# Three-boson problem at low energy and implications for dilute Bose-Einstein condensates

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It is shown that the effective interaction strength of three bosons at small collision energies can be extracted from their wave function at zero energy. Asymptotic expansions of this wave function at large interparticle distances are derived, from which is defined a quantity $D$ named three-body scattering hypervolume, which is an analog of the two-body scattering length. Given any finite-range interactions, one can thus predict the effective three-body force from a numerical solution of the Schrödinger equation. In this way, the constant $D$ for hard-sphere bosons is computed, leading to the first complete result for the ground-state energy per particle of a dilute Bose-Einstein condensate (BEC) of hard spheres to order $\rho^2$, where $\rho$ is the number density. Effects of $D$ are also demonstrated in the three-body energy in a finite box of size $L$, which is expanded to the order $L^{-7}$, and in the three-body scattering amplitude in vacuum. The three-body scattering amplitude calculated in this paper disagrees with an earlier calculation in the literature, because of the omission of the two-body effective range in that earlier work. Another key prediction is the condensate fractions of dilute BECs, which also disagree with an earlier work in the literature based on the effective field theory (EFT), as a result of short-range physics. An EFT prediction of the BEC ground-state energy, however, is corroborated.

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## I. INTRODUCTION

It has been known for many years that the ground-state energy per particle of a dilute Bose-Einstein condensate (BEC) is

$$E_0 = \frac{4\pi\hbar^2\rho a}{2m_{\text{boson}}}\left[1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2} + 8w\rho a^3 \ln(\rho a^3) + \rho a^3 \mathcal{E}_3'\right] \tag{1}$$

plus higher-order terms in number density $\rho$, where $a$ is the scattering length, $w \equiv 4\pi/3 - \sqrt{3} = 2.4567\cdots$, and $\mathcal{E}_3'$ is a constant. The first three terms in this expansion were discovered, respectively, in 1947 [1], 1957 [2–4], and 1959 [5–7].

The $\mathcal{E}_3'$ term has remained the least understood. It was known to Wu [5] that $\mathcal{E}_3'$ is given by a parameter $\mathcal{E}_3$ for the ground-state energy of three bosons in a periodic cubic volume [5], plus many-body corrections. Braaten and Nieto fully determined these many-body corrections using the effective field theory (EFT) [8] but, like Wu, they left undetermined a parameter $g_3(\kappa)$ for the three-body effective interaction near the scattering threshold [8], which is related to Wu's parameter $\mathcal{E}_3$ [5]. [The *difference*, $g_3(\kappa) - g_3(\kappa')$, is known for any momentum scales $\kappa$ and $\kappa'$ [8].]

For bosons with large scattering length, $g_3(\kappa)$ was recently computed using the EFT [9]. For other model interactions, Braaten *et al.* [10] used the Monte Carlo results of the energy density [11] to extract $\mathcal{E}_3'$ but, because of statistical uncertainties of the Monte Carlo data, they did not obtain satisfying results [10]. In summary, $g_3(\kappa)$ (and thus $\mathcal{E}_3'$) remains unknown for almost *all* bosonic systems.

In this paper, this effective three-body force [12] and a few related properties of the $\mathcal{N}$-body system are studied. Implications for dilute Bose-Einstein condensates are also explored.

We know that the interaction of *two* bosons at small collision energies ($E \ll \hbar^2/m_{\text{boson}} r_e^2$ and $E \ll \hbar^2/m_{\text{boson}} a^2$, $r_e$=range of interaction) is dominated by the *two-body scattering length a*, while $a$ is present in the small-momentum expansion of the two-body wave function at *zero* collision energy and zero orbital angular momentum,

$$\phi_{\mathbf{q}} = (2\pi)^3\delta(\mathbf{q}) - 4\pi a/q^2 + u_0 + O(q^2). \tag{2}$$

Analogously, the effective interaction strength of *three* identical bosons at low energy should be present in the small-$q$ expansion of the wave function of the same three bosons at *zero* collision energy and zero orbital angular momentum, $\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ ($\Sigma_{i=1}^3 \mathbf{k}_i \equiv \mathbf{0}$). It is shown in this paper that this is indeed the case. It is found that

$$\begin{aligned}\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} &= (2\pi)^6\delta(\mathbf{q}_1)\delta(\mathbf{q}_2) + G_{q_1q_2q_3} \\ &\quad\times\left\{\left[\sum_{i=1}^{3} -4\pi a(2\pi)^3\delta(\mathbf{q}_i) + 32\pi^2a^2/q_i^2 \right.\right. \\ &\quad\left.\left. - 16\pi^2wa^3/q_i - 64\pi wa^4\ln(q_i|a|)\right] - D\right\} \\ &\quad + u_0\sum_{i=1}^{3}[(2\pi)^3\delta(\mathbf{q}_i) - 8\pi a/q_i^2] + O(q^{-1})\end{aligned} \tag{3}$$

at small $q_i \sim q$, where $G_{q_1q_2q_3} \equiv 2/(q_1^2+q_2^2+q_3^2)$, and that $D$, named *three-body scattering hypervolume* (with dimension [length$^4$]), is a suitable parameter for the three-boson effective interaction [13].

The definition of the three-body parameter in Eq. (3) permits one to determine this parameter in an elementary way, namely by solving the three-body Schrödinger equation in vacuum and matching the solution to Eq. (3) at small momenta or its Fourier transform at large interparticle distances.

In Sec. II of the present paper, $\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ is expanded to the order $q^1$ at small momenta [Eqs. (40)] and, correspondingly, its Fourier transform is expanded to the order $R^{-7}$ at large relative distances $R$ [Eqs. (45)]. Although the parameter $D$ first appears in the latter expansion at the order $R^{-4}$, three higher-order corrections are determined to facilitate much more accurate determinations of $D$ from numerical solutions to the Schrödinger equation at not-so-large relative distances.

In Sec. III, the results of Sec. II are applied to bosons interacting through the hard-sphere (HS) potential. By solving the three-body Schrödinger equation numerically, the author found

$$D_{\mathrm{HS}} = (1761.5430 \pm 0.0024)a^4. \tag{4}$$

In Sec. IV, the ground state of three identical bosons in a large periodic cubic volume of side $L$ is determined perturbatively in powers of $L^{-1}$. The energy is expanded [14] to the order $L^{-7}$ ($\hbar = m_{\mathrm{boson}} = 1$),

$$\begin{aligned} E = \frac{12\pi a}{L^3}\Bigg[ & 1 + 2.837\,297\,479\,480\,619\,476\,67\frac{a}{L} \\ & + 9.725\,330\,808\,459\,240\,0570\frac{a^2}{L^2} \\ & + \Bigg(-39.307\,830\,355\,480\,219\,057 \ln\frac{L}{|a|} \\ & + 95.852\,723\,604\,821\,230\,29\Bigg)\frac{a^3}{L^3} + \frac{3\pi a^2 r_s}{L^3} \\ & + \Bigg(-669.168\,047\,948\,734\,849\,322 \ln\frac{L}{|a|} \\ & + 810.053\,286\,803\,649\,420\Bigg)\frac{a^4}{L^4} \\ & + 53.481\,797\,505\,510\,907\,636\frac{a^3 r_s}{L^4}\Bigg] + \frac{D}{L^6} \\ & + 17.023\,784\,876\,883\,716\,860\frac{aD}{L^7} + O(L^{-8}), \end{aligned} \tag{5}$$

where $r_s$ is the two-body effective range. Equation (5) holds for both $a \geqslant 0$ and $a < 0$, and holds for both $r_s \geqslant 0$ and $r_s < 0$.

In Sec. IV B, Wu's parameter $\mathcal{E}_3$ [5] is expressed in terms of $D$; $\mathcal{E}_3$ for hard-sphere bosons is then found [Eq. (109)].

In the last part of Sec. IV, we generalize this three-boson calculation to $\mathcal{N}$ bosons. General formulas for the ground-state energy and condensate fraction of dilute BECs in the thermodynamic limit are then obtained [Eqs. (118) and (119)]. The significance of the parameter $u_0$, defined in Eq. (2), is discussed.

In Sec. V, the scattering amplitude of three bosons at low energy is computed [Eqs. (135)]. After a discrepancy between Ref. [8] and our result at $r_s \neq 0$ is resolved, $g_3(\kappa)$ of Ref. [8] is expressed in terms of the scattering hypervolume $D$ [Eq. (136)]. The ground-state energy per particle of a dilute Bose gas of hard spheres is finally determined to order $\rho^2$ [Eq. (139)].

