n(R)$  is the hyperspherical potential energy eigenvalue for the  $n$ th channel, one obtains channel potentials free of the unphysical  $R^{-2}$  divergence.

The energy-dependent effective ranges do indeed regularize the three-body problem realistically in the adiabatic ap-

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proximation. However, use of an energy-dependent  $M(k^2)$  can only be carried out in the hyperspherical close-coupling formulation since it is necessary to replace  $k^2$  by a local three-body energy that is a function of  $R$ . In this case exact solutions obtained earlier [13] for constant  $M(k^2)$  cannot be employed.

More serious, however, is the problem that the adiabatic basis functions  $\Phi_n(R; \hat{\mathbf{R}})$  are not orthogonal if the boundary conditions are energy dependent. For this reason it is difficult to formulate an exact theory using an energy-dependent  $M(k^2)$ . Since we are interested in exact solutions we use a constant effective range and a constant cutoff  $R_0$  for which exact physical solutions can be found [13].

Zero-range potentials (ZRPs) are good models of actual three-body systems if the scattering length is much larger than the nominal range  $r_0$  of the two-body potential. This is the case for He atoms [4,15,17,18]. With the advent of magnetic tuning [19–21] it is also possible to tune scattering lengths so that  $a \gg r_0$  for a variety of atomic species. For this reason exact computations in the ZRP model are of physical interest.

Because of its wide significance for the description of threshold properties of few-body systems, it is important to understand the constant  $R_0$  as precisely as possible. To advance this end we have solved the three-body zero-range model for positive  $a$  exactly to obtain an expression that gives the dependence of an observable, namely, the phase shift for boson-diboson scattering for total angular momentum and energy equal to zero, on  $R_0$  in closed form. This rather special result is reported in an earlier manuscript [12,13]. There, small corrections of the order of 0.2% to the  $\ln(R_0/a)$  terms were found. These small correction terms add to the dominant  $\ln(R_0/a)$  term but the theory still has the universality property.

In this manuscript we further investigate the interaction of three Bosons of mass  $m$  in the zero-range or shape-independent model by deriving a quadrature solution for nonzero energies still with positive  $a$ . The functional dependence of all scattering matrix elements  $S_{0j}$ , where 0 denotes the diboson bound state with binding energy  $1/(ma^2)$  and  $j$  is any final state label, are deduced.

The two-body ZRPs [22] are defined by the scattering length  $a$  through the relation

$$\left. \frac{1}{r\psi} \frac{\partial(r\psi)}{\partial r} \right|_{r \rightarrow 0} = -1/a. \quad (1)$$

Such potentials can be used to model the asymptotic interactions of the atoms involved in the recombination processes, where the nominal range of the two-body interactions are much smaller than the mean radius of the three-body systems. A comparison between realistic effective potentials obtained using the hyperspherical adiabatic method [23] and those corresponding to ZRP derived using the Sturmian theory [24] has been done for a system of three helium atoms. The comparison shows that both calculations agree within the 17% and even 3% for some symmetries [24]. The ZRPs have been also applied to calculations of the recombination probabilities for three helium atoms using approxi-

mate analytical solutions to the problem [15,25]. These calculations have shown that the ZRP model properly describes some of the transitions occurring in real processes. Some exact numerical solutions of the three-body problem interacting via three ZRPs have been also reported [26]; however, the method applied is not completely familiar to the atomic physics community. One of the main aims of this paper is to present a closed-form solution for the three-body problem where the two-body interaction are given by ZRPs.

In a previous paper the solution of the three-body problem where two of the particles were interacting via ZRP and the third was free [27] was presented, henceforth called the model problem. This paper gives the solution of three interacting particles via ZRPs using the method developed for the three charged particles [28]. In the present case the three-body Schrödinger equation is just the free-particle equation, which is separable, but the ZRPs are represented by nonseparable boundary conditions. As for the model problem, an integral representation of the wave function is introduced to treat the nonseparable boundary conditions.

The Schrödinger equation for a system of three free particles can be solved in many coordinate systems by separation of variables. However, the inclusion of nonseparable boundary conditions is difficult if the appropriate coordinates are not used. We find that hyperspherical coordinates are best adapted to ZRPs. In the center of mass of the system these coordinates are a hyperradius  $R$ , with dimension of length, and five dimensionless angular coordinates  $\hat{\mathbf{R}}$ , namely, the hyperangle  $\alpha$ , a relative angle  $\theta$  between two Jacobi coordinate vectors, and three Euler angles [14]. The momentum  $K$ , conjugate to the hyperradius  $R$ , is given by  $E=K^2/2$  in mass scaled coordinates [25]. The general solution of the Schrödinger equation is a linear combination of products of Bessel functions  $Z_\nu(KR)$  and angular functions  $S_n(\nu, \hat{\mathbf{R}})$ . For general boundary conditions there are no restrictions on  $\nu$  thus the linear combination is, in general, a contour integral over the separation constant  $\nu$ . Thus we write

$$\Psi(R, \hat{\mathbf{R}}) = \frac{1}{R^2} \int_c A(\nu) S(\nu, \hat{\mathbf{R}}) Z_\nu(KR) \nu d\nu. \quad (2)$$

The expression for  $\Psi(R, \hat{\mathbf{R}})$  is a Kontorovich-Lebedev-like [27,29] representation where the integration contour it is not *a priori* defined. The function  $Z_\nu(KR)$  can be any of the Bessel function  $J_\nu(z)$ ,  $H_\nu^{(1,2)}(z)$  or  $K_\nu(z)$  [30], depending on the total energy  $E$ . When the energy is less than zero then the proper function is the  $K_\nu(z)$  and Eq. (2) is the Kontorovich-Lebedev representation. However, for  $E > 0$  more than one contour integral is needed to write the solution with the correct asymptotic behavior and then the representation becomes a generalization of the Kontorovich-Lebedev transform [27].

All of the interesting dynamics of the problem are incorporated in the coefficient  $A(\nu)$ . In Sec. II we show that the boundary conditions lead to a three-term recurrence relation (TTRR) for the coefficient  $A(\nu)$ . There are two linearly independent solutions of the TTRR and their exact asymptotic expressions are easily obtained. By using the asymptotic so-

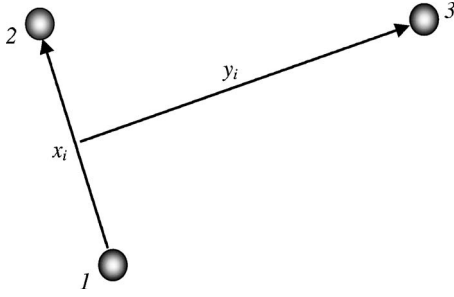


FIG. 1. One of three sets of Jacobi coordinates for three particles. Other sets are obtained by cyclic permutations.

lutions as starting points in the TTRR,  $A(\nu)$  can be evaluated in the entire complex plane of  $\nu$ . The details of how to construct  $A(\nu)$  are given in Sec. III. In Sec. IV we evaluate  $\Psi$  for large  $R$  and in Sec. V for small  $R$ . These two limits are then used to find physical solutions to obtain the elastic scattering  $S$  matrix  $S_{00}$  and the breakup matrix  $S_{R,0}$  in Sec. VI. Analytic results in the limit of zero energy are given in Sec. VII, and are applied to three-body recombination in Sec. VIII. Concluding remarks are given in Sec. IX.

## II. STATEMENT OF THE PROBLEM

The time-independent Schrödinger equation for three free identical particles in mass scaled Jacobi coordinates  $\mathbf{x}_i$  and  $\mathbf{y}_i$  (with  $i=1,2,3$ ) shown in Fig. (1) is

$$\left[ -\frac{1}{2}\nabla_{\mathbf{x}_i}^2 - \frac{1}{2}\nabla_{\mathbf{y}_i}^2 \right] \Psi = E\Psi. \quad (3)$$

As mentioned in the Introduction, the ZRP are included via the boundary condition where the logarithmic derivative of the function ( $x_i\Psi$ ) is fixed by

$$\left[ \frac{\partial(x_i\Psi)}{\partial x_i} + \frac{1}{a}(x_i\Psi) \right]_{x_i \rightarrow 0} = 0, \quad (4)$$

where  $a$  is the scattering length associates with the two-body interactions.

The hyperspherical coordinates are given by the hyperradius  $R = \sqrt{x_i^2 + y_i^2}$ , the hyperangle  $\alpha_i = \arctan(x_i/y_i)$ , and the direction vectors  $\hat{\mathbf{x}}_i$  and  $\hat{\mathbf{y}}_i$  [14]. In these coordinates the Schrödinger Eq. (3) is

$$\left[ \frac{1}{R^5} \frac{\partial}{\partial R} \left( R^5 \frac{\partial}{\partial R} \right) - \frac{\Lambda^2}{R^2} + K^2 \right] \Psi(R, \hat{\mathbf{R}}) = 0, \quad (5)$$

where  $K^2 = 2E$  and the operator  $\Lambda^2$  is defined by

$$\Lambda^2 = -\frac{1}{\sin^2 \alpha_i \cos^2 \alpha_i} \frac{\partial}{\partial \alpha_i} \left( \sin^2 \alpha_i \cos^2 \alpha_i \frac{\partial}{\partial \alpha_i} \right) + \frac{\mathbf{L}_{\mathbf{x}_i}^2}{\sin^2 \alpha_i} + \frac{\mathbf{L}_{\mathbf{y}_i}^2}{\cos^2 \alpha_i}, \quad (6)$$

and  $\mathbf{L}_{\mathbf{x}_i}^2$  and  $\mathbf{L}_{\mathbf{y}_i}^2$  are the angular momenta associated with the coordinates  $\mathbf{x}_i$  and  $\mathbf{y}_i$ . In these coordinates the boundary condition Eq. (4) becomes

$$\left[ \frac{\partial(\alpha_i \Psi)}{\partial \alpha_i} + \frac{R}{a}(\alpha_i \Psi) \right]_{\alpha_i \rightarrow 0} = 0, \quad (7)$$

which are clearly nonseparable in hyperspherical coordinates. In the last equation we replaced  $\sin \alpha_i$  by its small angle limit  $\alpha_i$  to simplify the notation. This change does not modify the boundary conditions on  $\Psi$ .

