

Three-body scattering hypervolume of particles with unequal masses

Zipeng Wang  and Shina Tan *

International Center for Quantum Materials, Peking University, Beijing 100871, China



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We analyze the collision of three particles with arbitrary mass ratio at zero collision energy, assuming arbitrary short-range potentials, and generalize the three-body scattering hypervolume D first defined for identical bosons in 2008. We solve the three-body Schrödinger equation asymptotically when the three particles are far apart or one pair and a third particle are far apart, deriving two asymptotic expansions of the wave function, and the parameter D appears at the order $1/B^4$, where B is the overall size of the triangle formed by the particles. We then analyze the ground state energy of three such particles with vanishing or negligible two-body scattering lengths in a large periodic volume of side length L , where the three-body parameter contributes a term of the order D/L^6 . From this result we derive some properties of a two-component Bose gas with negligible two-body scattering lengths: its energy density at zero temperature, the corresponding generalized Gross-Pitaevskii equation, the conditions for the stability of the two-component mixture against collapse or phase separation, and the decay rates of particle densities due to three-body recombination.

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I. INTRODUCTION

How do particles, composite or fundamental, such as atoms, molecules, ions, atomic nuclei, neutrons, protons, electrons, mesons, etc., interact at small collision energies? It depends on their electric charges. If at least one of two such particles is electrically neutral, usually the effective interaction between the two particles is dominated by the s -wave scattering length a , for collision energies that are so small that the de Broglie wavelength of each particle in the center-of-mass frame is much longer than the physical range of the interaction. If we need more precise knowledge of the effective pairwise interaction at small collision energies, we need to also know other parameters such as the s -wave effective range r_s , the p -wave scattering volume a_p , etc. All these parameters can be extracted from the wave functions for the two-body collision at collision energies equal to or close to zero, outside of the physical range of interaction. The s -wave scattering length a , for example, can be extracted from the wave function $\phi(\mathbf{s})$ of the two particles colliding at zero incoming kinetic energy and zero orbital angular momentum [1,2]:

$$\phi(\mathbf{s}) = 1 - \frac{a}{s}, \quad \text{if } s > r_e, \quad (1)$$

where \mathbf{s} is the spatial vector extending from one particle to the other, and r_e is the range of the microscopic interaction. The scattering length a is a key parameter in the quantum few-body and many-body physics for particles with small collision energies.

If we want to gain more precise knowledge of the effective interaction strengths of low-energy particles, we need to also study the wave function for the collision of three particles

at zero incoming kinetic energy. The three-body Schrödinger equation is usually not analytically solvable, even outside of the range of the microscopic interactions. But, in a prior paper by one of the present authors, the three-body Schrödinger equation was solved asymptotically for the collision of three identical bosons at zero incoming kinetic energy and zero orbital angular momentum, yielding well-controlled expansions of the three-body wave function $\Phi^{(3)}$ when three or two pairwise distances are large [3]. In such expansions, a three-body parameter named three-body scattering hypervolume D emerges [3]. When all three pairwise distances go to infinity simultaneously for a fixed ratio of pairwise distances, the three-body wave function has the following expansion, which may be called “111 expansion” (since each particle is alone when they are all far apart from each other):

$$\Phi^{(3)} = 1 - \Xi - \frac{\sqrt{3}D}{8\pi^3 B^4} + O(B^{-5} \ln B), \quad (2)$$

where $B = \sqrt{(s_1^2 + s_2^2 + s_3^2)/2}$ is the hyperradius of the triangle formed by the particles,

$$\mathbf{s}_1 \equiv \mathbf{r}_2 - \mathbf{r}_3, \quad \mathbf{s}_2 \equiv \mathbf{r}_3 - \mathbf{r}_1, \quad \mathbf{s}_3 \equiv \mathbf{r}_1 - \mathbf{r}_2, \quad (3)$$

\mathbf{r}_i is the position vector of the i th particle, and Ξ is a sum of a few terms due to a typically nonzero two-body scattering length. If $a = 0$, $\Xi = 0$. When two particles are kept at a fixed distance but the third particle is far away from the two, there is another expansion which may be called the “21 expansion” (since two particles are held at a fixed distance but the remaining particle is far apart):

$$\Phi^{(3)} = \sum_{q=0}^{\infty} S^{(-q)}, \quad (4)$$

*shinatan@pku.edu.cn

where $S^{(-q)}$ scales as R^{-q} for $q \leq 3$, and scales as R^{-q} times some polynomial of $\ln R$ for $q \geq 4$, and R is the distance between the center of mass of the two particles and the remaining particle. The function $S^{(-q)}$ is expressed in terms of the “two-body special functions” such as the $\phi(\mathbf{s})$ in Eq. (1), with coefficients that depend on R . The three-body scattering hypervolume D appears at the order R^{-4} .

The scattering hypervolume D is the three-body analog of the two-body scattering length a . It is a fundamental parameter determining the effective strength of three-body interactions at small collision energies, if the microscopic interactions vanish or become negligible beyond a certain range. For given microscopic interactions, one can numerically solve the Schrödinger equation for the zero-energy collision of the three particles and match the solution to either the 111 expansion or the 21 expansion to determine D numerically. D have been numerically computed in this way for identical bosons interacting with hard-sphere [3], Gaussian [4], square-well [5], and Lennard-Jones [6] potentials.

If the collision of the three particles is purely elastic, D is a real number. But if the two-body forces are so strongly attractive that they support two-body bound states, as is the case for most neutral atoms, then the three-body collisions are usually not purely elastic: two such particles may fall into one of the bound states, releasing the binding energy in the form of the center-of-mass kinetic energy of the two and the kinetic energy of the remaining free particle; these inelastic processes are called “three-body recombination” in cold atoms physics [7–14]. When there is three-body recombination, D becomes complex, and the three-body recombination rate constant is proportional to the imaginary part of D [4,15].

The three-body scattering hypervolume [3] determines the effective three-body coupling constant in the effective-field theoretical description of low-energy particles [3,14,16]. It is also directly related to the three-body parameters in three-meson systems [17,18].

The three-body scattering hypervolume provides a three-body effective interaction which, if repulsive, can stabilize dilute quantum droplets [19–21].