## II. ASYMPTOTICS OF $\phi^{(3)}$ AT SMALL MOMENTA OR LARGE RELATIVE DISTANCES

*Assumptions*. We consider identical bosons with instantaneous interactions that are translationally, rotationally, and Galilean invariant, and finite-ranged (i.e., limited within a finite interparticle distance $r_e$). So the two-body potential $\frac{1}{2}U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}$ conserves momentum, is invariant under rotation or any equal shift of $\mathbf{k}_i$'s ($1 \leqslant i \leqslant 4$), and is smooth. Also, because of Bose statistics, we can symmetrize $U$ with respect to the incoming (outgoing) momenta without losing generality [15]: $U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} = U_{\mathbf{k}_2\mathbf{k}_1\mathbf{k}_3\mathbf{k}_4} = U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_4\mathbf{k}_3} = U^*_{\mathbf{k}_4\mathbf{k}_3\mathbf{k}_2\mathbf{k}_1}$ (the last equality is the Hermiticity condition). We assume similar properties for the three-body potential, $\frac{1}{6}U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4\mathbf{k}_5\mathbf{k}_6}$. We will consider scattering states only. For few-body physics, the sign of $a$ is arbitrary, but for dilute BECs in the thermodynamic limit we assume that $a \geqslant 0$. Units such that $\hbar = m_{\mathrm{boson}} = 1$ are used.

*Summary of this section*. In Sec. II A, we introduce functions $\phi^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}$, $f^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}$, $g^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}, \ldots$, which are determined by the two-body potential only. We discuss their important properties for use later in the paper. In Sec. II B, we derive two asymptotic expansions of $\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ from the three-body Schrödinger equation that $\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ satisfies. In one of the expansions, $\phi^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}$, $f^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}$, $g^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}, \ldots$ enter as coefficients. These expansions are *very general* despite their complexity: they are valid for all bosonic systems satisfying the above assumptions. Certain quantities and functions, including $D$ and $d_{\mathbf{k}}$, naturally arise in the *derivation* of these expansions.

In this paper, the significance of $D$ will be clear.

In a future work, it will be shown that $d_{\mathbf{k}}$ enters in the low-density expansion of the anomalous average $\langle b_{\mathbf{k}} b_{-\mathbf{k}} \rangle$ in the many-body BEC (where $b_{\mathbf{k}}$ is the boson annihilation operator at momentum $\mathbf{k}$), so $d_{\mathbf{k}}$ is also important.

In Sec. II C, we derive two asymptotic expansions of $\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)$ from the Fourier transformation of the results in Sec. II B.

### A. Two-body special functions

This subsection is in preparation for the rest of the paper.

We define two-body special functions in the $l$-wave channel ($l$ is even for identical bosons), with zero magnetic quantum number along the direction $\hat{\mathbf{n}}$: $\phi^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}$, $f^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}$, $g^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}, \ldots$ [16],

$$(H\phi^{(l)}_{\hat{\mathbf{n}}})_{\mathbf{k}} = 0, \quad (Hf^{(l)}_{\hat{\mathbf{n}}})_{\mathbf{k}} = \phi^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}, \quad (Hg^{(l)}_{\hat{\mathbf{n}}})_{\mathbf{k}} = f^{(l)}_{\hat{\mathbf{n}}\mathbf{k}}, \tag{6}$$

$$(HX)_{\mathbf{k}} \equiv k^2 X_{\mathbf{k}} + \frac{1}{2}\int \frac{\mathrm{d}^3k'}{(2\pi)^3} U_{\mathbf{k}\mathbf{k}'} X_{\mathbf{k}'}, \tag{7}$$

where $U_{\mathbf{k}\mathbf{k}'} \equiv U_{\mathbf{k},-\mathbf{k},\mathbf{k}',-\mathbf{k}'}$. For $l=0$, we write these functions simply as $\phi_{\mathbf{k}}$, $f_{\mathbf{k}}$, $g_{\mathbf{k}}, \ldots$. For $l \geqslant 2$, we use usual symbols $d, g, i, \ldots$ to represent $l = 2, 4, 6, \ldots$. Let

$$\phi(\mathbf{r}) \equiv \int \frac{\mathrm{d}^3k}{(2\pi)^3} \phi_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

and similarly for the other functions. The amplitudes of these functions are fixed by the following equations at $r > r_e$:

$$\phi(\mathbf{r}) = 1 - a/r, \tag{8a}$$

$$f(\mathbf{r}) = -r^2/6 + ar/2 - ar_s/2, \tag{8b}$$

$$g(\mathbf{r}) = r^4/120 - ar^3/24 + ar_s r^2/12 - ar_s'/24, \tag{8c}$$

$$\phi_{\hat{\mathbf{n}}}^{(d)}(\mathbf{r}) = (r^2/15 - 3a_d/r^3)P_2(\hat{\mathbf{n}}\cdot\hat{\mathbf{r}}), \tag{8d}$$

$$f_{\hat{\mathbf{n}}}^{(d)}(\mathbf{r}) = (-r^4/210 - a_d r_d r^2/30 - a_d/2r)P_2(\hat{\mathbf{n}}\cdot\hat{\mathbf{r}}), \tag{8e}$$

$$\phi_{\hat{\mathbf{n}}}^{(g)}(\mathbf{r}) = (r^4/945 - 105a_g/r^5)P_4(\hat{\mathbf{n}}\cdot\hat{\mathbf{r}}), \tag{8f}$$

$$\phi_{\hat{\mathbf{n}}}^{(i)}(\mathbf{r}) = (r^6/135135 - 10395a_i/r^7)P_6(\hat{\mathbf{n}}\cdot\hat{\mathbf{r}}), \tag{8g}$$

where $P_l$ is the Legendre polynomial $[P_l(1)\equiv 1]$, and the $l$-wave scattering phase shift $\delta_l$ at low energy $k^2$ satisfies

$$k^{2l+1}\cot\delta_l(k) = -a_l^{-1} + r_l k^2/2! + r_l' k^4/4! + O(k^6), \tag{9}$$

where $a_0=a$, $r_0=r_s$, $r_0'=r_s'$, $a_2=a_d$, $r_2=r_d$, $a_4=a_g$, and $a_6=a_i$. Now define harmonic polynomials

$$Q_{\hat{\mathbf{n}}}^{(l)}(\mathbf{k}) \equiv k^l P_l(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}}). \tag{10}$$

The following more general formulas in the momentum space are directly related to Eqs. (8) by (Fourier transformation),

$$\phi_{\hat{\mathbf{n}}\mathbf{k}}^{(l)} = \frac{\mathrm{i}^l}{(2l+1)!!}Q_{\hat{\mathbf{n}}}^{(l)}(\nabla_k)(2\pi)^3\delta(\mathbf{k}) + \left(-\frac{4\pi a_l}{\mathrm{i}^l k^2} + \sum_{i=0}^{\infty} u_i^{(l)}k^{2i}\right)Q_{\hat{\mathbf{n}}}^{(l)}(\mathbf{k}), \tag{11a}$$

$$f_{\hat{\mathbf{n}}\mathbf{k}}^{(l)} = \left(\frac{\nabla_k^2}{2!!(2l+3)!!} - \frac{a_l r_l}{2!(2l+1)!!}\right)\mathrm{i}^l Q_{\hat{\mathbf{n}}}^{(l)}(\nabla_k)(2\pi)^3\delta(\mathbf{k}) + \left(-\frac{4\pi a_l Z}{\mathrm{i}^l k^4} + \sum_{i=0}^{\infty}\tilde{f}_i^{(l)}k^{2i}\right)Q_{\hat{\mathbf{n}}}^{(l)}(\mathbf{k}), \tag{11b}$$

$$g_{\hat{\mathbf{n}}\mathbf{k}}^{(l)} = \left(\frac{\nabla_k^4}{4!!(2l+5)!!} - \frac{a_l r_l\nabla_k^2}{2!2!!(2l+3)!!} - \frac{a_l r_l'}{4!(2l+1)!!}\right)\times\mathrm{i}^l Q_{\hat{\mathbf{n}}}^{(l)}(\nabla_k)(2\pi)^3\delta(\mathbf{k}) + \left(-\frac{4\pi a_l Z}{\mathrm{i}^l k^6} + \sum_{i=0}^{\infty}\tilde{g}_i^{(l)}k^{2i}\right)Q_{\hat{\mathbf{n}}}^{(l)}(\mathbf{k}), \tag{11c}$$

where $\mathrm{i}=\sqrt{-1}\neq i$, and $Z/k^4$ and $Z/k^6$ are generalized functions (in this paper $Z$ is merely a symbol and *not* a number),

$$\frac{Z}{k^4} = \frac{1}{k^4}\ (k>0), \quad \int_{\text{all }\mathbf{k}}\frac{Z}{k^4}\mathrm{d}^3k = 0,$$

$$\frac{Z}{k^6} = \frac{1}{k^6}\ (k>0), \quad \int_{\text{all }\mathbf{k}}\frac{Z}{k^6}\mathrm{d}^3k = \int_{\text{all }\mathbf{k}}k^2\frac{Z}{k^6}\mathrm{d}^3k = 0.$$

$Z/k^4$ and $Z/k^6$ have $-\infty$ values at $\mathbf{k}=\mathbf{0}$ to cancel certain integrals shown above. They inevitably arise from the Fourier transformation of functions such as $|\mathbf{r}|$. The $Z$ functions are more completely described in Appendix A.