This work treats the case where the total angular momentum of the system equals zero. The general case can also be solved, but is not considered in the present paper. Even though the total angular momenta  $\mathbf{L}$  equals zero,  $\mathbf{L}_{\mathbf{x}_i}^2$  and  $\mathbf{L}_{\mathbf{y}_i}^2$  could differ from zero.

Equation (5) can be solved by separation of variables where the angular and radial equations are given by

$$[\Lambda^2 - (\nu^2 - 4)]S(\nu, \hat{\mathbf{R}}) = 0, \quad (8)$$

$$\left[ \frac{1}{R^5} \frac{\partial}{\partial R} \left( R^5 \frac{\partial}{\partial R} \right) - \frac{\nu^2 - 4}{R^2} + K^2 \right] Z_\nu(KR) = 0, \quad (9)$$

and where  $\nu$  is the separation constant. The angular functions  $S(\nu, \hat{\mathbf{R}})$  are known [25] for general  $L$ ; however, this study is for the special case when  $L=0$  and identical bosons. Then the functions are given by

$$S(\nu, \hat{\mathbf{R}}) = \sum_{i=1}^3 \frac{\sin \left[ \nu \left( \frac{\pi}{2} - \alpha_i \right) \right]}{\sin \alpha_i \cos \alpha_i}. \quad (10)$$

Note that these functions are regular at  $\alpha_i = \pi/2$  but are irregular at  $\alpha_i = 0$ ,  $i=1,2,3$ . These irregularities are required in order to satisfy the zero-range boundary conditions of Eq. (7).

The radial equation Eq. (9) is solved in terms of Bessel functions. Different choices for these functions are available, namely, we can use the functions  $H_\nu^{(1)}(KR)$ ,  $H_\nu^{(2)}(KR)$ , and  $J_\nu(KR)$  with outgoing [30], incoming, and standing-wave asymptotic behavior when  $E > 0$ . For  $E < 0$  we use  $K_\nu(KR)$  [30], with  $\mathcal{K} = \pm iK$ .

The general solution  $\Psi$  of Eq. (5) is then given by Eq. (2) satisfying the following boundary condition:

$$\int_c A(\nu) \left\{ \frac{1}{R} \frac{\partial[\alpha_i S(\nu, \hat{\mathbf{R}})]}{\partial \alpha_i} Z_\nu(KR) + \frac{1}{a} [\alpha_i S(\nu, \hat{\mathbf{R}}) Z_\nu(KR)] \right\}_{\alpha_i \rightarrow 0} \nu d\nu = 0, \quad (11)$$

where the coefficient  $A(\nu)$  and the contour  $c$  are to be determined. To simplify the notation we define the function  $X(\nu)$  according to

$$X(\nu) = \frac{\partial[\alpha_i S(\nu, \hat{\mathbf{R}})]}{\partial \alpha_i} \Big|_{\alpha_i=0} = -\nu \cos \nu \frac{\pi}{2} + \frac{8}{\sqrt{3}} \sin \nu \frac{\pi}{6}. \quad (12)$$

The identity

$$\frac{2\nu}{KR}Z_\nu(KR) = Z_{\nu+1}(KR) \pm Z_{\nu-1}(KR), \quad (13)$$

where + is used for  $J_\nu$  and  $H_\nu^{(1,2)}$  and - for  $K_\nu$ , allows us to rewrite Eq. (11) as

$$\int_c A(\nu)X(\nu)Z_{\nu+1}(KR)d\nu \pm \int_c A(\nu)X(\nu)Z_{\nu-1}(KR)d\nu + \int_c A(\nu)\frac{2\nu}{aK}\sin\frac{\pi}{2}Z_\nu(KR)d\nu = 0. \quad (14)$$

At this point we introduce a restriction on the contour  $c$  and the coefficient  $A(\nu)$ . In Eq. (14) the Bessel functions are evaluated at different values of the indices  $\nu$  and  $\nu \pm 1$ . To obtain three integrals evaluated at the same value of  $\nu$  we close each of the contour  $c$  to connect the functions  $Z_{\nu \pm 1}$  with  $Z_\nu$ . This is possible because the contribution at infinity can be neglected and because we require that the function  $A(\nu)X(\nu)$  has no singularities inside of the contour connecting  $\nu$  and  $\nu \pm 1$ . With this constraint we can rewrite the last equation as

$$\int_c \left[ A(\nu-1)X(\nu-1) \pm A(\nu+1)X(\nu+1) + A(\nu)\frac{2\nu}{aKu(\nu)}\sin\frac{\pi}{2} \right] Z_\nu(KR)d\nu = 0. \quad (15)$$

If the integrand in Eq. (15) vanishes, then the integral will also. This requirement gives the three-term recurrence relation

$$A(\nu-1)X(\nu-1) \pm A(\nu+1)X(\nu+1) + A(\nu)\frac{2\nu}{aK}\sin\frac{\pi}{2} = 0. \quad (16)$$

Defining the quantity  $u(\nu)$  according to

$$u(\nu) = \frac{X(\nu)}{\cos\nu\frac{\pi}{2}}, \quad (17)$$

we write the recurrence relation Eq. (16) as

$$u(\nu-1)A(\nu-1) \mp u(\nu+1)A(\nu+1) = \frac{2\nu}{aK}A(\nu). \quad (18)$$

At this point the problem of solving the Schrödinger equation and boundary conditions Eqs. (5) and (7) has been transformed into the problem of solving the TTRR Eq. (18). The solution of these equations is described below in Sec. III C.

The appropriate integration contours have been determined for the model problem in Ref. [27]. These same contours are used in the present case and are explained more extensively in Sec. III B below. In the remainder of this work it is assumed that  $E > 0$ .

### III. SOLUTIONS AND INTEGRATION CONTOURS

#### A. Solutions of the three-term recurrence relation

To find the solutions of the TTRR we first find asymptotic solutions valid for large  $\nu$  then use the recurrence to step the solutions to all regions of the  $\nu$  plane. It is convenient to introduce the change of function  $B(\nu) = u(\nu)A(\nu)$  in Eq. (18), which leads us to an apparently simpler TTRR,

$$B(\nu-1) - B(\nu+1) = \frac{2\nu}{aKu(\nu)}B(\nu). \quad (19)$$

Two linearly independent solutions  $B_R$  and  $B_L$  [27] are defined by the asymptotic behavior for large  $\nu$  where  $u(\nu)/\nu \rightarrow 1$  provided  $\nu$  is not an odd integer. In this limit the two solutions are

$$\lim_{\nu \rightarrow \infty} B_R(\nu) = B_R^{(asy)}(\nu) = \exp[-\nu\alpha_K],$$

$$\lim_{\nu \rightarrow -\infty} B_L(\nu) = B_L^{(asy)}(\nu) = \exp[\nu\alpha_K]/\sin\pi\nu, \quad (20)$$

where  $\sinh\alpha_K = 1/(Ka)$ . Since  $\nu/u(\nu)$  is an even function of  $\nu$  it follows from Eq. (19) that

$$B_L(\nu) = B_R(-\nu)\frac{1}{\sin\pi\nu}. \quad (21)$$

Using  $B_R^{(asy)}$   $\nu$  for large positive  $\text{Re } \nu$  the recurrence relation is solved by stepping downward to obtain a coefficient  $B_R^{(1)}(\nu)$  for all  $\text{Re } \nu$  but especially on the interval  $0 < \text{Re } \nu \leq 2$ . Similarly the coefficient  $B_L^{(asy)}$  is found for all  $\text{Re } \nu$  but especially on the interval  $0 < \text{Re } \nu \leq 2$ . The restriction to positive  $\nu$  is required in order that the Hankel functions have correct properties for small values of  $R$  and in the limit that  $\nu \rightarrow \pm i\infty$ . The  $\text{Re } \nu$  interval must have length 2 and it turns out that any interval of length 2 is acceptable provided  $0 < \text{Re } \nu < 4$ . This larger interval is not used in the present work.

Both of these coefficients have a large number of poles in the interval  $0 < \text{Re } \nu \leq 2$  at  $\nu_j - m$  where  $\nu_j$  is a zero of  $u(\nu)$  and  $m$  is an integer such that  $\nu_j - m$  lies in the interval. The actual number of poles depends upon the large starting value of  $\nu$  and becomes infinite as the starting value becomes infinite. For any finite starting value, as used here, the number of poles is finite.

The specific starting values employed here use  $\nu = 2N + \delta\nu$  where  $N$  is a large integer,  $c/2N < \delta\nu < 1 - c/2N$  and  $c$  is some constant that is much less than unity. This excludes a small region in the complex  $\nu$  plane of radius  $c/2N$  about each integer. In general this leads to a discontinuity of order  $c/2N$  at the integers. When  $N$  becomes infinite the discontinuities disappear and we can suppose that the  $B(\nu)$ , thus obtained, is analytic at integer values of  $\nu$ . Actually, because  $u(\nu)$  vanishes at  $\nu = 4$  there is a pole of  $B_R(\nu)\cos\nu(\pi/2)$  at  $\nu = 2$  even when  $B_R(\nu)$  is continuous at integers greater than 3. This particular pole requires special treatment as discussed below.