In Sec. II of this paper, we generalize the 111 expansion and the 21 expansion to the collision of three particles with *unequal* masses, m_1 , m_2 , m_3 , for which we find that the expansions take much more complicated forms. We assume that two or three of the colliding particles are electrically neutral, and our expansions are also applicable to the collision of two neutral particles and one charged particle, such as two neutral mesons and one charged particle, as long as the neutral particles are not significantly electrically polarizable in the field of the charged particles. Although in a prior paper [3] the two expansions were carried out to the order B^{-7} and R^{-7} respectively, in this paper we will only expand $\Phi^{(3)}$ to the order B^{-4} and R^{-4} , respectively, the order at which the three-body scattering hypervolume first appears. If two of the particles have equal mass but are *not* spin-polarized identical fermions, and the third particle has a different mass, the expansions we find in this paper are also applicable. Our work is motivated by many cold atoms experiments in which two or three atomic species having different atomic masses are mixed together. But we believe our work will also be

of fundamental importance for other research areas such as nuclear physics.

In Sec. III we compute the ground state energy of three particles with unequal masses in a large periodic cubic volume, assuming vanishing or negligible two-body scattering lengths, such that the energy is dominated by the three-body scattering hypervolume D .

In Sec. IV we consider a zero-temperature Bose-Bose mixture having negligible two-body scattering lengths and derive its energy density in terms of the three-body scattering hypervolumes D_1 , D_{112} , D_{122} , and D_2 , and write down the corresponding generalized Gross-Pitaevskii equation. Here D_1 is the scattering hypervolume of three particles of type 1, and D_{112} is the scattering hypervolume of two particles of type 1 and one particle of type 2, and so on. We then give the criteria for stability of the mixture against collapse or phase separation. Finally we study the decay rates of the particle densities in such a mixture due to three-body recombination, in a shallow trap.

II. ASYMPTOTICS OF THE THREE-BODY WAVE FUNCTION

Consider three particles, labeled 1, 2, and 3, having masses m_1 , m_2 , and m_3 , respectively. Suppose that they have interactions that are invariant under translation, rotation, and Galilean transformations, and suppose the interactions vanish beyond a certain range. Particles 1 and 2 have scattering length a_3 , particles 2 and 3 have scattering length a_1 , and particles 3 and 1 have scattering length a_2 . If the three particles collide with zero energy and zero orbital angular momentum, the three-body wave function $\Phi^{(3)}$ satisfies the Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 - \frac{\hbar^2}{2m_3}\nabla_3^2 + V_1(s_1) + V_2(s_2) + V_3(s_3) + V_{123}(s_1, s_2, s_3) \right] \Phi^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = 0, \quad (5)$$

where \mathbf{r}_i is the position vector of particle i , and

$$\mathbf{s}_i \equiv \mathbf{r}_j - \mathbf{r}_k. \quad (6)$$

In the above equation and in the rest of the paper:

if $i = 1$, then $j = 2, k = 3$;

if $i = 2$, then $j = 3, k = 1$;

if $i = 3$, then $j = 1, k = 2$.

$V_i(s_i)$ is the interaction potential between particles j and k , and $V_{123}(s_1, s_2, s_3)$ is the three-body potential. Note that V_i and V_{123} are *not* zero-range pseudopotentials. They are real potentials that extend to some nonzero pairwise distances. But in this paper we assume that these potentials vanish beyond a certain range. $\Phi^{(3)}$ is translationally invariant because of the zero total linear momentum:

$$\Phi^{(3)}(\mathbf{r}_1 + \delta\mathbf{r}, \mathbf{r}_2 + \delta\mathbf{r}, \mathbf{r}_3 + \delta\mathbf{r}) = \Phi^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \quad (7)$$

for all $\delta\mathbf{r}$. $\Phi^{(3)}$ is also rotationally invariant because of the zero orbital angular momentum. As a result, $\Phi^{(3)}$ depends only on the pairwise distances s_1 , s_2 , and s_3 . We choose the

amplitude of $\Phi^{(3)}$ such that it approaches 1 when the three pairwise distances all go to infinity.

A. Jacobi coordinates, hyperradius, and hyperangles

For later use, we define \mathbf{R}_i as the vector extending from the center of mass of particles j and k to particle i :

$$\mathbf{R}_i \equiv \mathbf{r}_i - \frac{m_j \mathbf{r}_j + m_k \mathbf{r}_k}{m_j + m_k}. \tag{8}$$

$(\mathbf{s}_i, \mathbf{R}_i)$ are called Jacobi coordinates [15,22]. We define the hyperradius B as

$$B \equiv \sqrt{\frac{3}{2} \frac{m_1 m_2 s_3^2 + m_2 m_3 s_1^2 + m_3 m_1 s_2^2}{m_1 m_2 + m_2 m_3 + m_3 m_1}}. \tag{9}$$

If the particles have equal mass, the above definition of B reduces to the one in Ref. [3]. Let μ_i be the reduced mass of particles j and k , and v_i be the reduced mass of the particle i and the pair jk :

$$\frac{1}{\mu_i} \equiv \frac{1}{m_j} + \frac{1}{m_k}, \quad \frac{1}{v_i} \equiv \frac{1}{m_i} + \frac{1}{m_j + m_k}. \tag{10}$$

They satisfy

$$\mu_i v_i = \frac{m_1 m_2 m_3}{m_1 + m_2 + m_3}. \tag{11}$$

Define

$$\epsilon_i \equiv \sqrt{\frac{\mu_i}{v_i}}, \tag{12}$$

$$\lambda \equiv \frac{3}{2} \frac{m_1 + m_2 + m_3}{m_1 m_2 + m_2 m_3 + m_3 m_1}. \tag{13}$$

One can show that

$$B^2 = \lambda(v_i R_i^2 + \mu_i s_i^2) \tag{14}$$

for any $i \in \{1, 2, 3\}$. We also define three hyperangles:

$$\theta_i \equiv \arctan \frac{R_i}{\epsilon_i s_i}. \tag{15}$$

$s_i, R_i,$ and B satisfy

$$s_i = \frac{1}{\sqrt{\lambda \mu_i}} B \cos \theta_i, \quad R_i = \frac{1}{\sqrt{\lambda v_i}} B \sin \theta_i. \tag{16}$$