The infinite series such as $\sum_{i=0}^{\infty}u_i^{(l)}k^{2i}$ in Eqs. (11) account for the deviations of $\phi_{\hat{\mathbf{n}}}^{(l)}(\mathbf{r})$, $f_{\hat{\mathbf{n}}}^{(l)}(\mathbf{r})$, and $g_{\hat{\mathbf{n}}}^{(l)}(\mathbf{r})$ from Eqs. (8) at $r<r_e$. Since $r_e<\infty$, these series are convergent.

The superscripts of $u_i^{(l)}$ and $\tilde{f}_i^{(l)}$ will be omitted at $l=0$. From Eqs. (6) and (11), we derive that at small $\mathbf{k}$,

$$\frac{1}{2}\int\frac{\mathrm{d}^3k'}{(2\pi)^3}U_{\mathbf{k}\mathbf{k}'}\phi_{\hat{\mathbf{n}}\mathbf{k}'}^{(l)} = \left(\mathrm{i}^{-l}4\pi a_l - \sum_{i=0}^{\infty}u_i^{(l)}k^{2i+2}\right)Q_{\hat{\mathbf{n}}}^{(l)}(\mathbf{k}), \tag{12a}$$

$$\frac{1}{2}\int\frac{\mathrm{d}^3k'}{(2\pi)^3}U_{\mathbf{k}\mathbf{k}'}f_{\hat{\mathbf{n}}\mathbf{k}'}^{(l)} = \sum_{i=0}^{\infty}(u_i^{(l)}k^{2i} - \tilde{f}_i^{(l)}k^{2i+2})Q_{\hat{\mathbf{n}}}^{(l)}(\mathbf{k}), \tag{12b}$$

$$\frac{1}{2}\int\frac{\mathrm{d}^3k'}{(2\pi)^3}U_{\mathbf{k}\mathbf{k}'}g_{\mathbf{k}'} = \tilde{f}_0 + O(k^2). \tag{12c}$$

For any unknown $X_{\mathbf{k}}$ we have the uniqueness theorem [17],

$$(HX)_{\mathbf{k}}\equiv 0\ (\text{all }\mathbf{k})\text{ and }X_{\mathbf{k}} = o(k^{-3})\ (\text{small }\mathbf{k}) \Rightarrow X_{\mathbf{k}}\equiv 0. \tag{13}$$

The following identity is needed in the analysis of the momentum distribution of $\mathcal{N}$ particles at low density (Re stands for the real part) [18]:

$$\lim_{k_c\to 0^+}\int_{k>k_c}\frac{\mathrm{d}^3k}{(2\pi)^3}\left(|\phi_{\mathbf{k}}|^2 - \frac{16\pi^2a^2}{k^4}\right) = -2\pi a^2 r_s - 2\,\mathrm{Re}\,u_0. \tag{14}$$

### B. Asymptotics of $\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ at small momenta

From this point on, we let $\mathbf{q}$'s be small momenta and $q_i$'s scale like $q^1$, while $\mathbf{k}$'s will be independent from $\mathbf{q}$'s. We will derive the following two asymptotic expansions:

$$\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \sum_{s=-6}^{\infty}T^{(s)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}, \tag{15}$$

$$\phi_{\mathbf{k}}^{\mathbf{q}} \equiv \phi^{(3)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}} = \sum_{s=-3}^{\infty}S_{\mathbf{k}}^{(s)\mathbf{q}}, \tag{16}$$

where $T^{(s)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ and $S_{\mathbf{k}}^{(s)\mathbf{q}}$ both scale like $q^s$ (including possibly $q^s\ln^n q$, $n=1,2,\ldots$). The minimum values of $s$ in the above equations will be justified below.

The three-body Schrödinger equation can be written in two special forms [19],

$$G^{-1}_{q_1q_2q_3}\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = -\left(\sum_{i=1}^{3}\frac{1}{2}\int_{\mathbf{k}'}U_{\mathbf{p}_i\mathbf{k}'}\phi_{\mathbf{k}'}^{\mathbf{q}_i}\right) - U^{\phi}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}, \tag{17}$$

$$(H\phi^{\mathbf{q}})_{\mathbf{k}} + 3q^2\phi_{\mathbf{k}}^{\mathbf{q}}/4 + W_{\mathbf{k}}^{\mathbf{q}} = 0, \tag{18}$$

where $G_{q_1q_2q_3}=2/(q_1^2+q_2^2+q_3^2)$,

$$\mathbf{p}_1=(\mathbf{q}_2-\mathbf{q}_3)/2,\text{ and similarly for }\mathbf{p}_2,\mathbf{p}_3, \tag{19}$$

$$U^{\phi}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=\frac{1}{6}\int_{\mathbf{k}_1'\mathbf{k}_2'}U_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}\phi^{(3)}_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}, \tag{20}$$

$$W^{\mathbf{q}}_{\mathbf{k}}=\left(\frac{1}{2}\int_{\mathbf{k}'}U_{-\mathbf{q}/2+\mathbf{k},\mathbf{q}\mathbf{k}'\mathbf{k}''}\phi^{(3)}_{-\mathbf{q}/2-\mathbf{k},\mathbf{k}'\mathbf{k}''}+(\mathbf{q}\leftrightarrow-\mathbf{q})\right)+U^{\phi}_{-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k},\mathbf{q}}. \tag{21}$$

$\int_{\mathbf{k}'}$ is the shorthand for $\int\frac{d^3k'}{(2\pi)^3}$, and $\int_{\mathbf{k}'\mathbf{k}''}$ stand for $\int\int\frac{d^3k'}{(2\pi)^3}\frac{d^3k''}{(2\pi)^3}$.

At small $\mathbf{q}$'s we have Taylor expansions,

$$U^{\phi}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=\kappa_0+\kappa_1(q_1^2+q_2^2+q_3^2)+O(q^4), \tag{22a}$$

$$W^{\mathbf{q}}_{\mathbf{k}}=\sum_{s=0,2,4,\ldots}q^sW^{(s)}_{\hat{\mathbf{q}}\mathbf{k}},\quad W^{(0)}_{\hat{\mathbf{q}}\mathbf{k}}\equiv W^{(0)}_{\mathbf{k}}. \tag{22b}$$

Now we fix the overall amplitude of $\phi^{(3)}$ $(\Sigma_{i=1}^3\mathbf{q}_i\equiv0)$: $\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}\equiv(2\pi)^6\delta(\mathbf{q}_1)\delta(\mathbf{q}_2)+$higher-order terms. Because $\delta(\lambda\mathbf{q})=\lambda^{-3}\delta(\mathbf{q})$, $\delta(\mathbf{q})$ scales like $q^{-3}$. So $s\geqslant-6$ for $T^{(s)}$, and

$$T^{(-6)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=(2\pi)^6\delta(\mathbf{q}_1)\delta(\mathbf{q}_2). \tag{23}$$

So $T^{(-6)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}=(2\pi)^3\delta(\mathbf{q})(2\pi)^3\delta(\mathbf{k})\sim q^{-3}k^{-3}$, indicating that $s\geqslant-3$ for $S^{(s)\mathbf{q}}_{\mathbf{k}}$.

The following statement is now true at $s_1=-6$:

*Statement* $s_1$: All the functions $T^{(s)}$ for $s\leqslant s_1$, and all the $S^{(s)}$ for $s\leqslant s_1+2$, have been formally determined.

We can then do the following expansions at small $\mathbf{q}$, for $-6\leqslant s\leqslant s_1$:

$$T^{(s)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}=\sum_n t^{(n,s-n)}_{\mathbf{q},\mathbf{k}}, \tag{24}$$

where $t^{(n,s-n)}_{\mathbf{q},\mathbf{k}}$ scales like $q^nk^{s-n}$. Note also that $S^{(-3)\mathbf{q}}_{\mathbf{k}}+S^{(-2)\mathbf{q}}_{\mathbf{k}}+\cdots=T^{(-6)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}+T^{(-5)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}+\cdots$ $(=\phi^{(3)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}})$. Therefore, the asymptotic expansion of $S^{(s_1+3)\mathbf{q}}_{\mathbf{k}}$ at small $\mathbf{k}$ has been determined to the order $k^{-3}$,

$$S^{(s_1+3)\mathbf{q}}_{\mathbf{k}}=\sum_{m=-s_1-9}^{-3}t^{(s_1+3,m)}_{\mathbf{q},\mathbf{k}}+O(q^{s_1+3}k^{-2}). \tag{25a}$$

Equations (24) and (25a) ensure the continuity of the wave function $\phi^{(3)}$ across two connected regions. Extracting all the terms that scale like $q^{s_1+3}$ from Eq. (18), we get

$$(HS^{(s_1+3)\mathbf{q}})_{\mathbf{k}}=-3q^2S^{(s_1+1)\mathbf{q}}_{\mathbf{k}}/4-W^{(s_1+3)}_{\hat{\mathbf{q}}\mathbf{k}}q^{s_1+3}. \tag{25b}$$

If $W^{(s_1+3)}_{\hat{\mathbf{q}}\mathbf{k}}\neq0$ (i.e., if $s_1+3=0,2,4,\cdots$), we take it as formal input. Solving Eqs. (25), with the help of Eqs. (6) and (11), we thus determine $S^{(s_1+3)\mathbf{q}}_{\mathbf{k}}$. The uniqueness of the solution is guaranteed by Eq. (13).