Since any solution of the TTRR can be multiplied by an arbitrary function  $P(\nu)$  of  $\nu$  with period 1, i.e.,  $P(\nu) = P(\nu + 1)$

+1), it follows that the general solution is given by

$$B(\nu) = B_R(\nu)P_R(\nu) + B_L(\nu)P_L(\nu), \quad (22)$$

where  $P_R(\nu)$  and  $P_L(\nu)$  are arbitrary periodic functions. These functions and the contours must be chosen so that  $A(\nu)X(\nu)$  has no singularities in the region  $0 < \text{Re } \nu \leq 2$ . The contours are discussed in the next section and the periodic functions in Sec. III C.

### B. Integration contours

As discussed in Ref. [27] it is necessary to employ two contours with different Bessel functions to obtain convergent integrals for  $E > 0$ . Following that work we write

$$\begin{aligned} \Psi(\mathbf{R}) = & 2R^{-2} \int_{c_J} B_R(\nu)P_R(\nu)S(\nu, \hat{\mathbf{R}})J_\nu(KR) \frac{\nu d\nu}{u(\nu)} \\ & + R^{-2} \int_{c_1} B(\nu)S(\nu, \hat{\mathbf{R}})H_\nu^{(1)}(KR) \frac{\nu d\nu}{u(\nu)}, \end{aligned} \quad (23)$$

where  $c_J$  starts at  $i\infty$  goes to  $0+i\epsilon$  along the imaginary  $\nu$  axis and thence to  $+\infty$  along the positive real axis. The contour  $c_1$  starts at  $-i\infty$  and goes to  $+i\infty$  parallel to the imaginary axis. It crosses the real axis in the interval  $0 < \nu \leq 2$ . The contours are shown in Fig. 2. It must be emphasized that the separate terms in Eq. (23) do not converge since  $J_\nu(KR)$  increases exponentially as  $\nu \rightarrow i\infty$ . Only the combination converges, since then the increasing part of the first term is cancelled by the second term. This cancellation is apparent since  $2J_\nu(KR) - H_\nu^{(1)}(KR) = H_\nu^{(2)}(KR)$  and since  $H_\nu^{(2)}(KR)$  decreases exponentially as  $\nu \rightarrow i\infty$ .

The recurrence method used to solve for  $B_R(\nu)$  gives a function  $A(\nu)X(\nu)$  with no singularities in the upper right-hand quadrant of the  $\nu$  plane. The singularities in the right-hand quadrant appear only on the real axis and the contour is immediately above that axis. For that reason the contour  $c_J$  is readily shifted by one unit in  $\nu$  provided  $P_R(\nu)$  has no poles in the upper right quadrant.

Since  $B_R(\nu)$  and  $B_L(\nu)$  have poles on the interval  $0 < \nu \leq 2$  the contour  $c_1$  cannot be shifted two units as required by the derivation of the TTRR unless the periodic functions  $P_R(\nu)$  and  $P_L(\nu)$  are chosen so that the function  $B(\nu)\cos\pi\nu/2 = A(\nu)X(\nu)$  has no singularities on the strip  $0 < \text{Re } \nu \leq 2$  and

$$\lim_{\nu \rightarrow \pm i\infty} P_{R,L}(\nu) = \text{const} < \infty. \quad (24)$$

If these conditions are satisfied then the wave function of Eq. (23) is actually a mathematically acceptable solution of the Schrödinger equation since all integrals converge. In the next section we show that periodic functions satisfying the requisite conditions can indeed be found.

### C. Periodic functions $P_R(\nu)$ and $P_L(\nu)$

The periodic functions  $P_R(\nu)$  and  $P_L(\nu)$  that satisfy the above conditions have the form

$$P_R(\nu) = \lim_{N \rightarrow \infty} \prod_{j=0}^{N-1} \frac{\sin \pi(\nu - \nu_j) \sin \pi(\nu + \gamma_j^{(R)})}{\sin \pi(\nu - w_j) \sin \pi(\nu + w_j)}, \quad (25)$$

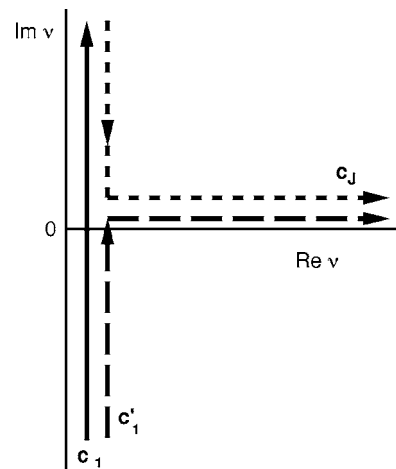


FIG. 2. Three contours  $c_1$ ,  $c_J$ , and  $c'_1$  in the complex  $\nu$  plane used to compute wave functions and scattering matrix elements.

$$\begin{aligned} P_L(\nu) = & \lim_{N \rightarrow \infty} iA \frac{\sin \pi(\nu - \nu_0)}{\sin \pi\nu} \\ & \times \prod_{j=0}^{N-1} \frac{\sin \pi(\nu + \nu_j) \sin \pi(\nu - \gamma_j^{(L)})}{\sin \pi(\nu - w_j) \sin \pi(\nu + w_j)}, \end{aligned} \quad (26)$$

where  $w_j$  is a zero of the Wronskian  $W(\nu)$

$$W(\nu) = B_R(\nu)B_L(\nu-1) - B_R(\nu-1)B_L(\nu), \quad (27)$$

and constants  $\gamma_j^{(R,L)}$  are to be chosen.

This form is surmised based upon experience with the exact solution in the special case  $K=0$ . Basically, the ratio  $\sin \pi(\nu - \nu_j)/\sin \pi(\nu - z_j)$  shifts poles from  $\nu_j$  to a set of points  $z_j \pm m$ ,  $m=0, 1, \dots$ . If the residue of  $B(\nu)$  at these new poles in the interval  $0 < \text{Re } \nu \leq 2$  vanishes, then  $B(\nu)$  is an acceptable coefficient.

Note that the Wronskian  $W(\nu)$  has twice as many poles on the interval  $0 < \nu < 2$  as do the coefficients  $B_R(\nu)$  or  $B_L(\nu)$ . Also, there are a similar number of zeros. Since the Wronskian  $W(\nu)$  is an even function of  $\nu$  then the zeros come in pairs which we label  $\pm w_j$ ,  $j=0, 1, \dots, N-1$ . We determine the constants  $\gamma_j^{(R)}$  and  $\gamma_j^{(L)}$  from  $2N$  equations so that the residues of  $B(\nu)$  Eq. (22) vanish at  $\nu = \pm w_n$ . The equation is

$$\text{Res}[B(\nu)]_{\nu=\pm w_n} = 0. \quad (28)$$

This choice of  $\gamma_j^{(R,L)}$ ,  $j=0, 1, \dots, N-1$  eliminates the poles at  $\pm w_n$ . Equation (28) is written in greater detail in Appendix A.

The point  $\nu=2$  is special, and is not included in the set  $\nu_j$ , yet the coefficients are singular at  $\nu=2$ . To eliminate the singularity at  $\nu=2$  we require that

$$B_R(2+\epsilon)P_R(2+\epsilon) + AB_L(2+\epsilon)P_L(2+\epsilon) = 0. \quad (29)$$

In the above equation it is understood that  $\epsilon$  is greater than or of the order of  $c/2N$ . In the limit that  $N \rightarrow \infty$  the value of  $\epsilon$  can be made arbitrarily small.

The  $2N+1$  equations Eqs. (28) and (29) determine the  $2N+1$  constants  $\gamma_j^{(R)}$ ,  $\gamma_j^{(L)}$  and  $A$ . With this construction we remove all the poles on the strip  $0 < \text{Re } \nu \leq 2$ .

The positions of the poles of  $B_R(\nu)$ , namely,  $\nu_j - m$ , does not depend upon the parameter  $Ka$ . In contrast,  $\gamma_j^{(R)}$ ,  $\gamma_j^{(L)}$ , and the zeros of the Wronskian  $\pm w_n$  depend upon  $Ka$  via the recurrence relation. As we shall see, this information allows us to identify parts of the  $S$  matrix that depend upon  $Ka$  and parts that do not.

It is necessary to know the values of the  $P_R(\nu)$  and  $P_L(\nu)$  in the limits that  $\nu \rightarrow \pm i\infty$ . One easily finds

$$\lim_{\nu \rightarrow \pm i\infty} P_R(\nu) \approx \exp \left[ \pm i\pi \sum_{j=0}^{\infty} (\nu_j - \gamma_j^{(R)}) \right],$$

$$\lim_{\nu \rightarrow \pm i\infty} P_L(\nu) \approx iA \exp \left[ \mp i\pi \sum_{j=0}^{\infty} (\nu_j - \gamma_j^{(L)}) \pm i\pi\nu_0 \right]. \quad (30)$$

In the following we take  $\nu_0 = it_0$ , where  $\pm it_0$  is a complex zero of  $u(\nu)$  and all other  $\nu_j$ ,  $j \geq 1$  are real. It also proves necessary to construct functions with  $\nu_0 = -it_0$ . The two functions, denoted by  $u$  and  $d$ , respectively, are constructed by identical procedures, thus only the  $u$  choice is described in detail. For simplicity of notation, the  $u$  label is omitted until these two functions are combined to get physical solutions.