B. Two-body special functions

For $i = 1, 2,$ or $3,$ we define the two-body special functions $\phi_{i,\hat{\mathbf{n}}}^{(l)}(\mathbf{s}), f_{i,\hat{\mathbf{n}}}^{(l)}(\mathbf{s}), g_{i,\hat{\mathbf{n}}}^{(l)}(\mathbf{s}), \dots$ for the collision of particles j and k with orbital angular momentum quantum number l and zero magnetic quantum number along the direction specified by the unit vector $\hat{\mathbf{n}}$ [3]:

$$\tilde{H}_i \phi_{i,\hat{\mathbf{n}}}^{(l)} = 0, \quad \tilde{H}_i f_{i,\hat{\mathbf{n}}}^{(l)} = \phi_{i,\hat{\mathbf{n}}}^{(l)}, \quad \tilde{H}_i g_{i,\hat{\mathbf{n}}}^{(l)} = f_{i,\hat{\mathbf{n}}}^{(l)}, \dots, \tag{17}$$

where $\tilde{H}_i = \hbar^2 \tilde{H}_i / 2\mu_i$ is the two-body Hamiltonian for the collision of particles j and k in the center-of-mass frame, and

$$\tilde{H}_i \equiv -\nabla_s^2 + \frac{2\mu_i}{\hbar^2} V_i(s). \tag{18}$$

Unlike the case of identical bosons [3], here l may be odd.

To complete the definition of $\phi_{i,\hat{\mathbf{n}}}^{(l)}$, we need to specify its overall amplitude. Since the potential $V_i(s)$ vanishes beyond a finite range $r_e,$ $\phi_{i,\hat{\mathbf{n}}}^{(l)}$ takes a simple form at $s > r_e:$

$$\phi_{i,\hat{\mathbf{n}}}^{(l)}(\mathbf{s}) = \left[\frac{s^l}{(2l+1)!!} - \frac{(2l-1)!! a_{i,l}}{s^{l+1}} \right] P_l(\hat{\mathbf{n}} \cdot \hat{\mathbf{s}}), \tag{19}$$

where we have fixed the overall amplitude of $\phi_{i,\hat{\mathbf{n}}}^{(l)}$ by specifying the coefficient of the term $\propto s^l.$ Here P_l is the Legendre polynomial. The parameter $a_{i,l}$ is determined by solving the two-body Schrödinger equation at zero collision energy, $\tilde{H}_i \phi_{i,\hat{\mathbf{n}}}^{(l)} = 0,$ using the two-body potential $V_i(s)$ at $s < r_e,$ and matching the solution with Eq. (19) at $s > r_e.$

The solution to the equation $\tilde{H}_i f_{i,\hat{\mathbf{n}}}^{(l)} = \phi_{i,\hat{\mathbf{n}}}^{(l)}$ is not unique, because if $f_{i,\hat{\mathbf{n}}}^{(l)}(s)$ satisfies this equation, then $f_{i,\hat{\mathbf{n}}}^{(l)}(s) + (\text{arbitrary coefficient}) \times \phi_{i,\hat{\mathbf{n}}}^{(l)}(s)$ also satisfies this equation. To complete the definition of $f_{i,\hat{\mathbf{n}}}^{(l)}(s),$ we specify that in the expansion of $f_{i,\hat{\mathbf{n}}}^{(l)}(s)$ at $s > r_e$ we do not have the term $\propto s^{-l-1}$ (if such a term exists, we can add a suitable coefficient times $\phi_{i,\hat{\mathbf{n}}}^{(l)}(s)$ to $f_{i,\hat{\mathbf{n}}}^{(l)}(s)$ to cancel this term). Then at $s > r_e$ we have the following analytical formula for $f_{i,\hat{\mathbf{n}}}^{(l)}(s):$

$$f_{i,\hat{\mathbf{n}}}^{(l)}(\mathbf{s}) = \left[-\frac{s^{l+2}}{2(2l+3)!!} - \frac{a_{i,l} r_{i,l} s^l}{2(2l+1)!!} - \frac{(2l-3)!!}{2} a_{i,l} s^{l-1} \right] P_l(\hat{\mathbf{n}} \cdot \hat{\mathbf{s}}). \tag{20}$$

This completes the definition of $f_{i,\hat{\mathbf{n}}}^{(l)}(s).$ We can similarly fix the definitions of $g_{i,\hat{\mathbf{n}}}^{(l)}(s),$ etc. For brevity we do not show the formula for $g_{i,\hat{\mathbf{n}}}^{(l)}(\mathbf{s})$ at $s > r_e$ as it is not explicitly used in this paper.

Given the two-body special functions $\phi_{i,\hat{\mathbf{n}}}^{(l)}, f_{i,\hat{\mathbf{n}}}^{(l)}, g_{i,\hat{\mathbf{n}}}^{(l)}, \dots,$ we can express the wave function for the collision of particles j and k at any small nonzero energy $E = \hbar^2 k^2 / 2\mu_i$ as an infinite series in $k^2:$

$$\phi_{i,\hat{\mathbf{n}}}^{(l,k)}(\mathbf{s}) = \phi_{i,\hat{\mathbf{n}}}^{(l)}(\mathbf{s}) + k^2 f_{i,\hat{\mathbf{n}}}^{(l)}(\mathbf{s}) + k^4 g_{i,\hat{\mathbf{n}}}^{(l)}(\mathbf{s}) + \dots \tag{21}$$

It is easy to verify that this series satisfies the Schrödinger equation at nonzero energy $E,$ namely,

$$\tilde{H}_i \phi_{i,\hat{\mathbf{n}}}^{(l,k)}(\mathbf{s}) = k^2 \phi_{i,\hat{\mathbf{n}}}^{(l,k)}(\mathbf{s}). \tag{22}$$

On the other hand, if $s > r_e,$ then $V_i(s) = 0$ and Eq. (22) can be solved analytically to yield

$$\phi_{i,\hat{\mathbf{n}}}^{(l,k)}(\mathbf{s}) = \alpha_{i,l}(k) [j_l(ks) \cot \delta_{i,l} - n_l(ks)] P_l(\hat{\mathbf{n}} \cdot \hat{\mathbf{s}}), \tag{23}$$

where j_l and n_l are spherical Bessel functions of the first kind and the second kind, respectively, $\delta_{i,l}$ is the scattering phase shift, and the overall coefficient $\alpha_{i,l}(k)$ is to be determined. Comparing Eq. (23) with Eq. (21), and using the definitions of $\phi_{i,\hat{\mathbf{n}}}^{(l)}$ and $f_{i,\hat{\mathbf{n}}}^{(l)},$ etc., we find that $\alpha_{i,l}(k) = -k^{l+1} a_{i,l}$ and

$$k^{2l+1} \cot \delta_{i,l}(k) = -\frac{1}{a_{i,l}} + \frac{1}{2} r_{i,l} k^2 + O(k^4). \tag{24}$$

Equation (24) is in fact the well-known effective range expansion [23]. We now see that $a_{i,l}$ which first appears in Eq. (19)

is the two-body l -wave scattering length (or volume or hypervolume) of particles j and k , and $r_{i,l}$ which first appears in Eq. (20) is the two-body l -wave effective range.