Once $S^{(s_1+3)}$ is determined, the right-hand side of Eq. (17) can be determined up to the order $q^{s_1+3}$, if the coefficients of the Taylor expansion of $U^{\phi}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ [see Eq. (22a)] are regarded as formal input. Solving Eq. (17), and noting that $G^{-1}_{q_1q_2q_3}\sim q^2$, we thus determine $T^{(s_1+1)}$.

So now the truth of Statement $(s_1+1)$ is established.

We can thus formally determine all the functions $T^{(s)}$ and $S^{(s)}$ by repeating the above routine, starting from $s_1=-6$. The results of this program are shown below.

*Step 1.* $S^{(-3)\mathbf{q}}_{\mathbf{k}}=(2\pi)^3\delta(\mathbf{q})(2\pi)^3\delta(\mathbf{k})+O(q^{-3}k^{-2})$ at small $\mathbf{k}$, and $(HS^{(-3)\mathbf{q}})_{\mathbf{k}}=0$, so

$$S^{(-3)\mathbf{q}}_{\mathbf{k}}=(2\pi)^3\delta(\mathbf{q})\phi_{\mathbf{k}}. \tag{26}$$

*Step 2.* With the help of Eqs. (12), and noting that $\Sigma_{i=1}^3\mathbf{q}_i\equiv0$, we get

$$T^{(-5)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=\sum_{i=1}^3-(4\pi a/p_i^2)(2\pi)^3\delta(\mathbf{q}_i). \tag{27}$$

Expanding $T^{(-5)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}$ at small $\mathbf{q}$, we get all the functions $t^{(n,m)}_{\mathbf{q}k}$ for $n+m=-5$; shown below are those in the range $-2\leqslant n\leqslant3$ (zeros are omitted),

$$t^{(-2,-3)}_{\mathbf{q}\mathbf{k}}=-(8\pi a/q^2)(2\pi)^3\delta(\mathbf{k}), \tag{28a}$$

$$t^{(0,-5)}_{\mathbf{q}\mathbf{k}}=-\pi a(\hat{\mathbf{q}}\cdot\nabla_{\mathbf{k}})^2(2\pi)^3\delta(\mathbf{k}), \tag{28b}$$

$$t^{(2,-7)}_{\mathbf{q}\mathbf{k}}=-(\pi a/48)(\hat{\mathbf{q}}\cdot\nabla_{\mathbf{k}})^4(2\pi)^3\delta(\mathbf{k})q^2. \tag{28c}$$

*Step 3.* $S^{(-2)\mathbf{q}}_{\mathbf{k}}=t^{(-2,-3)}_{\mathbf{q}k}+O(q^{-2}k^{-2})$ at small $\mathbf{k}$, and $(HS^{(-2)\mathbf{q}})_{\mathbf{k}}=0$, so

$$S^{(-2)\mathbf{q}}_{\mathbf{k}}=-(8\pi a/q^2)\phi_{\mathbf{k}}. \tag{29}$$

*Step 4.* Using the same method as in Step 2, we get

$$T^{(-4)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=32\pi^2a^2G_{q_1q_2q_3}\sum_{i=1}^3q_i^{-2}. \tag{30}$$

At small $\mathbf{q}$ we have the following expansions (named "$Z$-$\delta$ expansions;" see Appendix B for details):

$$\begin{aligned}(k^2+3q^2/4)^{-1}&=k^{-2}-\sqrt{3}(2\pi)^3\delta(\mathbf{k})q/8\pi-3q^2Z/4k^4\\&\quad+\sqrt{3}\nabla_k^2(2\pi)^3\delta(\mathbf{k})q^3/64\pi+9q^4Z/16k^6\\&\quad-3\sqrt{3}\nabla_k^4(2\pi)^3\delta(\mathbf{k})q^5/5120\pi+O(q^6),\end{aligned} \tag{31a}$$

$$\begin{aligned}&(|\mathbf{k}+\mathbf{q}/2|^{-2}+|\mathbf{k}-\mathbf{q}/2|^{-2})/(k^2+3q^2/4)\\&=(2\pi)^3\delta(\mathbf{k})/6q+2Z/k^4+[-\nabla_k^2/48+(1/24\\&\quad-\sqrt{3}/16\pi)Q^{(d)}_{\hat{\mathbf{q}}}(\nabla_k)](2\pi)^3\delta(\mathbf{k})q+(4ZQ^{(d)}_{\hat{\mathbf{q}}}(\mathbf{k})/3k^8\\&\quad-4Z/3k^6)q^2+[\nabla_k^4/1280-(1/448-3\sqrt{3}/896\pi)\\&\quad\times\nabla_k^2Q^{(d)}_{\hat{\mathbf{q}}}(\nabla_k)+(19/10080-3\sqrt{3}/896\pi)Q^{(g)}_{\hat{\mathbf{q}}}(\nabla_k)]\\&\quad\times(2\pi)^3\delta(\mathbf{k})q^3+O(q^4),\end{aligned} \tag{31b}$$

so $T^{(-4)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}=\Sigma_{n=-2}^{\infty}t^{(n,-4-n)}_{\mathbf{q},\mathbf{k}}$, where

$$t^{(-2,-2)}_{\mathbf{q},\mathbf{k}}=32\pi^2a^2/q^2k^2, \tag{32a}$$

$$t^{(-1,-3)}_{\mathbf{q},\mathbf{k}}=4\pi wa^2(2\pi)^3\delta(\mathbf{k})/q, \tag{32b}$$

$$t^{(0,-4)}_{\mathbf{q},\mathbf{k}}=40\pi^2a^2Z/k^4, \tag{32c}$$

and for brevity higher-order terms [which can readily be obtained from Eqs. (31)] are not shown.

*Step 5.* $S^{(-1)\mathbf{q}}_{\mathbf{k}}=t^{(-1,-3)}_{\mathbf{q},\mathbf{k}}+O(q^{-1}k^{-2})$ at small $\mathbf{k}$, and $(HS^{(-1)\mathbf{q}})_{\mathbf{k}}=0$, so

$$S^{(-1)\mathbf{q}}_{\mathbf{k}}=(4\pi w a^2/q)\phi_{\mathbf{k}}. \tag{33}$$

*Step 6.* This is similar to Steps 2 and 4.

$$T^{(-3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=-16\pi^2 w a^3 G_{q_1q_2q_3}\sum_{i=1}^{3} q_i^{-1}+u_0\sum_{i=1}^{3}(2\pi)^3\delta(\mathbf{q}_i). \tag{34}$$

Doing the $Z$-$\delta$ expansion (Appendix B), one finds that $T^{(-3)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}=\sum_{n=-3}^{\infty}t^{(n,-3-n)}_{\mathbf{q},\mathbf{k}}$. For brevity, only one of the terms is shown here (to be used in the next step),

$$t^{(0,-3)}_{\mathbf{q},\mathbf{k}}=[16wa^3\ln(q|a|)+2u_0+(14\pi/\sqrt{3}-16)wa^3]\times(2\pi)^3\delta(\mathbf{k})-32\pi^2wa^3Z_{1/|a|}(k)/k^3. \tag{35}$$

This equation remains *unaffected* if both $|a|$'s in the logarithm and in the subscript of $Z$ are replaced by any other length scale simultaneously, because of Eq. (A10).