#### IV. WAVE FUNCTIONS AT LARGE $R$

Having found solutions of the Schrödinger equation for three particles interacting via ZRPs, it is now necessary to extract the scattering matrix elements. These quantities are found by evaluating the integral in Eq. (23) for large  $R$ . When  $R$  is large a steepest descent analysis shows that the dominant part of the wave function comes from regions where  $\nu$  is large and imaginary. The analysis is carried out as described in Ref. [27].

The steepest descent evaluation finds three nonvanishing contributions, namely, a contribution to the incoming wave  $H_\nu^{(2)}(KR)$  from the first term as  $\nu \rightarrow +i\infty$ , and two contributions to the outgoing wave  $H_\nu^{(1)}(KR)$ . The latter two contributions come from  $B_R(\nu)H_\nu^{(1)}(KR)$  as  $\nu \rightarrow -i\infty$  and from  $B_L \nu H_\nu^{(1)}(KR)$  as  $\nu \rightarrow +i\infty$ .

When the limits  $R \rightarrow \infty$ ,  $x_i = \text{const}$  are taken under the integral and the stationary phase approximation [27] is used to evaluate the integral we obtain

$$\Psi_i \rightarrow -i \frac{e^{-r_i/a}}{r_i} \left[ e^{-s^{(R)}} e^{-i\delta_\infty^{(R)}} \frac{e^{-iks_i}}{s_i} - e^{s^{(R)}} e^{i\delta_\infty^{(R)}} \frac{e^{iks_i}}{s_i} - A e^{s^{(L)}} e^{i\delta_\infty^{(L)}} \frac{e^{iks_i}}{s_i} \right], \quad (31)$$

where

$$\delta_\infty^{(R,L)} = -\pi \sum_{j=0}^{\infty} \text{Re}(\nu_j - \gamma_j^{(R,L)}), \quad (32)$$

$$s^{(R)} = \pi t_0 - \pi \sum_{j=0}^{\infty} \text{Im} \gamma_j^{(R)},$$

$$s^{(L)} = -\pi \sum_{j=0}^{\infty} \text{Im} \gamma_j^{(L)}, \quad (33)$$

and where we have set  $r_i = x_i$  and  $s_i = \sqrt{3}y_i/2$ . One immediately sees that only the bound state channel appears in the large  $R$  limit when  $r_i$  is held fixed.

The limit with  $r_i$  fixed is only one part of the circle at infinity. It is also necessary to examine the limit as  $R \rightarrow \infty$  with  $\alpha$  held fixed. To evaluate this limit advantage can be taken of the fact that all integrals converge when the integration over  $\nu$  and the limits are interchanged. Then the limiting forms of the Bessel functions, namely,

$$H_\nu^{(1)}(KR) \rightarrow \sqrt{\frac{2}{\pi KR}} e^{i(KR - \pi/2\nu - \pi/4)}, \quad (34)$$

$$H_\nu^{(2)}(KR) \rightarrow \sqrt{\frac{2}{\pi KR}} e^{-i(KR - \pi/2\nu - \pi/4)}, \quad (35)$$

with  $2J_\nu(x) = H_\nu^{(1)}(x) + H_\nu^{(2)}(x)$  are taken underneath the integrals. With these substitutions in Eq. (23), the incoming waves corresponding to  $H_\nu^{(2)}$  appear under the integral around contour  $c_j$ . This contour may be closed in the upper quadrant without enclosing any poles of  $B_R(\nu)$  thus the coefficient of the incoming waves vanishes, verifying that the wave function of Eq. (23) satisfies physical boundary conditions at large  $R$ , and  $\alpha_i$ ,  $i = 1, 2, 3$  fixed.

For future reference the coefficient of the outgoing wave is also needed. By joining the lower part of the contour  $c_1$  with the part of  $c_j$  along the real axis to define a new contour  $c'_1$  shown in Fig. 2, we have that the coefficient  $S_{0,\hat{R}}$  is given by

$$S_{\hat{R},0} = \frac{1}{\pi} e^{-i\pi/4} \left[ \int_{c'_1} \frac{P_R(\nu)B_R(\nu)}{u(\nu)} S(\nu, \hat{R}) e^{-i(\pi/2)\nu} \nu d\nu \times \int_{c_1} \frac{P_L(\nu)B_L(\nu)}{u(\nu)} S(\nu, \hat{R}) e^{-i(\pi/2)\nu} \nu d\nu \right]. \quad (36)$$

#### V. WAVE FUNCTIONS AT SMALL $R$

If the wave function satisfies appropriate boundary conditions in the limit  $R \rightarrow 0$  then the coefficient  $S_{0,\hat{R}}$  would be the fragmentation matrix element for the reaction

$$B + B_2 \rightarrow B + B + B. \quad (37)$$

To examine the wave function at small values  $R = R_0$  of  $R$ , note that the integral representation in Eq. (23) converges, thus the limit  $R \rightarrow 0$  may be taken before integration. The limit of the Bessel functions  $J_\nu(KR)$  and  $H_\nu^{(1)}(KR)$  and for small  $R = R_0$  and  $\text{Re } \nu > 0$  are

$$J_\nu(KR_0) \rightarrow \frac{1}{\Gamma(\nu+1)} \left( \frac{1}{2}KR_0 \right)^\nu,$$

$$H_\nu^{(1)}(KR_0) \rightarrow \frac{1}{i\pi} \Gamma(\nu) \left( \frac{1}{2}KR_0 \right)^{-\nu}. \quad (38)$$

After substituting these expressions onto Eq. (23) we may close the contour  $c_j$  in the right-hand quadrant of the complex  $\nu$  plane without enclosing any singularities of the integrand. It follows that the first term vanishes as  $R \rightarrow 0$ . The only contribution comes from the contour  $c_1$  as  $R \rightarrow 0$ . Again, after substituting the limiting form of  $H_\nu^{(1)}(KR_0)$  in this term the integral can be evaluated by closing the contour around a semicircle at infinity in the left-hand  $\nu$  plane. In this case many poles of the integrand are enclosed since both  $B_R(\nu)$  and  $B_L(\nu)$  have poles in the left-hand plane. Those on the real axis have negative real parts that are greater in magnitude than  $\nu_2=4$ . It follows that the residues at these poles vanish as  $R_0^{\nu_j-2}$  for  $j \geq 1$ . The pole in  $1/u(\nu)$  at  $\nu=0$  is cancelled by the angular wave function  $S(\nu; \hat{\mathbf{R}})$  so there is no contribution from this pole.

There is also a pole in  $B_R(\nu)/u(\nu)$  at the purely imaginary point  $\nu=-\nu_0$ . Because  $R_0^{\pm\nu_0}$  has unit magnitude, the pole at  $\nu_0$  gives the dominant contribution to the wave function at vanishingly small  $R_0$ . This contribution is readily evaluated using the residue theorem for the residue at  $u(\nu) \approx u'(-\nu_0)(\nu + \nu_0)=0$ . We have

$$\lim_{R_0 \rightarrow 0} \psi(R_0 \hat{\mathbf{R}}) = R_0^{-2} \beta S(-\nu_0, \hat{\mathbf{R}})$$

$$= 2 \frac{B_R(-\nu_0) P_R(-\nu_0)}{u'(-\nu_0) R_0^2} \Gamma(-\nu_0 + 1)$$

$$\times S(-\nu_0, \hat{\mathbf{R}}) (KR_0/2)^{\nu_0}, \quad (39)$$

which defines the quantity  $\beta$ . Since  $\nu_0$  could be either  $\mp it_0$  in Eq. (39) we see that there are two solutions which are denoted by  $u$  when  $\nu_0=it_0$  and  $d$  when  $\nu_0=-it_0$ . The coefficient in the limiting value of the  $u$  solution will be denoted by  $\beta$ . The limiting value of the  $d$  solution is then  $\beta^* S(it_0, \hat{\mathbf{R}})$ . Since  $S(\nu, \hat{\mathbf{R}})$  is an odd function of  $\nu$ , it follows that the linear combination

$$\Psi(\mathbf{R}) = \beta \psi^{(d)}(\mathbf{R}) + \beta^* \psi^{(u)}(\mathbf{R}) \quad (40)$$

vanishes at  $R=R_0$ .

The function  $\Psi(\mathbf{R})$  satisfies the Schrödinger equation for all  $R, \hat{\mathbf{R}}$  in the region  $R > R_0$  and vanishes at the boundary  $R_0$ . It therefore corresponds to a physical system where a hard-core three-body potential

$$V_r(R) \rightarrow \infty, \quad R \leq R_0,$$

$$V_r(R) = 0, \quad R > R_0, \quad (41)$$

has been added to the Hamiltonian.

This potential is in addition to the two-body interactions represented by the ZRPs. In effect, this explicit three-body potential is introduced to compensate or renormalize away

unphysical effects of the ZRPs when the positions of all three particles coalesce. Thus this potential will be referred as the renormalization potential.