For $l = 0$, we write the functions $\phi_{i,\hat{\mathbf{n}}}^{(0)}(\mathbf{s})$, $f_{i,\hat{\mathbf{n}}}^{(0)}(\mathbf{s})$, and $g_{i,\hat{\mathbf{n}}}^{(0)}(\mathbf{s})$ simply as $\phi_i(\mathbf{s})$, $f_i(\mathbf{s})$, and $g_i(\mathbf{s})$. We use symbols s, p, d, f, \dots to represent $l = 0, 1, 2, 3, \dots$. For later convenience we simply write the s -wave scattering length $a_{i,s}$ as a_i .

The two-body special functions will appear in the expansion of the three-body wave function $\Phi^{(3)}$ when two particles are held at a fixed distance and the third particle is far away from the two.

C. Asymptotics of $\Phi^{(3)}$ at large distances

When particle i is far away from particles j and k , but particles j and k are held at a fixed distance s_i , the pairwise interaction potentials $V_j(s_j)$ and $V_k(s_k)$ and the three-body potential $V_{123}(s_1, s_2, s_3)$ vanish, and Eq. (5) is simplified as

$$\left[-\nabla_{\mathbf{s}_i}^2 + \frac{2\mu_i}{\hbar^2} V_i(s_i) - \frac{\mu_i}{v_i} \nabla_{\mathbf{R}_i}^2 \right] \Phi^{(3)} = 0. \quad (25)$$

The following partial-wave expansion is the formal solution to the above equation:

$$\Phi^{(3)} = \sum_{l=0}^{\infty} [A_i^{(l)}(R_i) \phi_{i,\hat{\mathbf{R}}_i}^{(l)}(\mathbf{s}_i) + B_i^{(l)}(R_i) f_{i,\hat{\mathbf{R}}_i}^{(l)}(\mathbf{s}_i) + C_i^{(l)}(R_i) g_{i,\hat{\mathbf{R}}_i}^{(l)}(\mathbf{s}_i) + \dots], \quad (26)$$

where the function $A_i^{(l)}(R_i)$ has a well-controlled expansion at large R_i , and $B_i^{(l)}(R_i)$, $C_i^{(l)}(R_i)$, \dots satisfy

$$B_i^{(l)}(R_i) = \frac{\mu_i}{v_i} \left[\frac{1}{R_i^2} \frac{d}{dR_i} R_i^2 \frac{d}{dR_i} - \frac{l(l+1)}{R_i^2} \right] A_i^{(l)}(R_i), \quad (27a)$$

$$C_i^{(l)}(R_i) = \frac{\mu_i}{v_i} \left[\frac{1}{R_i^2} \frac{d}{dR_i} R_i^2 \frac{d}{dR_i} - \frac{l(l+1)}{R_i^2} \right] B_i^{(l)}(R_i), \quad (27b)$$

and so on. We may also group the terms according to the powers of $1/R_i$:

$$\Phi^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \sum_{q=0}^{\infty} S_i^{(-q)}(\mathbf{R}_i, \mathbf{s}_i), \quad (28)$$

where $S_i^{(-q)}$ scales as R_i^{-q} times some polynomial of $\ln R_i$ (such a logarithmic dependence on R_i could be absent for a small q), and satisfies

$$\begin{aligned} \tilde{H}_i S_i^{(0)} &= 0, \\ \tilde{H}_i S_i^{(-1)} &= 0, \\ \tilde{H}_i S_i^{(-q)} &= \frac{\mu_i}{v_i} \nabla_{\mathbf{R}_i}^2 S_i^{(-q+2)} \quad (q \geq 2). \end{aligned} \quad (29)$$

Equation (28) is the 21 expansion.

When the three particles are all far apart from each other, such that s_1, s_2, s_3 go to infinity simultaneously for any fixed ratio $s_1 : s_2 : s_3$, we may expand $\Phi^{(3)}$ in powers of $1/B$:

$$\Phi^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \sum_{p=0}^{\infty} T^{(-p)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3), \quad (30)$$

where $T^{(-p)}$ scales as B^{-p} times some polynomial of $\ln B$ (such a logarithmic dependence on $\ln B$ could be absent for a small p), and satisfies the free Schrödinger equation:

$$\left(-\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 - \frac{\hbar^2}{2m_3} \nabla_3^2 \right) T^{(-p)} = 0 \quad (31)$$

if the pairwise distances s_i are all nonzero. Equation (30) is the 111 expansion.

We start from the leading-order term in the 111 expansion:

$$T^{(0)} = 1, \quad (32)$$

and first derive $S_i^{(0)}$, and then derive $T^{(-1)}$, and then derive $S_i^{(-1)}$, and then derive $T^{(-2)}$, and so on, all the way until $S_i^{(-4)}$. At every step, we require the 111 expansion and the 21 expansion to be consistent in the region $r_e \ll s_i \ll R_i$. See the Appendix for details. Our resultant 111 expansion is

$$\begin{aligned} \Phi^{(3)} &= 1 - \frac{\sqrt{3}D}{8\pi^3 B^4} + \sum_{i=1}^3 \left\{ -\frac{a_i}{s_i} + \frac{2b_i \theta_i}{\pi R_i s_i} - \frac{2\lambda v_i w_i a_i}{\pi B^2 s_i} + \frac{m_s}{B^4} J_i^{(s)} \left[\left(\ln \frac{B}{\sqrt{\lambda v_i |a_i|}} \right) + \gamma - 1 - \theta_i \cot(2\theta_i) \right] \right. \\ &\quad \left. + \frac{d_p}{B^4} J_i^{(p)} \frac{\sin(4\theta_i) - 4\theta_i}{\sin^2(2\theta_i)} (\hat{\mathbf{R}}_i \cdot \hat{\mathbf{s}}_i) \right\} + O(B^{-5} \ln^n B), \end{aligned} \quad (33)$$