*Step 7.* Substituting $s_1=-3$ into Eq. (25b), we get $(HS^{(0)\mathbf{q}})_{\mathbf{k}}=6\pi a\phi_{\mathbf{k}}-W^{(0)}_{\mathbf{k}}$. Because the right-hand side does not depend on $\hat{\mathbf{k}}$ or $\mathbf{q}$, we can introduce a single function $d_{\mathbf{k}}$, which is independent of $\hat{\mathbf{k}}$ and satisfies

$$(Hd)_{\mathbf{k}}=6\pi a\phi_{\mathbf{k}}-W^{(0)}_{\mathbf{k}}, \tag{36a}$$

and get $S^{(0)\mathbf{q}}_{\mathbf{k}}=d_{\mathbf{k}}+(\text{linear combination of}\,\phi^{(l)}_{\hat{\mathbf{q}}\mathbf{k}})$. Equation (36a) does not completely determine $d_{\mathbf{k}}$, since $d_{\mathbf{k}}+\eta\phi_{\mathbf{k}}$ satisfies the same equation. At small $\mathbf{k}$ [Eq. (25a)],

$$S^{(0)\mathbf{q}}_{\mathbf{k}}=[-2\pi a Q^{(d)}_{\hat{\mathbf{q}}}(\boldsymbol{\nabla}_k)/3+16wa^3\ln(q|a|)](2\pi)^3\delta(\mathbf{k})+d_a(\mathbf{k})+O(k^{-2}),$$

where

$$d_a(\mathbf{k})\equiv-(\pi a/3)\boldsymbol{\nabla}_k^2(2\pi)^3\delta(\mathbf{k})+40\pi^2a^2Z/k^4+[2u_0+(14\pi/\sqrt{3}-16)wa^3](2\pi)^3\delta(\mathbf{k})-32\pi^2wa^3Z_{1/|a|}(k)/k^3 \tag{36b}$$

does not depend on $\hat{\mathbf{k}}$ or $\mathbf{q}$. Noting Eq. (11a), we can now complete our defintion of $d_{\mathbf{k}}$ [20] and determine $S^{(0)\mathbf{q}}_{\mathbf{k}}$,

$$d_{\mathbf{k}}=d_a(\mathbf{k})+O(k^{-2})\ \text{at small}\ \mathbf{k}. \tag{36c}$$

$$S^{(0)\mathbf{q}}_{\mathbf{k}}=16wa^3\ln(q|a|)\phi_{\mathbf{k}}+10\pi a\phi^{(d)}_{\hat{\mathbf{q}}\mathbf{k}}+d_{\mathbf{k}}. \tag{37}$$

*Step 8.* This is similar to Steps 2, 4, and 6. Extracting all the terms that scale like $q^0$ from both sides of Eq. (17), and solving the resultant equation, we get

$$T^{(-2)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=G_{q_1q_2q_3}[-64\pi wa^4\ln(q_1q_2q_3|a|^3)-D]-\sum_{i=1}^{3}8\pi a u_0/q_i^2, \tag{38}$$

$$D\equiv\frac{3}{2}\int_{\mathbf{k}'}U_{0,\mathbf{k}'}d_{\mathbf{k}'}+\frac{1}{6}\int_{\mathbf{k}_1'\mathbf{k}_2'}U_{0,0,0,\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}\phi^{(3)}_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}-18\pi a u_0. \tag{39}$$

The subsequent steps are similar to the above ones but considerably lengthier; details will not be shown. At the completion of Step 14, the following results are accumulated:

$$\begin{aligned}\phi^{(3)}_{-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k},\mathbf{q}}=&\bigg((2\pi)^3\delta(\mathbf{q})-\frac{8\pi a}{q^2}+\frac{4\pi wa^2}{q}+16wa^3\ln(q|a|)+24\sqrt{3}wa^4q\ln(q|a|)+\xi_1q-\frac{32\sqrt{3}wa^5}{\pi}q^2\ln^2(q|a|)\\&-\xi_2q^2\ln(q|a|)-\zeta_3q^3\ln(q|a|)+\xi_3q^3\bigg)\phi_{\mathbf{k}}+\bigg(-3\pi wa^2q-12wa^3q^2\ln(q|a|)-18\sqrt{3}wa^4q^3\ln(q|a|)-\frac{3\xi_1}{4}q^3\bigg)f_{\mathbf{k}}\\&+\frac{9\pi w}{4}a^2q^3g_{\mathbf{k}}+[10\pi a-10\pi(2\pi-3\sqrt{3})a^2q-4wa^3q^2\ln(q|a|)+\xi_3^{(d)}q^3]\phi^{(d)}_{\hat{\mathbf{q}}\mathbf{k}}+\frac{15\pi}{2}(2\pi-3\sqrt{3})a^2q^3f^{(d)}_{\hat{\mathbf{q}}\mathbf{k}}\\&+\bigg(-\frac{9\pi}{2}aq^2+\frac{3\pi}{4}(76\pi-135\sqrt{3})a^2q^3\bigg)\phi^{(g)}_{\hat{\mathbf{q}}\mathbf{k}}+d_{\mathbf{k}}+q^2d^{(2)}_{\hat{\mathbf{q}}\mathbf{k}}+O(q^4),\end{aligned} \tag{40a}$$

$$\begin{aligned}\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=&(2\pi)^3\delta(\mathbf{q}_1)(2\pi)^3\delta(\mathbf{q}_2)+\frac{2}{q_1^2+q_2^2+q_3^2}\sum_{i=1}^{3}\bigg(-4\pi a(2\pi)^3\delta(\mathbf{q}_i)+\frac{32\pi^2a^2}{q_i^2}-\frac{16\pi^2wa^3}{q_i}-64\pi wa^4\ln(q_i|a|)-\frac{D}{3}\\&-96\sqrt{3}\pi wa^5q_i\ln(q_i|a|)-4\pi a\xi_1q_i+128\sqrt{3}wa^6q_i^2\ln^2(q_i|a|)+4\pi a\xi_2q_i^2\ln(q_i|a|)+40\pi^2aa_dQ^{(d)}_{\hat{\mathbf{q}}_i}(\mathbf{p}_i)+4\pi a\zeta_3q_i^3\ln(q_i|a|)\\&-4\pi a\xi_3q_i^3-40\pi^2(2\pi-3\sqrt{3})a^2a_dq_iQ^{(d)}_{\hat{\mathbf{q}}_i}(\mathbf{p}_i)\bigg)+\sum_{i=1}^{3}\bigg((2\pi)^3\delta(\mathbf{q}_i)(u_0+u_1p_i^2+u_2p_i^4)-\frac{8\pi a}{q_i^2}(u_0+u_1p_i^2)\\&+\frac{4\pi wa^2}{q_i}(u_0+u_1p_i^2)+16wa^3\ln(q_i|a|)u_0+24\sqrt{3}wa^4q_i\ln(q_i|a|)u_0+\xi_1q_iu_0-3\pi wa^2q_i\tilde{f}_0\bigg)+\chi_0+O(q^2),\end{aligned} \tag{40b}$$

where $q^2 d^{(2)}_{\hat{\mathbf{q}}\mathbf{k}}$ is a quadratic *polynomial* of $\mathbf{q}$ [and for any rotation $r$, $d^{(2)}_{r\hat{\mathbf{q}},r\mathbf{k}} = d^{(2)}_{\hat{\mathbf{q}}\mathbf{k}}$], and

$$\xi_1 \equiv \sqrt{3}D/8\pi - 8(\sqrt{3} - \pi/3)wa^4 - 3\pi wa^3 r_s/2, \quad (41a)$$

$$\xi_2 \equiv aD/\sqrt{3}\pi^2 - (260/9 + 128/\sqrt{3}\pi)wa^5 + 2wa^4 r_s, \quad (41b)$$

$$\xi_3^{(d)} \equiv 5(9\sqrt{3} - 4\pi)wa^4/3 + 15\pi(2\pi - 3\sqrt{3})a^2 a_d r_d/4, \quad (41c)$$

$$\zeta_3 \equiv (24/\pi + 16/\sqrt{3})wa^6 + 9\sqrt{3}wa^5 r_s, \quad (41d)$$

$$\xi_3 \equiv -[(1/8\pi^2 + 1/12\sqrt{3}\pi)a + 3\sqrt{3}r_s/64\pi]aD + (17\sqrt{3}/2 + 22/\pi + 353\pi/27)wa^6 + (11\sqrt{3}/4 - 7\pi/6)wa^5 r_s + 9\pi wa^4 r_s^2/16 + 3\pi wa^3 r_s'/32 + (10\pi^2 - 45\sqrt{3}\pi/4)aa_d, \quad (41e)$$

$$\chi_0 \equiv 9\pi a u_1 - 3\omega_1/2 - 2\kappa_1 - \int_{\mathbf{k}'} U_{0\mathbf{k}'} d^{(2)}_{\hat{\mathbf{q}}\mathbf{k}'}. \quad (42)$$

$\kappa_1$ is defined in Eq. (22a), $\int_{\mathbf{k}'} \equiv \int \frac{d^3k'}{(2\pi)^3}$, and $\omega_1$ is a coefficient in the following Taylor expansion at small $\mathbf{k}$:

$$\frac{1}{2}\int_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} d_{\mathbf{k}'} = \omega_0 + \omega_1 k^2 + O(k^4). \quad (43)$$

The other symbols in Eqs. (40) were defined previously: $a$, $r_s$, $r_s'$, $a_d$, and $r_d$ in Eq. (9); $\phi_{\mathbf{k}}$, $f_{\mathbf{k}}$, $g_{\mathbf{k}}$, $\phi^{(d)}_{\hat{\mathbf{q}}\mathbf{k}}$, $f^{(d)}_{\hat{\mathbf{q}}\mathbf{k}}$, and $\phi^{(g)}_{\hat{\mathbf{q}}\mathbf{k}}$ in Eqs. (6) and (11); $u_i$ and $\tilde{f}_0$ in Eqs. (11) with $l=0$, $w \equiv 4\pi/3 - \sqrt{3}$, $\Sigma_{i=1}^3 \mathbf{q}_i \equiv \mathbf{0}$; $\mathbf{p}_i$ in Eq. (19); $Q^{(d)}$ in Eq. (10) with $l=2$; and $d_{\mathbf{k}}$ in Eqs. (36).