## VI. S MATRIX

With the introduction of the renormalization potential, the wave function  $\Psi(\mathbf{R})$  is acceptable everywhere including on the circle at infinity. From the asymptotic expression Eq. (31) one has for the  $S_{00}$  matrix element the result

$$S_{00} = \exp(2i\delta_\infty^{(R)}) \left( \frac{\beta e^{s^{(R)}} + \beta^* e^{-s^{(R)}}}{\beta e^{-s^{(R)}} + \beta^* e^{s^{(R)}}} \right.$$

$$\left. + e^{i\delta_\infty^{(L)} - i\delta_\infty^{(R)}} \frac{A \beta e^{s^{(L)}} - A^* \beta^* e^{-s^{(L)}}}{\beta e^{-s^{(R)}} + \beta^* e^{s^{(R)}}} \right), \quad (42)$$

where we define

$$A \equiv A^{(u)} = -[A^{(d)}]^*,$$

$$\delta_\infty^{(R,L)} \equiv [\delta_\infty^{(R,L)}]^{(u)} = [\delta_\infty^{(R,L)}]^{(d)},$$

$$s^{(R,L)} \equiv [s^{(R,L)}]^{(u)} = -[s^{(R,L)}]^{(d)}. \quad (43)$$

The total cross section for the process

$$B + B_2 \rightarrow B + B + B$$

is calculated from the  $S$  matrix element

$$S_{\hat{\mathbf{R}},0} = \beta S_{\hat{\mathbf{R}},0}^{(u)} + \beta^* S_{\hat{\mathbf{R}},0}^{(d)} \quad (44)$$

by integrating the squared matrix element over  $\hat{\mathbf{R}}$ . Alternatively the total cross section can be computed using  $S_{00}$  and unitarity. It is convenient to define the quantity  $|S_{01}|^2$  according to

$$|S_{01}|^2 = \int |S_{\hat{\mathbf{R}},0}|^2 d\hat{\mathbf{R}}, \quad (45)$$

so that the unitarity relation reads

$$|S_{00}|^2 + |S_{01}|^2 = 1, \quad (46)$$

from which  $|S_{01}|^2$  is readily computed.

## VII. CALCULATIONS IN THE LIMIT $K \rightarrow 0$

The shape-independent representation of two-body interactions is generally employed for energies such that  $Ka \leq 1$ . When the energy is greater than  $1/ma^2$ , higher order terms in the expansion of the two-body phase shift may be important, thus interest attaches to cross sections and rate coefficients in the limit that  $Ka \rightarrow 0$ . It is also found that in this limit  $w_j \rightarrow 0$ ,  $\gamma_j^{(R,L)} \rightarrow 0$  and

$$B_L(\nu) P_L \nu = i A B_R(-\nu) P_R(-\nu) \frac{\sin \pi(\nu - \nu_0)}{\sin^2 \pi \nu}. \quad (47)$$

In this region we can use that  $B_R(\nu) = (Ka)^\nu Q(\nu)$ , where to lowest order in  $(Ka)^2$  the reduced coefficient  $Q(\nu)$  satisfies the two-term recurrence relation

$$Q(\nu - 1) = \frac{2\nu}{u(\nu)} Q(\nu), \quad (48)$$

so that  $\lim_{\epsilon \rightarrow 0} Q(\epsilon)/Q(-\epsilon) \rightarrow 1$  from which one easily finds

$$A = (Ka)^4 \lim_{\epsilon \rightarrow 0} \frac{Q(\epsilon + 2) \sin^2 \pi \epsilon}{Q(-\epsilon - 2) \sinh(\pi t_0)} \quad (49)$$

$$\begin{aligned} &= \left(\frac{Ka}{2}\right)^4 \lim_{\epsilon \rightarrow 0} \frac{u(1-\epsilon)u(\epsilon)u(-1-\epsilon)u(-2) \sin^2 \pi \epsilon}{(1-\epsilon)\epsilon(-1-\epsilon)(-2) \sinh \pi t_0} \\ &= -(Ka)^4 \left(1 - \frac{4\pi}{3\sqrt{3}}\right) \frac{8}{\sinh \pi t_0}, \end{aligned} \quad (50)$$

and we have used Eq. (17) to evaluate  $u(\nu)$  and  $u'(\nu)$ . Note that  $Q\nu$  differs slightly from the similar function  $C(\nu) = Q\nu\nu/2u(\nu)$  employed in Ref. [13]. This difference is reflected in the two-term recurrence relation Eq. (48).

Equation (42) for  $S_{00}$  in the limit  $K \rightarrow 0$  has the form

$$S_{00} = \exp(2i\delta_\infty) \left( \frac{\beta e^{\pi t_0} + \beta^* e^{-\pi t_0} + A(\beta - \beta^*)}{\beta e^{-\pi t_0} + \beta^* e^{\pi t_0}} \right). \quad (51)$$

Using Eq. (51) and defining  $\delta_0$  according to

$$\beta = |\beta| e^{i\Delta(R_0)} \quad (52)$$

and

$$\Delta(R_0) = \delta_0 + t_0 \ln(R_0/a) \quad (53)$$

gives the expression for  $S_{00}$

$$\begin{aligned} S_{00} &= e^{i2\delta_\infty - i2\Delta(R_0)} [1 + e^{-2\pi t_0 + i2\Delta(R_0)} \\ &\quad + i2A e^{-\pi t_0} e^{i\Delta(R_0)} \sin \Delta(R_0)] [1 + e^{-2\pi t_0 - i2\Delta(R_0)}] \\ &= e^{i2\delta_\infty - i2\Delta(R_0)} \left( 1 + \frac{2iA e^{-\pi t_0} e^{i\Delta(R_0)} \sin \Delta(R_0)}{1 + e^{-2\pi t_0} e^{2i\Delta(R_0)}} \right). \end{aligned} \quad (54)$$

The term in round brackets on the right-hand side of Eq. (54) can be written

$$1 + 2iP e^{i\Delta_r(R_0)} \sin \Delta_r(R_0), \quad (55)$$

where

$$P = \frac{A}{2 \sinh(\pi t_0)} = \left( \frac{4\pi}{\sqrt{3}} - 1 \right) \frac{4(Ka)^4}{\sinh^2 \pi t_0}, \quad (56)$$

and where

$$\Delta_r(R_0) = \Delta(R_0) - \arctan \left( \frac{e^{-2\pi t_0} \sin 2\Delta(R_0)}{1 + e^{-2\pi t_0} \cos 2\Delta(R_0)} \right). \quad (57)$$

With these definitions the elastic scattering  $S$  matrix is

$$S_{00} = e^{2i\delta_\infty - 2i\Delta_r(R_0)} (1 + 2iP e^{i\Delta_r(R_0)} \sin \Delta_r(R_0)), \quad (58)$$

and the squared matrix element  $|S_{01}|^2$  becomes

$$|S_{01}|^2 = 4P(1 - P) \sin^2 \Delta_r(R_0), \quad (59)$$

which is exactly the form given by the hidden-crossing approximation. Equation (59) shows that the hidden-crossing form is exact at  $E=0$  for the zero-range model. Furthermore the exact ‘‘probability’’  $P$  is independent of  $R_0$  just as in the

hidden-crossing theory. The renormalization enters only through the phase  $\Delta_r(R_0)$ , but now the phase differs from the hidden-crossing result owing to the second term on the right-hand side of Eq. (57).

This renormalized ‘‘Stuekelberg’’ phase is closely related to the exact elastic scattering phase at the breakup threshold given by Eq. (58) with  $P=0$  which was previously obtained by our group [13]. In terms of the elastic scattering phase  $\delta(R_0) = \delta_\infty - \Delta_r(R_0)$  we have that  $\Delta_r(R_0)$  is given by

$$\Delta_r(R_0) = \delta_\infty - \delta(R_0), \quad (60)$$

where  $\delta_\infty$  is defined by Eq. (32). Clearly, if the renormalized phase for elastic scattering is set for the zero-range model, the ‘‘Stuekleberg’’ phase relevant to breakup or to three-body recombination at threshold is easily determined simply by finding the zeros  $\nu_j$  of the  $X(\nu)$  in order to compute  $\delta_\infty$  using Eq. (32).

The  $\sin^2$  factor was previously obtained in the hidden crossing calculations of Ref. [15], in the hyperspherical close coupling calculations of Ref. [31], and as a fitting function for the exact zero-energy calculations of Ref. [26]. It is remarkable that our exact theory shows that the same form holds exactly at zero energy. In particular, the renormalization constant  $R_0$  enters into the cross section formulae only through the phase of  $\sin \Delta_r(R_0)$ , just as in the fit to the exact numerical results of Ref. [26]. The main difference between our exact result and the exact numerical results is the additional small oscillatory factor in the definition of  $\Delta(R_0)$ . Since the amplitude of this factor is of the order of 0.002 and since the functional form fits the numerical results with an error of  $\pm 0.7\%$  the exact results given above are fully consistent with the essentially exact results of Ref. [26].

Equation (59) and the results of Ref. [13] show that most important physical quantities can be computed exactly for the zero-range model using our method. To summarize the technique one first solves Eq. (19) for  $B_R(\nu)$  using Eq. (20) for the starting value at large positive  $\nu$ . The coefficient  $B_L(\nu)$  is found by a similar procedure. The zeros  $w_n$  of the Wronskian of the two solutions on the interval  $0 < \text{Re } \nu < 1$  are then found. These zeros are functions of the energy  $E$ , the poles  $\nu_j$  of the solutions are also found, by the simpler task of locating the zeros of  $\rho(\nu)$ . They are independent of  $E$ . These quantities are then used to form the periodic functions  $P_R(\nu)$  and  $P_L(\nu)$  and to compute the constant  $A$  from Eq. (49), the phase  $\delta_\infty$  from Eq. (32), and the phase  $\delta_0$  from Eq. (54). All of these physical quantities depend upon the energy  $E$ .

They also depend upon the renormalization constant  $R_0$  found by fitting one of the physical quantities to its measured value at some energy. Alternatively the physical quantity can be computed by, e.g., the hyperspherical close-coupling method, using realistic two-body potentials and that value used to obtain  $R_0$ . In either case, the renormalization constant, thus obtained, incorporates the details of the two-body interaction that are most relevant for low energy three-body interactions.