where $\gamma = 0.57721566\dots$ is Euler's constant, n is a non-negative integer (we conjecture here $n = 1$, just like the case of identical bosons [3]), and

$$b_i = a_i(a_j + a_k), \quad (34a)$$

$$w_i = -\epsilon_i b_i + \frac{\beta_k b_j}{\eta_{ik}} + \frac{\beta_j b_k}{\eta_{ij}}, \quad (34b)$$

$$\eta_{\mu\nu} = \frac{m_\mu}{m_\mu + m_\nu}, \quad \text{for } \mu, \nu \in \{1, 2, 3\}, \quad (34c)$$

$$\beta_i = \arctan \sqrt{\frac{m_j m_k}{m_i(m_1 + m_2 + m_3)}}, \quad (34d)$$

$$m_s = \frac{18(m_1 m_2 m_3)^{3/2} \sqrt{m_1 + m_2 + m_3}}{\pi^2 (m_1 m_2 + m_2 m_3 + m_3 m_1)^2}, \quad (34e)$$

$$d_p = \frac{27 m_1 m_2 m_3 (m_1 + m_2 + m_3)}{2\pi (m_1 m_2 + m_2 m_3 + m_3 m_1)^2}, \quad (34f)$$

$$J_i^{(s)} = a_i \left(\frac{w_j a_j}{\mu_j} + \frac{w_k a_k}{\mu_k} \right), \quad (34g)$$

$$J_i^{(p)} = a_{i,p} \frac{m_j a_j - m_k a_k}{m_j + m_k}. \quad (34h)$$

D is the *three-body scattering hypervolume*, and its dimension is $[\text{length}]^4$. It is the generalization of the scattering

hypervolume for identical bosons defined in Ref. [3]. The value and sign of the scattering hypervolume in each three-particle system depend on the details of two-body and three-body potentials, as well as the masses of the three particles. For very weakly repulsive potentials D is small and positive. For very weakly attractive potentials D is small and negative. As one increases the strength of attractive interactions such that they nearly support a three-body bound state, D becomes large and negative. At the critical attraction strength at which the three-body s -wave bound state energy is zero, D is divergent. As one slightly increases the strength of attraction further, then D becomes large and positive. Fur-

ther increasing the strength of attraction, one can make D smaller. D will pass zero and turn negative as one further increases the strength of attraction. If the two-body potentials are sufficiently strongly attractive such that there are two-body bound states, D will in general acquire some imaginary part which determines the three-body recombination rate constant for dilute gases consisting of the relevant particles (the rate constant is proportional to $\text{Im}D$) [4]. If there are multiple two-body bound states, then $\text{Im}D$ contains the contributions from the three-body recombination processes to all these two-body bound states.

Our resultant 21 expansion is

$$\begin{aligned} \Phi^{(3)} = & \left[1 - \frac{a_j + a_k}{R_i} + \frac{2w_i}{\pi R_i^2} - \frac{2\mu_i}{\pi R_i^3} \left(\frac{w_j a_j}{\mu_j} + \frac{w_k a_k}{\mu_k} \right) + \frac{W_i}{R_i^4} + \frac{8\epsilon_i \mu_i J^{(s)}}{\pi^2 R_i^4} \ln \frac{R_i}{|a_i|} \right] \phi_i(\mathbf{s}_i) \\ & + \left(\frac{3}{R_i^2} \frac{m_j a_j - m_k a_k}{m_j + m_k} + \frac{3c_i}{R_i^3} + \frac{\#_{ip}}{R_i^4} \right) \phi_{i,\hat{\mathbf{R}}_i}^{(p)}(\mathbf{s}_i) + \left[-\frac{15}{R_i^3} \frac{m_j^2 a_j + m_k^2 a_k}{(m_j + m_k)^2} + \frac{\#_{id}}{R_i^4} \right] \phi_{i,\hat{\mathbf{R}}_i}^{(d)}(\mathbf{s}_i) \\ & + \frac{105}{R_i^4} \frac{m_j^3 a_j - m_k^3 a_k}{(m_j + m_k)^3} \phi_{i,\hat{\mathbf{R}}_i}^{(f)}(\mathbf{s}_i) + \frac{4\epsilon_i^2 w_i}{\pi R_i^4} f_i(\mathbf{s}_i) + O(R_i^{-5} \ln^n R_i), \end{aligned} \quad (35)$$

where $\phi_{i,\hat{\mathbf{R}}_i}^{(l)}$ and f_i are the two-body special functions for particles j and k as defined in Sec. II B, and

$$J^{(s)} = J_1^{(s)} + J_2^{(s)} + J_3^{(s)}, \quad (36a)$$

$$c_i = -\frac{2b_j}{\pi \eta_{ik}^2} [\epsilon_j \eta_{jk} + (2\eta_{jk} \eta_{ik} - 1)\beta_k] + \frac{2b_k}{\pi \eta_{ij}^2} [\epsilon_k \eta_{kj} + (2\eta_{kj} \eta_{ij} - 1)\beta_j], \quad (36b)$$

$$\#_{ip} = \frac{6\mu_i^2}{\pi} \left(\frac{w_j a_j}{\mu_j m_k} - \frac{w_k a_k}{\mu_k m_j} \right), \quad (36c)$$

$$\begin{aligned} \#_{id} = & \frac{10}{\pi} \left\{ 3b_j \left[\frac{\epsilon_j \mu_i}{\eta_{ik}^2 \mu_j} (2\eta_{jk} \eta_{ik} - 1) + \frac{1}{\eta_{ik}^3} (1 - 2\eta_{jk} \eta_{ik} + 2\eta_{jk}^2 \eta_{ik}^2) \beta_k - \epsilon_i^2 \frac{2\beta_k}{3\eta_{ik}} \right] \right. \\ & \left. + 3b_k \left[\frac{\epsilon_k \mu_i}{\eta_{ij}^2 \mu_k} (2\eta_{kj} \eta_{ij} - 1) + \frac{1}{\eta_{ij}^3} (1 - 2\eta_{kj} \eta_{ij} + 2\eta_{kj}^2 \eta_{ij}^2) \beta_j - \epsilon_i^2 \frac{2\beta_j}{3\eta_{ij}} \right] \right\}, \end{aligned} \quad (36d)$$