At the order $q^2$ in the expansion of $\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$, one will encounter another three-body parameter, $D'$, in the term $-D' G_{q_1 q_2 q_3} \Sigma_{i=1}^4 q_i^4$. [Another contribution at the same order, $\chi_1(q_1^2+q_2^2+q_3^2)$, is smooth and contributes nothing to the Fourier-transformed wave function at large relative distances.] $D'$ is independent from $D$ for general interactions.

In general, if one expands $\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ to the order $q^m$, one will encounter a total of exactly

$$N_3(m) = \mathcal{R}(m'^2/48 + m'/3 + 89/72) \quad (44)$$

independent three-body parameters that contribute to the Fourier transform of $\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ at large relative distances, where $m'=m$ (if $m$ is even), $m'=m-1$ (if $m$ is odd), and "$\mathcal{R}$" rounds to the nearest integer.

### C. Asymptotics of $\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)$ at large relative distances

Let

$$\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) \equiv \int \frac{d^3k_1}{(2\pi)^3}\frac{d^3k_2}{(2\pi)^3}\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}\exp\left(\sum_{i=1}^3 i\mathbf{k}_i\cdot\mathbf{r}_i\right),$$

where $\Sigma_{i=1}^3 \mathbf{k}_i \equiv \mathbf{0}$. We consider the asymptotic expansions of $\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)$ in two different limits: (i) the distance $r$ between two bosons is fixed, but the distance between their center of mass and the third boson, $R$, is large, or (ii) all three interparticle distances, $s_1$, $s_2$, and $s_3$, are large but their ratio is fixed. These two expansions are, respectively,

$$\phi^{(3)}(\mathbf{r}/2,-\mathbf{r}/2,\mathbf{R}) = \left(1 - \frac{2a}{R} + \frac{2wa^2}{\pi R^2} - \frac{4wa^3}{\pi R^3} + \frac{24\sqrt{3}wa^4(\tau-3/2)-\xi_1}{\pi^2 R^4} + \frac{32\sqrt{3}wa^5(6\tau-11)-3\pi\xi_2}{2\pi^2 R^5} + \frac{\zeta_3(12\tau-25)+12\xi_3}{\pi^2 R^6} + \frac{\zeta_4(60\tau-137)+30\xi_4}{\pi R^7}\right)\phi(\mathbf{r}) + \left(\frac{3wa^2}{\pi R^4} - \frac{18wa^3}{\pi R^5} + \frac{18\sqrt{3}wa^4(12\tau-25)-9\xi_1}{\pi^2 R^6} + \frac{48\sqrt{3}wa^5(60\tau-137)-45\pi\xi_2}{2\pi^2 R^7}\right)f(\mathbf{r}) + \left(\frac{27wa^2}{\pi R^6} - \frac{270wa^3}{\pi R^7}\right)g(\mathbf{r}) + \left(-\frac{15a}{2R^3} + \frac{40(2\pi-3\sqrt{3})a^2}{\pi R^4} - \frac{15wa^3}{\pi R^5} + \frac{24\xi_3^{(d)}}{\pi^2 R^6} - \frac{12\sqrt{3}wa^5(210\tau-457)}{7\pi^2 R^7} + \frac{105\xi_4^{(d)}}{2\pi R^7}\right)\phi^{(d)}_{\hat{\mathbf{R}}}(\mathbf{r}) + \left(\frac{180(2\pi-3\sqrt{3})a^2}{\pi R^6} - \frac{315wa^3}{2\pi R^7}\right)f^{(d)}_{\hat{\mathbf{R}}}(\mathbf{r}) + \left(-\frac{945a}{8R^5} + \frac{144(76\pi-135\sqrt{3})a^2}{\pi R^6} - \frac{945wa^3}{4\pi R^7}\right)\phi^{(g)}_{\hat{\mathbf{R}}}(\mathbf{r}) - \frac{135135a}{32R^7}\phi^{(i)}_{\hat{\mathbf{R}}}(\mathbf{r}) + O(R^{-8}), \quad (45a)$$

$$\phi^{(3)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = 1 + \left(\sum_{i=1}^{3} - \frac{a}{s_i} + \frac{4a^2\theta_i}{\pi R_i s_i} - \frac{2wa^3}{\pi B^2 s_i} + \frac{8\sqrt{3}wa^4(t-1-\theta_i\cot 2\theta_i)}{\pi^2 B^4}\right) - \frac{\sqrt{3}D}{8\pi^3 B^4} + \sum_{i=1}^{3}\left\{\frac{36wa^5[(2t-3)\sin 3\theta_i - 2\theta_i\cos 3\theta_i] - \sqrt{3}a\xi_1\sin 3\theta_i}{\pi^2 B^5\sin 2\theta_i} - \frac{96wa^6[3\theta_i^2\sin 4\theta_i + (6t-11)\theta_i\cos 4\theta_i]}{\pi^3 B^6\sin 2\theta_i} + \frac{3\sqrt{3}a\xi_2\theta_i\cos 4\theta_i}{\pi^2 B^6\sin 2\theta_i} + \frac{45\sqrt{3}aa_d(24\theta_i - 8\sin 4\theta_i + \sin 8\theta_i)}{8\pi B^6\sin^3 2\theta_i}P_2(\hat{\mathbf{R}}_i\cdot\hat{\mathbf{s}}_i) + \frac{\sqrt{3}a\zeta_3[12\theta_i\cos 5\theta_i + (25-12t)\sin 5\theta_i]}{\pi^2 B^7\sin 2\theta_i} - \frac{12\sqrt{3}a\xi_3\sin 5\theta_i}{\pi^2 B^7\sin 2\theta_i} - 45\left(2\sqrt{3}-\frac{9}{\pi}\right)\frac{a^2 a_d\sin^2\theta_i(9+10\cos 2\theta_i + 2\cos 4\theta_i)}{B^7\cos^3\theta_i}P_2(\hat{\mathbf{R}}_i\cdot\hat{\mathbf{s}}_i)\right\} + O(B^{-8}), \quad (45b)$$

where $\tau \equiv \ln(\tilde{\gamma}R/|a|)$, $t \equiv \ln(\tilde{\gamma}B/|a|)$, $\tilde{\gamma} \equiv e^{\gamma} = 1.78107\ldots$, $\gamma$ is Euler's constant, and

$$\mathbf{s}_1 = \mathbf{r}_2 - \mathbf{r}_3, \quad \mathbf{s}_2 = \mathbf{r}_3 - \mathbf{r}_1, \quad \mathbf{s}_3 = \mathbf{r}_1 - \mathbf{r}_2, \quad (46)$$

$$\mathbf{R}_1 = \mathbf{r}_1 - (\mathbf{r}_2 + \mathbf{r}_3)/2, \text{ and similarly for } \mathbf{R}_2 \text{ and } \mathbf{R}_3,$$

$$B = \sqrt{(s_1^2 + s_2^2 + s_3^2)/2}, \quad \theta_i = \arctan(2R_i/\sqrt{3}s_i).$$

$$\zeta_4 \equiv 42\sqrt{3}wa^6 r_s/5\pi - (48/5\pi^2 + 32/5\sqrt{3}\pi)wa^7, \quad (47a)$$

$$\xi_4 \equiv [(1/10\pi^3 + 1/15\sqrt{3}\pi^2)a - 7\sqrt{3}r_s/80\pi^2]a^2 D - (536/25\pi^2 + 124/27 - 86/25\sqrt{3}\pi)wa^7 + (65/3 + 309\sqrt{3}/25\pi)wa^6 r_s - 6wa^5 r_s^2/5 - (60\pi - 87\sqrt{3})a^2 a_d - 9wa^4 r_s'/20, \quad (47b)$$

$$\xi_4^{(d)} \equiv \sqrt{3}aD/28\pi^2 - (416/21 - 8384\sqrt{3}/245\pi)wa^5 - 3wa^4 r_s/7 - 3wa^3 a_d r_d/2. \quad (47c)$$

$R_i = B\sin\theta_i$, $s_i = \frac{2}{\sqrt{3}}B\cos\theta_i$, and $\Sigma_{i=1}^3\cos 2\theta_i \equiv 0$.