### VIII. APPLICATIONS

Since we are concerned with cold ensembles of atoms, it is natural to employ the zero-range model at total energies  $E=0$ . Calculations of elastic scattering at  $E=0$  have been given in Ref. [13]. In this section we report computations of the three-body recombination rate  $K_3$  at  $E=0$  given by [15],

$$\begin{aligned} K_3 &= 2(2\pi)^2 3^{3/2} \frac{|S_{01}|^2 \hbar}{(Ka)^4 m} a^4 \\ &= 32\pi^2 3^{3/2} \frac{P(1-P)}{(Ka)^4} \sin^2 \Delta_r(R_0) \frac{\hbar}{m} a^4. \end{aligned} \quad (61)$$

Using  $P$  from Eq. (56) gives

$$K_3 = 2^7 \pi^2 (4\pi - 3\sqrt{3}) \frac{\sin^2 \Delta_r(R_0) \hbar}{\sinh^2 \pi t_0 m} a^4 \equiv C_3 \sin^2 \Delta_r \frac{\hbar}{m} a^4. \quad (62)$$

In this way the coefficient

$$C_3 = 2^7 \pi^2 (4\pi - 3\sqrt{3}) / \sinh^2 \pi t_0 \quad (63)$$

of  $(\hbar/m)\sin^2 \Delta(R_0)$  is found in closed form. Numerically, it is equal to  $C_3=67.1177\dots$ , in excellent agreement with the fit  $C_3=67.1\pm 0.7\%$  to the exact numerical computations of  $K_3$  reported in Ref. [26]. This value is also in good agreement with the hidden-crossing approximation [15], namely,  $C_{HC}=68.4$ . The hidden-crossing result is derived in detail in Appendix B. After completing this work [12] we learned that exactly the same coefficient was obtained independently by Petrov [32].

The phase of the ‘‘Stuekelbeg’’ oscillations  $\Delta_r(R_0)$  is a sum of constant term  $\delta_0$  and terms that depend upon  $R_0$ . The dependence upon  $R_0$  is given in closed form by Eq. (57). An expression for  $\delta_0$  of Eq. (53) was obtained in Ref. [13]. It is given in terms of a rather complicated combination of gamma functions and  $P_R(-\nu_0)$ , but can also be considered a closed form result. In any event, the value  $\delta_0=1.588$  was obtained.

For comparison the phase and amplitude are also evaluated in the hidden-crossing approximation in Appendix B. There we find that

$$K_3(HC) = 68.4 \sin^2 [t_0 \ln(R_0/a) + 1.5742] \frac{\hbar}{m} a^4. \quad (64)$$

Clearly, when  $K=0$  the hidden-crossing amplitude and phase agree with the exact result to order 2%. Since the hidden-crossing amplitude is rather easy to compute it can be used to get a good estimate of the essential features of three-body interactions in the limit of large scattering length.

To check the good agreement between the hidden-crossing and exact amplitudes we compute corrections to  $B(\nu)$  to higher order in  $(Ka)^2$  in Appendix C. It should be noted that the expansion about  $Ka=0$  is not valid for regions of  $\nu$  where the correction terms are larger than unity. This excludes regions around integer values of  $\nu$ . For that reason we only use the expansion at  $\nu=\pm t_0$  and for values of  $(Ka)$  such that the correction to  $B(-it_0)$  is much less than unity. This means that we cannot use the power series expansion to

compute the energy-dependent zeros of the Wronskian nor the phases  $\delta_\infty(Ka)$  and  $\delta_0(Ka)$ . We can use the expansion at  $\nu=\pm t_0$  and for all values of  $(Ka)$  such that the correction to  $B(-it_0)$  is much less than unity. Then the power series expansion gives

$$\delta_0 = 1.588 + 0.944(Ka)^2 + \delta_p(Ka) - \delta_p(0), \quad (65)$$

where  $\delta_p(Ka)$  is the phase of the periodic function  $P_R(Ka)$  at  $\nu=-it_0$  for a given  $Ka$ .

To evaluate  $\delta_p(Ka)$  we note that  $\delta_p$  and  $\delta_\infty$  differ by factors of the order of  $e^{-2\pi t_0}$ . Since  $e^{-2\pi t_0}$  is less than 0.5% we will assume exact equality recognizing that this may introduce negligibly small errors. Then Eq. (65) gives us the approximate result

$$\delta_\infty - \delta_0 = 0.148 - 0.94(Ka)^2, \quad (66)$$

while the hidden-crossing theory gives

$$\delta_\infty(HC) - \delta_0(HC) = 0.1623 - 0.52(Ka)^2. \quad (67)$$

Although these results differ by only 0.014 rad at  $E=0$ , they rapidly diverge for larger values of  $E$ . To some extent this rapid divergence may be due to the failure of the hidden-crossing or JWKB approximation at the boundary of the hard-core renormalization potential so that the divergence between exact and hidden-crossing phases may not be so strong for two-body interactions that are realistic when  $R \leq R_0$ . In any case, agreement is very good at threshold but the region where the hidden-crossing approximation is accurate appears to be limited to a small energy range near  $E=0$ .

Our result shows that the coefficient  $C_3$  is a universal constant, i.e., it does not depend upon  $R_0$  or  $a$ . Other universal constants are  $\delta_\infty(E=0)$  and  $\delta_0(E=0)$ . They also do not depend upon  $R_0$  or  $a$ . Of course, at nonzero energies these quantities depend upon  $a$ . That dependence, however, can be scaled out so that these observable depend only upon the product  $Ka$ . In that sense they are also universal functions applicable whenever the zero-range representation is valid for two-body interactions.

Other physical quantities that depend upon the phase  $\Delta_r(R_0)$  are not as universal as those that depend only  $a$ , since they depend upon details of two-body interactions not included in the scattering length. Even so, once this quantity is fixed all of the physical quantities are readily computed if the  $R_0$  independent functions  $\delta_\infty(Ka)$ ,  $A(Ka)$ , and  $\delta_0(Ka)$  are known. It is not necessary to recompute these quantities when  $R_0$  changes. In this way two- and three-body boson interactions characterized by a scattering length and the parameter  $R_0$  are truly universal as discussed in Ref. [3].

The Schrödinger equation has been solve by the essentially standard method of separating variables and writing the solution as a contour integral over the single separation constant  $\nu$ . The contours that we use, however, are not standard and were extracted earlier by solving a model problem [27]. They generalize the known Kantarovich-Lebedev representation [29]. The ZRP boundary conditions then gave a three-term recurrence relation for the expansion coefficients  $A(\nu)$ . Three-term recurrence relations also occur in power series

expansions of special functions [30]. In both cases, multiplication of the coefficients by a periodic function gives a new coefficient, but for power series this periodic function plays no role since it may be factored out and subsumed in a normalization constant. In contrast, the periodic functions cannot be factored out of the integral representation; indeed, they play a crucial role in finding coefficients with correct analytic properties determined by boundary conditions. There is no standard means to find such periodic functions, but a general method to move poles around has been devised in this work. We use this method to move poles to the zeros of the coefficients for two- and three-term recurrence relations. Using the general technique, it is possible to completely determine the three-particle wave function.

The solution obtained here is exact, and can be made without reference to more standard techniques such as the hyperspherical adiabatic representation, the Sturmian representation, and the hyperspherical close-coupling method. To connect to these known techniques we indicate how the quantities employed here relate to the hyperspherical adiabatic potentials  $U_n(R)$  and the hyperspherical adiabatic wave functions.

The quantity  $X(\nu)$  was introduced in this work purely for notational convenience, but if we set

$$\rho(\nu) = -a \frac{X(\nu)}{\sin(\nu) \frac{\pi}{2}}, \quad (68)$$

then we recognize  $\rho(\nu)$  as the single pseudo-Sturmian eigenvalue for this problem defined by the equation

$$\left[ \frac{\partial \alpha_i S(\nu, \hat{\mathbf{R}})}{\partial \alpha_i} + \rho(\nu) \alpha_i S(\nu, \hat{\mathbf{R}}) \right] = 0. \quad (69)$$

The Sturmian eigenvalue  $\rho(\nu)$  does not equal the physical radius  $R$ , but if we set  $\rho(\nu) = R$  and solve for  $\nu$  as a function of  $R$  we obtain an infinite set of roots  $\nu_n(R)$ . These roots define the adiabatic energy eigenvalues according to

$$U_n(R) = \frac{\nu_n(R)^2 - 1/4}{2R^2}, \quad (70)$$

while the adiabatic wave functions  $\Phi_n(R; \hat{\mathbf{R}})$  are given by

$$\Phi_n(R; \hat{\mathbf{R}}) = N_n(R) S(\nu_n(R), \hat{\mathbf{R}}), \quad (71)$$

where  $N_n(R)$  is a normalization constant. The adiabatic eigenvalue thus obtained is used in Appendix A to compute the hidden-crossing approximation for the recombination coefficient  $K_3$ .

## IX. CONCLUDING REMARKS

The Schrödinger equation for a system of three particles interacting via ZRP has been solved in quadrature form. The solution for total angular momentum equal to zero has been written as a contour integral over the product of Bessel and pseudo-Sturmian functions weighted by a function obtained from a three-term recurrence relation. The integration is per-

formed over the indices of the Bessel functions around contours fixed by asymptotic conditions. The indices of the Bessel functions are separation constants in the Schrödinger equation and can be understood as generalized angular momenta.