$$\begin{aligned} W_i = & -\frac{(m_1 m_2 + m_2 m_3 + m_3 m_1)^2 D}{6\sqrt{3}\pi^3 m_i^2 (m_j + m_k)^2} + \frac{2\epsilon_i^2 w_i a_i r_{i,s}}{\pi} + \frac{8\epsilon_i \mu_i}{\pi^2} \left\{ J_i^{(s)} \left(\gamma - \frac{3}{2} \right) + J_j^{(s)} \left[\gamma + \ln \left(\sqrt{\frac{v_i}{v_j}} \frac{|a_i|}{|a_j|} \right) - 1 - \beta_k \cot 2\beta_k \right] \right. \\ & \left. + J_k^{(s)} \left[\gamma + \ln \left(\sqrt{\frac{v_i}{v_k}} \frac{|a_i|}{|a_k|} \right) - 1 - \beta_j \cot 2\beta_j \right] \right\} + \frac{6\epsilon_i^2}{\pi} \left[J_j^{(p)} \frac{\sin(4\beta_k) - 4\beta_k}{\sin^2(2\beta_k)} - J_k^{(p)} \frac{\sin(4\beta_j) - 4\beta_j}{\sin^2(2\beta_j)} \right]. \end{aligned} \quad (36e)$$

III. THE GROUND STATE ENERGY OF THREE PARTICLES IN A PERIODIC BOX

In this section, we consider the ground state of three particles in a large periodic cubic box with side length L . Their wave function satisfies the periodic boundary condition:

$$\begin{aligned} \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) &= \Psi(\mathbf{r}_1 + \mathbf{L}, \mathbf{r}_2, \mathbf{r}_3) \\ &= \Psi(\mathbf{r}_1, \mathbf{r}_2 + \mathbf{L}, \mathbf{r}_3) = \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3 + \mathbf{L}), \end{aligned} \quad (37)$$

where $\mathbf{L} = L(n_x \hat{\mathbf{e}}_x + n_y \hat{\mathbf{e}}_y + n_z \hat{\mathbf{e}}_z)$. Here \mathbf{e}_x , \mathbf{e}_y , and \mathbf{e}_z are unit vectors along the sides of the cube, and n_x , n_y , and n_z are integers.

Here we assume the two-body s -wave scattering lengths a_1, a_2, a_3 are 0, while the three-body scattering hypervolume D is not. If there are no two-body or three-body bound states,

the three-body ground state wave function takes a simple form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \approx 1 - \frac{\sqrt{3}D}{8\pi^3 B^4} \quad (38)$$

at $r_e \ll s_i \ll L$, where r_e is the maximum range of two-body and three-body interactions. The wave function should also satisfy the free Schrödinger equation

$$-\frac{\hbar^2}{2} (\nabla_1^2/m_1 + \nabla_2^2/m_2 + \nabla_3^2/m_3) \Psi = E \Psi \quad (39)$$

if s_1, s_2 , and s_3 are all greater than r_e . Because the ground state has zero total momentum, Ψ depends only on (s_2, s_3) , and can be written as $\Psi = \Psi(s_2, s_3)$. We multiply both sides of Eq. (39) by $d^3 s_2 d^3 s_3$ and integrate over s_2 and s_3 in the domain $B > B_0$ (where $r_e \ll B_0 \ll L$): the right-hand side yields approximately EL^6 , and the left-hand side can be computed by

using Gauss's theorem and Eq. (38). We get

$$E = \frac{\hbar^2 \tilde{D}}{L^6}, \quad (40)$$

where

$$\tilde{D} \equiv \frac{\sqrt{3}(m_1 m_2 + m_2 m_3 + m_3 m_1)^2}{9(m_1 m_2 m_3)^{3/2} \sqrt{m_1 + m_2 + m_3}} D. \quad (41)$$

The dimension of \tilde{D} is [length]⁴/[mass].

If there are three-body bound states but no two-body bound states, Eqs. (38)–(41) are applicable to the lowest-energy three-body scattering state although this is no longer the three-body ground state.

If there are two-body bound states, Eq. (38) would describe a metastable state rather than the ground state. This is analogous to real ultracold atomic gases which are after all not the true ground state of atoms (the true ground state of multiple atoms having attractive interactions is a tiny solid or liquid). One can tune the two-body interactions between ultracold atoms such that the scattering lengths are zero [24], and then the three-body scattering hypervolumes will be among the dominant parameters for low-energy effective interactions.

IV. IMPLICATIONS FOR A DILUTE BOSE-BOSE MIXTURE

We consider an interacting mixture of two Bose-Einstein condensed gases [25–34]. If the scattering lengths are tuned to zero near a Feshbach resonance for cold atoms [24,35] or if they are accidentally close to zero, or if the particles are near a low-energy three-body resonance, the interactions of the particles could be dominated by the three-body scattering hypervolumes. For a two-component Bose gas, consisting of bosons of types 1 and 2, there are four scattering hypervolumes, D_1 , D_{112} , D_{122} , and D_2 . Here D_1 is the intraspecies scattering hypervolume of three bosons of type 1, D_{112} is the scattering hypervolume of two bosons of type 1 and one boson of type 2, D_{122} is the scattering hypervolume of one boson of type 1 and two bosons of type 2, and D_2 is the intraspecies scattering hypervolume of three bosons of type 2.