Equation (45b) derives from Eq. (40b).

The terms up to the order $R^{-6}$ on the right-hand side of Eq. (45a) derive from Eq. (40a); those of the order $R^{-7}$, however, are inferred from Eq. (45b) and the continuity of $\phi^{(3)}(\mathbf{r}/2, -\mathbf{r}/2, \mathbf{R})$ across two connected regions: $r \sim O(r_e)$ and $r \sim O(R)$ (they join at $r_e \ll r \ll R$), and also the Schrödinger equation at large $R$,

$$(\tilde{H} - 3\nabla_R^2/4)\phi^{(3)}(\mathbf{r}/2, -\mathbf{r}/2, \mathbf{R}) = 0, \quad (48)$$

where $\tilde{H}$ is the coordinate representation of the Hamiltonian $H$ for two-body relative motion [Eq. (7)].

### III. LOW-ENERGY EFFECTIVE INTERACTION OF THREE HARD-SPHERE BOSONS

In this section, we consider the hard-sphere (HS) interaction. The two-body potential $V(r)=0$ $(r>1)$, $V(r)=+\infty$ $(r<1)$ ($a=1$ in this section), and there is no three-body potential. We numerically solve the Schrödinger equation at zero energy in the coordinate representation, in conjunction with Eq. (45a) at large $R$, to determine $D$ [21].

For three-body configurations excluded by the repulsive interaction, $\phi^{(3)}$ vanishes; for allowed configurations, $\phi^{(3)}$ satisfies the free Schrödinger equation. So $\Sigma_{i=1}^3\nabla_i^2\phi^{(3)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ is nonzero on the boundary $\mathcal{B}$ between these two regions only (in fact, it has a $\delta$-function singularity on $\mathcal{B}$). Thus

$$\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) = 1 - \frac{4\sqrt{3}}{\pi}\int_{-1}^{1}dc'\int_{R_{\min}(c')}^{\infty}F(R',c')R'^2 dR' \times \{\mathcal{G}[s_1,s_2,s_3;1,s_-(R',c'),s_+(R',c')] + \mathcal{G}[s_1,s_2,s_3;s_-(R',c'),1,s_+(R',c')] + \mathcal{G}[s_1,s_2,s_3;s_-(R',c'),s_+(R',c'),1]\} \quad (49)$$

for some function $F(R',c')$, where $s_i$'s are defined in Eq. (46), $c'$ is the cosine of the angle formed by the line connecting two bosons with distance 1 and the line connecting their center-of-mass to the third boson,

$$R_{\min}(c') = (|c'| + \sqrt{c'^2 + 3})/2, \quad (50a)$$

$$s_{\pm}(R',c') = \sqrt{1/4 \pm R'c' + R'^2}, \quad (50b)$$

and

$$\mathcal{G}(s_1s_2s_3;s_1's_2's_3') \equiv \{[(s_1^2+s_2^2+s_3^2+s_1'^2+s_2'^2+s_3'^2)^2 - 2(5s_1^2s_1'^2 - s_1^2s_2'^2 - s_1^2s_3'^2 + 5s_2^2s_2'^2 - s_2^2s_1'^2 - s_2^2s_3'^2 + 5s_3^2s_3'^2 - s_3^2s_1'^2 - s_3^2s_2'^2)]^2 - 36(2s_1^2s_2^2 + 2s_2^2s_3^2 + 2s_3^2s_1^2 - s_1^4 - s_2^4 - s_3^4) \times (2s_1'^2s_2'^2 + 2s_2'^2s_3'^2 + 2s_3'^2s_1'^2 - s_1'^4 - s_2'^4 - s_3'^4)\}^{-1/2} \quad (51a)$$

is the translationally and rotationally invariant Green function, satisfying [$s_i$'s are defined in Eq. (46)]

$$\sum_{i=1}^{3}\nabla_i^2\mathcal{G}(s_1s_2s_3;s_1's_2's_3') = -\frac{\pi}{2\sqrt{3}s_1's_2's_3'}\prod_{i=1}^{3}\delta(s_i - s_i'). \quad (51b)$$

Because $\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)$ vanishes on $\mathcal{B}$, the unknown function $F(R',c')$ in Eq. (49) satisfies an integral equation,

$$\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)=0 \text{ at } s_1=1, \quad s_{2,3}=s_{\mp}(R,c), \tag{52}$$

where $-1<c<1$ and $R>R_{\min}(c)$.

From Eqs. (49) and (51b), we get

$$(\nabla_r^2+3\nabla_R^2/4)\phi^{(3)}(\mathbf{r}/2,-\mathbf{r}/2,\mathbf{R})=F(R,c)\delta(r-1) \tag{53}$$

at $|\mathbf{R}\pm\mathbf{r}/2|>1$, where $c=\hat{\mathbf{R}}\cdot\hat{\mathbf{r}}$.

From Eq. (53), it is clear that $F(R,-c)=F(R,c)$.

The two-boson special functions satisfy Eqs. (8) at $r\geqslant 1$ and vanish at $r\leqslant 1$, so

$$a=1, \quad r_s=2/3, \quad r_s'=8/15, \quad a_d=1/45, \quad r_d=-150/7,$$

$$a_g=1/99\,225, \quad a_i=1/1\,404\,728\,325.$$

Applying $(\nabla_r^2+3\nabla_R^2/4)$ to Eq. (45a), and comparing the result with Eq. (53), we get the asymptotic expansion of $F(R,c)$ at large $R$,

$$F(R,c)=F_a^{(1)}(R,c)+QF_a^{(2)}(R,c)+O(R^{-8}), \tag{54a}$$

$$\begin{aligned}F_a^{(1)}(R,c)={}&1-\frac{2}{R}+\frac{2w}{\pi R^2}-\frac{4w}{\pi R^3}+\left(\frac{24\sqrt{3}w}{\pi^2}\ln R+\frac{12}{\pi^2}-\frac{8}{\sqrt{3}\pi}\right.\\&\left.-\frac{14}{9}\right)R^{-4}+\left(\frac{96\sqrt{3}w}{\pi^2}\ln R+\frac{460}{9}+\frac{48}{\pi^2}\right.\\&\left.-\frac{161}{\sqrt{3}\pi}\right)R^{-5}+\left(\frac{4(72+43\sqrt{3}\pi)w}{\pi^3}\ln R+\frac{10885}{54}\right.\\&\left.+\frac{48\sqrt{3}}{\pi^3}+\frac{105}{\pi^2}-\frac{5005}{8\sqrt{3}\pi}\right)R^{-6}\\&+\left(\frac{64(7\sqrt{3}\pi-9)w}{\pi^3}\ln R+\frac{61279}{135}-\frac{96\sqrt{3}}{\pi^3}+\frac{492}{\pi^2}\right.\\&\left.-\frac{27733}{20\sqrt{3}\pi}\right)R^{-7}+\left\{-\frac{5}{2R^3}+\left(\frac{80}{3}-\frac{40\sqrt{3}}{\pi}\right)R^{-4}\right.\\&-\frac{5w}{\pi R^5}+\left(\frac{730}{\sqrt{3}\pi}-\frac{820}{9}-\frac{360}{\pi^2}\right)R^{-6}\\&+\left(-\frac{120\sqrt{3}w}{\pi^2}\ln R+\frac{15865}{4\sqrt{3}\pi}-\frac{4115}{9}\right.\\&\left.\left.-\frac{2220}{\pi^2}\right)R^{-7}\right\}P_2(c)+\left[-\frac{9}{8R^5}+\left(\frac{3648}{35}\right.\right.\\&\left.\left.-\frac{1296\sqrt{3}}{7\pi}\right)\frac{1}{R^6}-\frac{9w}{4\pi R^7}\right]P_4(c)-\frac{13P_6(c)}{32R^7},\end{aligned} \tag{54b}$$

$$\begin{aligned}F_a^{(2)}(R,c)={}&-\frac{6\sqrt{3}}{\pi R^4}-\frac{24\sqrt{3}}{\pi R^5}-\left(\frac{72}{\pi^2}+\frac{43\sqrt{3}}{\pi}\right)R^{-6}+\left(\frac{144}{\pi^2}\right.\\&\left.-\frac{112\sqrt{3}}{\pi}+\frac{30\sqrt{3}P_2(c)}{\pi}\right)R^{-7},\end{aligned} \tag{54c}$$

where $Q$ is directly related to $D$,

$$\begin{aligned}D={}&48\pi^2Q-192\pi w(1-\gamma)-12\pi^2=473.741\,011\,252\,289Q\\&-744.946\,799\,290\,500.\end{aligned} \tag{55}$$

It can be shown from Eqs. (52) (at large $R$) and (54) that

$$\begin{aligned}Q={}&\lim_{R\to\infty}\int_0^1 dc'\int_{R_{\min}(c')}^{R}F(R',c')R'^2dR'-[R^3/3-R^2\\&+2wR/\pi-(4w/\pi)\ln R].\end{aligned} \tag{56}$$

Solving Eqs. (52) and (56) for $F(R,c)$ and $Q$ numerically [using $F_a^{(1)}(R',c')+QF_a^{(2)}(R',c')$ to approximate $F(R',c')$ for $R'$ greater than some sufficiently large value in these two equations, and discretizing $F(R',c')$ for $R'$ less than this value], the author finds

$$Q=5.290844\pm 0.000005.$$

Substituting this result into Eq. (55), we obtain Eq. (4).