A renormalization constant  $R_0$  is needed to obtain wave functions that are defined in the limit as  $R \rightarrow 0$ . This constant represents the radius of an explicit three-body potential that becomes infinite when the hyperradius  $R$  is less than  $R_0$ . With this constant fixed we show how the scattering matrix can be obtained from the asymptotic form of our wave function. The fundamental formulae of the theory are illustrated by a computation of the three-body recombination rate in the limit of zero energy. In this case a completely analytic expression is obtained for the rate. The expression is compared with previous exact and approximate results. Agreement with the exact numerical results of Ref. [26] is excellent. Agreement with the hidden crossing approximation is also good showing that the quasi-classical theory is reliable for three-body recombination at the threshold for this process.

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## APPENDIX A: EQUATIONS FOR $\gamma_j^{(R,L)}$

Equation (28) for  $\gamma_j^{(R,L)}$  is written in a compact form in the main text. By evaluating the residues explicitly we have

$$\prod_{j=0}^N \frac{\sin \pi(w_n + \gamma_j^{(R)})}{\sin \pi(w_n - \gamma_j^{(L)})} = iA \frac{\sin \pi(w_n - \nu_0)}{\sin^2 \pi w_n} \times \frac{B_R^{(N)}(-w_n)}{B_R^{(N)}(w_n)} \prod_{j=0}^N \frac{\sin \pi(w_n + \nu_j)}{\sin \pi(w_n - \nu_j)}, \quad (A1)$$

and

$$\prod_{j=0}^N \frac{\cos 2\pi \gamma_j^{(R)} - \cos 2\pi w_n}{\cos 2\pi \gamma_j^{(L)} - \cos 2\pi w_n} = 2A^2 \frac{\cos 2\pi \nu_0 - \cos 2\pi w_n}{(1 - \cos 2\pi w_n)^2}. \quad (A2)$$

These are highly nonlinear equations. They can be solved iteratively by starting with some known value of  $\gamma_j^{(R,L)}$  and linearizing the equations to obtain a correction  $\delta \gamma_j^{(R,L)}$ . The processes is repeated until convergence is obtained.

## APPENDIX B: HIDDEN CROSSING THEORY FOR ZERO-RANGE POTENTIALS

The hidden-crossing theory was originally developed by Sulev'ev [33] as an asymptotic expansion in powers of  $1/\nu$

for transition matrix elements in the semiclassical theory of atomic collisions where the internuclear distance is represented by a classical trajectory  $R_n(t, v)$ . Extension of this theory to a wave representation of relative motion leads to the hyperspherical adiabatic representation [34] of Ref. [14]. The hyperspherical hidden-crossing theory employs this representation and is derived in Ref. [28]. In the wave representation the hidden-crossing approximation for the squared transition matrix element  $|S_{01}|^2$  is given by

$$|S_{01}|^2 = 4P_{\text{HC}}(1 - P_{\text{HC}})\sin^2\Delta_{\text{HC}}, \quad (\text{B1})$$

where

$$P = e^{-2\text{Im} I}, \quad (\text{B2})$$

$$\Delta_{\text{HC}} = \text{Re} I, \quad (\text{B3})$$

with

$$I = \int_{R_0}^{R_1} \sqrt{K^2 - 2U(R) + \frac{1/4}{R^2}} dR. \quad (\text{B4})$$

The function  $U(R)$  is the adiabatic eigenvalue [14],  $K$  is the wave vector for hyperradial motion,  $R_0$  is the classical turning point in the initial channel, 0, and  $R_1$  is the classical turning point in the final channel. In order to connect the initial and final channels the integration contour must go into the complex plane to encircle branch points where the initial branch  $U_0(R)$  of  $U(R)$  connects with the final branch  $U_1(R)$ .

This approximation has been extensively employed to treat ion-atom collisions and has seen some limited use in the hyperspherical representation. Its use for zero-range potentials presents special problems owing the Thomas-effect divergences of  $U(R)$  near  $R \approx 0$ . With the renormalization procedure where  $R_0$  is some finite constant quantity chosen to fit a three-body observable, one can apply the theory for a system of three bosons interacting via zero-range potentials.

To compute  $I$  it only necessary to find the function  $U(R)$ . This is easily done for zero-range potentials by solving the equation

$$\rho(\nu) = R \quad (\text{B5})$$

for  $\nu(R)$  and forming

$$U(\nu) = \frac{\nu(R)^2 - 1/4}{2R^2}. \quad (\text{B6})$$

Even though  $\rho(\nu)$  is a relatively simple known function integration in the complex plane must be carried out numerically. The integral, however, diverges at the lower limit as  $R_0 \rightarrow 0$  and at the upper limit as  $E \rightarrow 0$  so the expression given by Eq. (B4) is not convenient for zero-range potentials.

A more tractable expression is obtained by adding and subtracting terms that given explicit closed-form expressions for the divergent parts. If we suppose that there is only one dominant branch point  $R_b$  connecting initial and final channels, then we may form

$$\begin{aligned} \mathcal{I} = & \int_{R_0}^{R_b} (\sqrt{K^2 - \nu^2/R^2} - \sqrt{K^2 - (it_0)^2/R^2}) dR \\ & + \int_{R_b}^{R_1} (\sqrt{K^2 - \nu^2/R^2} - \sqrt{K^2 - 2^2/R^2}) dR \\ & + \int_{R_0}^{R_b} \sqrt{K^2 - (it_0)^2/R^2} dR + \int_{R_b}^{R_1} \sqrt{K^2 - 2^2/R^2} dR. \end{aligned} \quad (\text{B7})$$

The first two terms are now finite in the limits that  $R_0 \rightarrow 0$  and  $E \rightarrow 0$  so that these limits may be taken before integration. These terms give a constant that is computed by numerical integration. The third and fourth terms are evaluated analytically so that the divergent factors are exhibited explicitly. The fourth term gives the  $E^2 a^4$  threshold law for breakup, while the third term is just  $t_0 \ln(R_b/R_0)$ . Using the value of  $R_b$  from Ref. [15] in Eq. (B7) to evaluate  $\mathcal{I}$  then substituting the result into Eq. (B1) with Eq. (61) we find the hidden-crossing approximation for  $K_3$ , namely

$$K_3(\text{HC}) = 68.4 \sin^2(t_0 \ln(a/R_0) + 1.5742 + 0.17K^2) \frac{\hbar}{m} a^4, \quad (\text{B8})$$

where we have added  $\pi/4$  to  $\text{Re} I$  to allow for the hard core at  $R_0$ . This is the result quoted in the text at  $Ka=0$ .

### APPENDIX C: SOLUTION OF INHOMOGENEOUS RECURRENCE RELATIONS

Near  $Ka=0$  it is tempting to expand the three-term recurrence relation in powers of  $Ka$ . Such expansions are asymptotic since one cannot obtain the exact solution, namely  $\exp[-\alpha_k] \equiv \zeta = (Ka)/[1 + \sqrt{1 + (Ka)^2}]$  in the limit that  $\nu \rightarrow \infty$  with a finite number of terms. A more realistic expansion about the point  $E=0$  is obtained by expanding in powers of  $\zeta$ . This is done by setting  $B(\nu) = \zeta^\nu Q(\nu) \tilde{B}(\nu)$  where  $Q(\nu)$  is the exact solution for  $E=0$ . The form of this solution is not needed here, rather only the defining property

$$Q(\nu - 1) = \frac{\nu}{\nu + b(\nu)} Q(\nu) \quad (\text{C1})$$

is employed.

The TTR becomes

$$\begin{aligned} \zeta^2 \left[ - \left( 1 + \frac{b(\nu)}{\nu} \right) \left( 1 + \frac{b(\nu+1)}{\nu+1} \right) \tilde{B}(\nu+1) + \tilde{B}(\nu) \right] \\ = \tilde{B}(\nu) - \tilde{B}(\nu-1). \end{aligned} \quad (\text{C2})$$

Expanding  $\tilde{B}(\nu)$  in a power series in  $\zeta^2$

$$\tilde{B}(\nu) = \sum_{k=0}^{\infty} \tilde{B}^{(k)}(\nu) \zeta^{2k}, \quad (\text{C3})$$

where  $\tilde{B}^{(0)}(\nu)=1$  gives an inhomogeneous recurrence relation for  $\tilde{B}^{(1)}$ , namely,

$$-\left[\frac{b(\nu)}{\nu} + \frac{b(\nu+1)}{\nu+1} + \frac{b(\nu)b(\nu+1)}{\nu(\nu+1)}\right] \equiv D(\nu) = \tilde{B}^{(1)}(\nu) - \tilde{B}^{(1)}(\nu-1), \tag{C4}$$

where the driving term  $D(\nu)$  is defined by Eq. (C4). One readily verifies that the expression

$$\tilde{B}^{(1)}(\nu) = -\lim_{N \rightarrow \infty} \sum_{n=0}^N D(\nu+n+1) \tag{C5}$$

is a solution of the inhomogeneous recurrence relation Eq. (C4). Other solutions are obtained by adding a periodic function to the principal solution of Eq. (C5); however, such solutions do not vanish in the limit  $\nu \rightarrow \infty$ , thus they play no role in the present application.

The sum over the driving terms can be carried out in essentially closed form using the summation properties of hypergeometric functions. To carry out these sums we may use the definition

$${}_2F(\nu, 1, \nu+1, e^{ip\pi/s}) = \nu \sum_{n=0}^{\infty} \frac{\exp[inp\pi/s]}{\nu+n}, \tag{C6}$$

where  $s$  and  $p$  are integers. Of course, the sum already defines a hypergeometric function; however, such functions are not convenient for numerical evaluation since  $\exp(i\pi/s)$  has unit magnitude.