We consider N_1 bosons of type 1 and N_2 bosons of type 2 having vanishing or negligible intraspecies and interspecies two-body scattering lengths ($a_{11} = a_{12} = a_{22} = 0$) in a large cubic box of side length L , and impose the periodic boundary condition. Using Eq. (40), and assuming low enough densities such that the total ground state energy E may be approximated as a sum of the three-particle energies, we get

$$E = \frac{\hbar^2}{L^6} (C_{N_1}^3 \tilde{D}_1 + C_{N_1}^2 C_{N_2}^1 \tilde{D}_{112} + C_{N_1}^1 C_{N_2}^2 \tilde{D}_{122} + C_{N_2}^3 \tilde{D}_2), \quad (42)$$

where $C_N^n = N!/[n!(N-n)!]$. According to the general relations between \tilde{D} and D in Eq. (41),

$$\tilde{D}_1 = \frac{D_1}{m_1}, \quad (43a)$$

$$\tilde{D}_{112} = \frac{(m_1 + 2m_2)^2}{3m_1 m_2 \sqrt{3m_2(2m_1 + m_2)}} D_{112}, \quad (43b)$$

$$\tilde{D}_{122} = \frac{(2m_1 + m_2)^2}{3m_1 m_2 \sqrt{3m_1(m_1 + 2m_2)}} D_{122}, \quad (43c)$$

$$\tilde{D}_2 = \frac{D_2}{m_2}, \quad (43d)$$

where m_1 is the mass of each boson of type 1, and m_2 is the mass of each boson of type 2. In the thermodynamic limit, in which $N_1, N_2, L \rightarrow \infty$ while the densities $n_1 = N_1/L^3$ and $n_2 = N_2/L^3$ are fixed, we get

$$\frac{E}{\hbar^2 \Omega} = \frac{1}{6} \tilde{D}_1 n_1^3 + \frac{1}{6} \tilde{D}_2 n_2^3 + \frac{1}{2} \tilde{D}_{112} n_1^2 n_2 + \frac{1}{2} \tilde{D}_{122} n_1 n_2^2, \quad (44)$$

where $\Omega = L^3$ is the volume of the system. The energy can also be calculated using the effective field theory (EFT) [16].

Taking the partial derivative of the energy with respect to the densities n_1 or n_2 , we get the chemical potentials μ_1 and μ_2 . Further adding the kinetic energy operators and the external potentials, we find that the two-component Bose-Einstein condensate (BEC) can be described by the following coupled Gross-Pitaevskii equations [36,37]:

$$i\hbar \frac{\partial}{\partial t} \Psi_1 = \left[-\frac{\hbar^2 \nabla^2}{2m_1} + V_1(\mathbf{r}, t) + \frac{\hbar^2}{2} \tilde{D}_1 |\Psi_1|^4 + \hbar^2 \tilde{D}_{112} |\Psi_1|^2 |\Psi_2|^2 + \frac{\hbar^2}{2} \tilde{D}_{122} |\Psi_2|^4 \right] \Psi_1, \quad (45a)$$

$$i\hbar \frac{\partial}{\partial t} \Psi_2 = \left[-\frac{\hbar^2 \nabla^2}{2m_2} + V_2(\mathbf{r}, t) + \frac{\hbar^2}{2} \tilde{D}_{112} |\Psi_1|^4 + \hbar^2 \tilde{D}_{122} |\Psi_1|^2 |\Psi_2|^2 + \frac{\hbar^2}{2} \tilde{D}_2 |\Psi_2|^4 \right] \Psi_2, \quad (45b)$$

where $\Psi_1 = \Psi_1(\mathbf{r}, t)$ and $\Psi_2 = \Psi_2(\mathbf{r}, t)$ are the macroscopic wave functions whose norm squares are the densities n_1 and n_2 , respectively, and $V_1(\mathbf{r}, t)$ and $V_2(\mathbf{r}, t)$ are the external potentials experienced by the bosons of types 1 and 2, respectively. The terms containing $|\Psi_1|^4$, $|\Psi_1|^2 |\Psi_2|^2$, or $|\Psi_2|^4$ in the above two equations generalize the three-body coupling term in the Gross-Pitaevskii equation for a single-component BEC [38,39]. We have related the three-body coupling constants to the wave functions for the zero-energy collisions of three particles, facilitating numerical determinations of these constants for any given microscopic interactions.

In a two-component BEC, if the two-body scattering lengths a_{ij} are not zero, the system is stable when $g_{11} > 0$, $g_{22} > 0$, and $|g_{12}| < \sqrt{g_{11} g_{22}}$ [1,2], where $g_{ij} = 2\pi \hbar^2 a_{ij} / \mu_{ij}$ is the two-body coupling constant, and μ_{ij} is the reduced mass of m_i and m_j . The first and second conditions ensure stability against collapse when only one component exists. The third condition ensures the two species are mixed together, rather than phase separated [25,26,40–43].

Now we derive the conditions for the stability of the two-component BEC with only three-body scattering hypervolumes and negligible two-body scattering lengths. The zero-temperature state energy of a homogeneous gaseous

mixture of the two components is given by Eq. (44). The mixture should be dynamically stable against local density fluctuations [1] if

$$\partial^2 E / \partial n_i^2 > 0 \quad (46)$$

and

$$\left(\frac{\partial^2 E}{\partial n_1^2} \right) \left(\frac{\partial^2 E}{\partial n_2^2} \right) > \left(\frac{\partial^2 E}{\partial n_1 \partial n_2} \right)^2. \quad (47)$$

Substituting Eq. (44) into the above inequalities, we get

$$\begin{aligned} \tilde{D}_{1n_1} + \tilde{D}_{112n_2} &> 0, \\ \tilde{D}_{2n_2} + \tilde{D}_{122n_1} &> 0, \end{aligned} \quad (48)$$

$$(\tilde{D}_{1n_1} + \tilde{D}_{112n_2})(\tilde{D}_{2n_2} + \tilde{D}_{122n_1}) > (\tilde{D}_{112n_1} + \tilde{D}_{122n_2})^2. \quad (49)$$

If the scattering hypervolumes become complex (with negative imaginary parts [4]), the energy in Eq. (44) gains a negative imaginary part, indicating the decaying of the BEC. Within a short time Δt , the probability that no recombination occurs is $\exp(-2|\text{Im}E|\Delta t/\hbar) \simeq 1 - 2|\text{Im}E|\Delta t/\hbar$. Then the probability for one recombination is $2|\text{Im}E|\Delta t/\hbar$. If the BEC is contained in a shallow trap (whose depth is small compared to the energy released in a three-body recombination event), after each recombination event, three atoms escape from the trap. This leads to the decay rates of the atomic densities within the trap:

$$\begin{aligned} \frac{1}{\hbar} \frac{dn_1}{dt} &= -|\text{Im}\tilde{D}_1|n_1^3 - 2|\text{Im}\tilde{D}_{112}|n_1^2n_2 - |\text{Im}\tilde{D}_{122}|n_1n_2^2, \\ \frac{1}{\hbar} \frac{dn_2}{dt} &= -|\text{Im}\tilde{D}_2|n_2^3 - 2|\text{Im}\tilde{D}_{122}|n_1n_2^2 - |\text{Im}\tilde{D}_{112}|n_1^2n_2. \end{aligned} \quad (50)$$