To take advantage of integer values of  $p$  and  $s$  we set  $n = sk+j$  where  $k$  and  $j$  are integers. Then the sum is written

$$F = \frac{\nu}{s} \sum_{j=1}^{s-1} \exp(ipj\pi/s) \sum_{k=0}^{\infty} \frac{\exp(ikp\pi)}{k + (\nu+j)/s} = \frac{\nu}{s} \sum_{j=1}^{s-1} \exp(ipj\pi/s) \frac{1}{a_j} {}_2F(a_j, 1; a_j+1; \exp(ip\pi)), \tag{C7}$$

where  $a_j = (\nu+j)/s$ . When  $p$  is even we may use that

$$\sum_{j=0}^{s-1} \exp(ipj\pi/s) = 0 \tag{C8}$$

in Eq. (15.3.10) of Ref. [30] to evaluate the sum over hypergeometric functions of unit argument. One obtains

$$F = -\frac{\nu}{s} \sum_{j=0}^{s-1} \exp(ipj\pi/s) \psi(a_j), \tag{C9}$$

where  $\psi(a_j)$  is the digamma function.

Alternatively, when  $\exp(ip\pi) = -1$  use of Eq. (15.1.23) of Ref. [30] gives

$$F = \frac{\nu}{2s} \sum_{j=0}^{s-1} \exp(ipj\pi/s) [\psi(1/2 + a_j/2) - \psi(a_j/2)], \tag{C10}$$

where  $a_j$  is defined above. Actually, this expression may be derived from Eq. (C9) by replacing  $p$  and  $s$  by  $2p$  and  $2s$ . In any case, the relatively simple closed-form expression given by Eq. (C9) is readily evaluated.

We first write the driving term in the form

$$-D(\nu) = \frac{\alpha(\nu)}{\nu} + \frac{\beta(\nu+1)}{\nu+1}, \tag{C11}$$

where

$$\alpha(\nu) = b(\nu)(1 + b(\nu+1)), \tag{C12}$$

$$\beta(\nu+1) = b(\nu+1)(1 - b(\nu)). \tag{C13}$$

Then the sum becomes

$$-\sum_{n=0}^{\infty} D(\nu+n+1) = \sum_{n=0}^{\infty} \frac{\alpha(\nu+n+1) + \beta(\nu+n+1)}{\nu+n+1} = -\frac{\beta(\nu+1)}{\nu+1}. \tag{C14}$$

Now

$$b(\nu+1)[b(\nu+2) - b(\nu)] = -\left(-\frac{8}{\sqrt{3}}\right)^2 \frac{\sin \pi(\nu+1)/6}{\cos \pi(\nu+1)/2} \left[ \frac{\sin[\pi(\nu+1)/6 + \pi/6] + \sin[\pi(\nu+1)/6 - \pi/6]}{\sin \pi(\nu+1)/2} \right] = -\left(-\frac{8}{\sqrt{3}}\right)^2 4 \frac{\sin^2[\pi(\nu+1)/6] \cos(\pi/6)}{\sin \pi(\nu+1)} = -\sqrt{3} \left(-\frac{8}{\sqrt{3}}\right)^2 \frac{1 - \cos[\pi(\nu+1)/3]}{\sin[\pi(\nu+1)]}. \tag{C15}$$

We also need the term with  $2b(\nu+1)$  for which

$$\begin{aligned}
 2b(\nu+1) &= 2\left(-\frac{8}{\sqrt{3}}\right)\frac{\sin \pi(\nu+1)/6}{\cos \pi(\nu+1)/2} \\
 &= 2\left(-\frac{8}{\sqrt{3}}\right)\frac{\sin \pi(\nu+1)/6 \sin \pi(\nu+1)/2}{\cos \pi(\nu+1)/2 \sin \pi(\nu+1)/2} \\
 &= 2\left(-\frac{8}{\sqrt{3}}\right)\frac{\cos \pi(\nu+1)/3 - \cos 2\pi(\nu+1)/3}{\sin \pi(\nu+1)}.
 \end{aligned}
 \tag{C16}$$

From this we see that we need three sums, namely,

$$\begin{aligned}
 f_1(\nu+1) &= \frac{1}{\sin \pi(\nu+1)} \sum_n \frac{e^{i\pi n}}{\nu+n+1} \\
 &= \frac{1}{\sin \pi(\nu+1)} \frac{1}{\nu+1} F(\nu+1, 1; \nu+2; -1) \\
 &= \frac{1}{\sin \pi(\nu+1)} \frac{1}{2} \left[ \psi\left(\frac{1}{2} + \frac{\nu+1}{2}\right) - \psi\left(\frac{\nu+1}{2}\right) \right],
 \end{aligned}
 \tag{C17}$$

$$\begin{aligned}
 f_2(\nu+1) &= \sum_{n=0}^{\infty} \frac{\cos \pi(\nu+1+n)/3}{\sin \pi(\nu+1+n)(\nu+1+n)} \\
 &= \text{Re} \left[ \frac{e^{i\pi(\nu+1)/3}}{\sin \pi(\nu+1)} \sum_n \frac{e^{i4\pi n/3}}{\nu+n+1} \right] \\
 &= \text{Re} \left[ \frac{e^{i\pi(\nu+1)/3}}{\sin \pi(\nu+1)} \frac{1}{\nu+1} F(\nu+1, 1; \nu+2; e^{i4\pi/3}) \right] \\
 &= \text{Re} \left[ \frac{e^{i\pi(\nu+1)/3}}{\sin \pi(\nu+1)} \left(-\frac{1}{3}\right) \sum_{j=0}^2 e^{i4j\pi/3} \psi\left(\frac{\nu+1+j}{3}\right) \right] = \\
 &\quad - \frac{1}{3 \sin \pi(\nu+1)} \sum_{j=0}^2 \cos \pi(\nu+1 \\
 &\quad + 4j)/3 \psi\left(\frac{\nu+1+j}{3}\right),
 \end{aligned}$$

$$\begin{aligned}
 f_3(\nu+1) &= \sum_{n=0}^{\infty} \frac{\cos 2\pi(\nu+1+n)/3}{\sin \pi(\nu+1+n)(\nu+1+n)} \\
 &= \text{Re} \left[ \frac{e^{i2\pi(\nu+1)/3}}{\sin \pi(\nu+1)} \sum_{n=0}^{\infty} \frac{e^{i5\pi n/3}}{\nu+n+1} \right] \\
 &= \text{Re} \left[ \frac{e^{i2\pi(\nu+1)/3}}{\sin \pi(\nu+1)} \frac{1}{\nu+1} F(\nu+1, 1; \nu+2; e^{i5\pi/3}) \right]
 \end{aligned}$$

$$\begin{aligned}
 &= \text{Re} \left\{ \frac{e^{i2\pi(\nu+1)/3}}{\sin \pi(\nu+1)} \left(\frac{1}{6}\right) \sum_{j=0}^2 e^{i5\pi j/3} \left[ \psi\left(\frac{1}{2} + \frac{\nu+1+j}{6}\right) \right. \right. \\
 &\quad \left. \left. - \psi\left(\frac{\nu+1+j}{6}\right) \right] \right\} \\
 &= \frac{1}{6 \sin \pi(\nu+1)} \sum_{j=0}^2 \cos \pi[2(\nu+1)+j5]/3 \\
 &\quad \times \left[ \psi\left(\frac{1}{2} + \frac{\nu+1+j}{6}\right) - \psi\left(\frac{\nu+1+j}{6}\right) \right].
 \end{aligned}
 \tag{C18}$$

Our final answer is

$$\begin{aligned}
 \tilde{B}^{(1)}(\nu) &= 2\left(-\frac{8}{\sqrt{3}}\right)[f_2(\nu+1) - f_3(\nu+1)] - \sqrt{3}\left(-\frac{8}{\sqrt{3}}\right)^2 \\
 &\quad \times [f_1(\nu+1) - f_2(\nu+1)] - \frac{\beta(\nu+1)}{\nu+1},
 \end{aligned}
 \tag{C19}$$

where

$$\begin{aligned}
 \beta(\nu+1) &= \left(-\frac{8}{\sqrt{3}}\right)\frac{\sin \pi(\nu+1)/6}{\cos \pi(\nu+1)/2} \left[ 1 - \left(-\frac{8}{\sqrt{3}}\right)\frac{\sin \pi\nu/6}{\cos \pi\nu/2} \right] \\
 &= 2\left(-\frac{8}{\sqrt{3}}\right)\frac{\sin \pi(\nu+1)/6}{\sin \pi(\nu+1)} \\
 &\quad \times \left[ \cos \pi\nu/2 - \left(-\frac{8}{\sqrt{3}}\right)\sin \pi\nu/6 \right].
 \end{aligned}
 \tag{C20}$$

For the special case of  $\nu = -it_0$  we get  $\tilde{B}^{(1)}(-it_0) = 1 + i0.6924$ . This value is used in the text to compute an energy-dependent phase  $\delta_0$ . Taking into account that

$$\left(\frac{2\xi}{Ka}\right)^{-it_0} \approx 1 + \frac{it_0}{4}(Ka)^2,
 \tag{C21}$$

we obtain

$$\begin{aligned}
 \arg[\beta/P_R(-it_0)] &= 1.588 + \left(0.6924 + \frac{it_0}{4}\right)(Ka)^2 \\
 &= 1.588 + i0.944(Ka)^2,
 \end{aligned}
 \tag{C22}$$

where  $\beta$  is defined by Eq. (39).

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