V. SUMMARY

We studied the wave function for the collision of three particles of unequal masses with short-range interactions at zero incoming kinetic energy and zero orbital angular momentum. We derived the asymptotic expansions of such a wave function when two particles are held at a fixed distance and the third particle is far away from the two, or when all three particles are far away from each other. From these expansions we defined the three-body scattering hypervolume for the three particles. This generalizes the definition of three-body scattering hypervolume for identical bosons in Ref. [3]. We then computed the ground state energy of three particles of unequal masses with short-range interactions in a large cubic box, assuming vanishing two-body scattering lengths. This result enabled us to compute the zero-temperature energy of a dilute two-component BEC having vanishing or negligible two-body scattering lengths, to write down the corresponding Gross-Pitaevskii equation for such a BEC in some external potentials, to derive conditions for the stability of the mixture, and to find the decay rates of particle densities due to three-body recombination events.

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APPENDIX: PROCEDURE FOR DETERMINING THE 1-1-1 EXPANSION AND 2-1 EXPANSION

If $s_i \ll R_i$, we can expand $T^{(-p)}$ as

$$T^{(-p)} = \sum_n t_i^{(n, -p-n)}, \quad (A1)$$

where $t_i^{(n, m)}$ scales like $R_i^n s_i^m$ (with a possible extra factor that scales like a polynomial of $\ln R_i$). If $s_i \gg r_e$, we can expand $S_i^{(-q)}$ as

$$S_i^{(-q)} = \sum_m t_i^{(-q, m)}. \quad (A2)$$

Because the three-body wave function $\Phi^{(3)}$ may be expanded as $\sum_p T^{(-p)}$ at $B \rightarrow \infty$, and may also be expanded as $\sum_q S^{(-q)}$ at $R_i \rightarrow \infty$, the $t_i^{(n, m)}$ in the above two expansions should be the same. In fact the wave function has a double expansion $\Phi^{(3)} = \sum_{n, m} t_i^{(n, m)}$ in the region $r_e \ll s_i \ll R_i$.

We choose the overall amplitude of $\Phi^{(3)}$ such that $T^{(0)} = 1$. Therefore

$$\begin{aligned} t_i^{(0, 0)} &= 1, \\ t_i^{(-1, 1)} &= 0, \\ t_i^{(-2, 2)} &= 0, \\ &\dots \end{aligned} \quad (A3)$$

From

$$\hat{H}_i S_i^{(0)} = 0, \quad (A4)$$

we deduce that $S_i^{(0)}$ takes the form

$$S_i^{(0)} = \sum_l c_l \phi_{i, \mathbf{R}_i}^{(l)}(\mathbf{s}_i). \quad (A5)$$

Using the expansion $S_i^{(0)} = t_i^{(0, 0)} + t_i^{(0, -1)} + \dots$ at $s_i \gg r_e$, we find that here the coefficient $c_0 = 1$ but $c_l = 0$ for $l \geq 1$. So

$$S_i^{(0)} = \phi_i(\mathbf{s}_i). \quad (A6)$$

If $s_i > r_e$ we get

$$S_i^{(0)} = 1 - \frac{a_i}{s_i}. \quad (A7)$$

This leads to

$$t_i^{(0, -1)} = -\frac{a_i}{s_i}, \quad (A8)$$

and it will contribute to $T^{(-1)}$.

$T^{(-1)}$ should satisfy Eq. (31) outside the interaction range, and $T^{(-1)} = t_i^{(0, -1)} + t_i^{(-1, 0)} + t_i^{(-2, 1)} + \dots$ if $s_i \ll R_i$. From

these conditions we can determine $T^{(-1)}$:

$$T^{(-1)} = \sum_{i=1}^3 -\frac{a_i}{s_i}. \quad (\text{A9})$$

Expanding $T^{(-1)}$ at $s_i \ll R_i$, we get

$$\begin{aligned} t_i^{(-1,0)} &= -\frac{a_j + a_k}{R_i}, \\ t_i^{(-2,1)} &= (\eta_{jk}a_j - \eta_{kj}a_k) \frac{s_i}{R_i^2} P_1(\hat{\mathbf{R}}_i \cdot \hat{\mathbf{s}}_i), \\ t_i^{(-3,2)} &= -(\eta_{jk}^2 a_j + \eta_{kj}^2 a_k) \frac{s_i^2}{R_i^3} P_2(\hat{\mathbf{R}}_i \cdot \hat{\mathbf{s}}_i), \\ t_i^{(-4,3)} &= (\eta_{jk}^3 a_j - \eta_{kj}^3 a_k) \frac{s_i^3}{R_i^4} P_3(\hat{\mathbf{R}}_i \cdot \hat{\mathbf{s}}_i), \end{aligned} \quad (\text{A10})$$

and so on. From the expansion $S_i^{(-1)} = t_i^{(-1,1)} + t_i^{(-1,0)} + t_i^{(-1,-1)} + \dots$ at $s_i \gg r_e$, and

$$\hat{H}_i S_i^{(-1)} = 0, \quad (\text{A11})$$

we find

$$S_i^{(-1)} = -\frac{a_j + a_k}{R_i} \phi_i(\mathbf{s}_i). \quad (\text{A12})$$

This leads to

$$t_i^{(-1,-1)} = \frac{a_i(a_j + a_k)}{R_i s_i}, \quad (\text{A13})$$

and it will contribute to $T^{(-2)}$.

Repeating this procedure, we can successively determine $T^{(-2)}$, $S_i^{(-2)}$, ..., $T^{(-4)}$, and $S_i^{(-4)}$. In this way we computed the three-body wave function order by order, and finally arrived at the 111 expansion Eq. (33) and the 21 expansion Eq. (35).

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