## IV. GROUND STATE OF THREE BOSONS IN A PERIODIC CUBIC VOLUME AND IMPLICATIONS FOR THE MANY-BODY PHYSICS

In this section, we return to the general interactions considered in Sec. II. The bosons are now placed in a large periodic cubic volume of side $L$, and

$$\epsilon\equiv 1/L \tag{57}$$

is a small parameter.

In Sec. IV A, we derive asymptotic expansions of the ground-state wave function and energy of three bosons (assumed to be in a scattering state). These calculations are *very general* despite their complexity.

In Sec. IV B, we find the relation between Wu's parameter $\mathcal{E}_3$ [5] and our quantity $D$. For the hard-sphere interaction, we subtitute our numerical result of $D$ into this relation to obtain the value of $\mathcal{E}_3$.

We summarize the results for the wave function in Sec. IV C, from which we derive asymptotic expansions of the momentum distribution of the three bosons in Sec. IV D. In particular, it is found that the population of the zero-momentum state depends on the parameter $u_0$. In Sec. IV E, we discuss the implications of this dependence.

In Sec. IV F, the author generalizes the above expansions to the case of $\mathcal{N}$ bosons ($\mathcal{N}$ is fixed, $a$ may be either positive or negative, and $L$ is large), from which we infer low-density expansions of the energy and condensate fraction in the thermodynamic limit ($\mathcal{N}/L^3$ is fixed, $a\geqslant 0$, and $\mathcal{N}$ and $L^3$ are large).

### A. Ground-state wave function and energy

Let $A_{\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3}$ ($\Sigma_{i=1}^3\mathbf{n}_i\equiv\mathbf{0}$) be proportional to the probability amplitude that the bosons have momenta $2\pi\epsilon\mathbf{n}_i$ ($i=1,2,3$). We shall call $\mathbf{n}_i$ an *integral vector*, since its Cartesian components (along the sides of the cubic volume) are integers. The Schrödinger equation ($\hbar=m_{\text{boson}}=1$)

$$[2\pi^2\epsilon^2(n_1^2+n_2^2+n_3^2)-E]A_{\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3} + \frac{1}{6L^6}U_{2\pi\epsilon\mathbf{n}_1,2\pi\epsilon\mathbf{n}_2,2\pi\epsilon\mathbf{n}_3,2\pi\epsilon\mathbf{n}_1',2\pi\epsilon\mathbf{n}_2',2\pi\epsilon\mathbf{n}_3'}A_{\mathbf{n}_1'\mathbf{n}_2'\mathbf{n}_3'} + \frac{1}{2L^3}U_{2\pi\epsilon\mathbf{n}_1,2\pi\epsilon\mathbf{n}_2,2\pi\epsilon\mathbf{n}',2\pi\epsilon\mathbf{n}''}A_{\mathbf{n}'\mathbf{n}''\mathbf{n}_3}+\cdots=0, \tag{58}$$

where summation over dumb momenta is implicit, and "⋯" stands for two other similar pairwise interaction terms, is rewritten as

$$[(k_1^2+k_2^2+k_3^2)/2-E]\psi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + \frac{1}{6}I_\epsilon(\mathbf{k}_1)I_\epsilon(\mathbf{k}_2)\int_{\mathbf{k}_1'\mathbf{k}_2'}U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}\psi_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'} + \frac{1}{2}I_\epsilon(\mathbf{k}_1)\int_{\mathbf{k}'}U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}'\mathbf{k}''}\psi_{\mathbf{k}'\mathbf{k}''\mathbf{k}_3}+\cdots=0, \tag{59}$$

$$\psi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} \equiv \sum_{\mathbf{n}_1\mathbf{n}_2} A_{\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3}\prod_{i=1}^{2}(2\pi\epsilon)^3\delta(\mathbf{k}_i-2\pi\epsilon\mathbf{n}_i), \tag{60}$$

where $\Sigma_{i=1}^3\mathbf{k}_i\equiv 0$, $\int_{\mathbf{k}'}\equiv\int\frac{d^3k'}{(2\pi)^3}$, $\int_{\mathbf{k}_1'\mathbf{k}_2'}\equiv\int\int\frac{d^3k_1'}{(2\pi)^3}\frac{d^3k_2'}{(2\pi)^3}$, and

$$I_\epsilon(\mathbf{k}) \equiv \sum_{\mathbf{n}}(2\pi\epsilon)^3\delta(\mathbf{k}-2\pi\epsilon\mathbf{n}). \tag{61}$$

$$J_\epsilon(\mathbf{k}) \equiv \sum_{\mathbf{n}\neq 0}(2\pi\epsilon)^3\delta(\mathbf{k}-2\pi\epsilon\mathbf{n}). \tag{62}$$

In the following, $\mathbf{k}$'s will be taken as independent of $\epsilon$ but $\mathbf{q}$'s be small momenta such that $\mathbf{q}/\epsilon$'s are independent of $\epsilon$. Also, $I_\epsilon(\mathbf{k})$ and $J_\epsilon(\mathbf{k})$ will be simply written as $I(\mathbf{k})$ and $J(\mathbf{k})$, respectively.

Let

$$A_{0,0,0}\equiv L^6, \tag{63}$$

so $\psi_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=\Pi_{i=1}^2(2\pi)^3\delta(\mathbf{q}_i)+o(\epsilon^{-6})$.

The following expansions will be found:

$$\psi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}=\sum_{s\geq 0}\mathcal{R}^{(s)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}, \tag{64a}$$

$$\psi_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}=\sum_{s\geq -3}\mathcal{S}^{(s)\mathbf{q}}_{\mathbf{k}}, \tag{64b}$$

$$\psi_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=\sum_{s\geq -6}\mathcal{T}^{(s)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}, \tag{64c}$$

$$E=\sum_{s\geq 3}E^{(s)}, \tag{64d}$$

where $\mathcal{R}^{(s)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$, $\mathcal{S}^{(s)\mathbf{q}}_{\mathbf{k}}$, $\mathcal{T}^{(s)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$, and $E^{(s)}$ scale with $\epsilon$ like $\epsilon^s$ (*not* excluding $\epsilon^s\ln\epsilon$). Equation (64a) is understood in the following sense: we expand the Fourier transform of $\psi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ within a large but *fixed* spatial region in powers of $\epsilon$, and then transform the result back to the $\mathbf{k}_i$ space term by term, to obtain $\Sigma_s\mathcal{R}^{(s)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$. Equation (64b) is similar: we expand the partial Fourier transform, $\int_{\mathbf{k}}\psi_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r})$, within a large but fixed region of the $\mathbf{r}$ space, for fixed $\mathbf{q}/\epsilon$, in powers of $\epsilon$, and then transform the result back to the $\mathbf{k}$ space term by term, to obtain $\Sigma_s\mathcal{S}^{(s)\mathbf{q}}_{\mathbf{k}}$.

Obviously

$$\mathcal{T}^{(-6)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}=(2\pi)^3\delta(\mathbf{q}_1)(2\pi)^3\delta(\mathbf{q}_2). \tag{65}$$

Therefore, $\mathcal{T}^{(-6)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}=(2\pi)^3\delta(\mathbf{k}_1)(2\pi)^3\delta(\mathbf{k}_2)$ and $\mathcal{T}^{(-6)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}=(2\pi)^3\delta(\mathbf{q})(2\pi)^3\delta(\mathbf{k})$, indicating that the minimum values of $s$ for $\mathcal{R}^{(s)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ and $\mathcal{S}^{(s)\mathbf{q}}_{\mathbf{k}}$ are 0 and $-3$, respectively. Since the energy is dominated by pairwise mean-field interactions, $E\sim\epsilon^3$.

The Fourier transform of $I(\mathbf{k})$ becomes $\delta(\mathbf{r})$ within any *fixed* spatial region, when $\epsilon$ is sufficiently small. Using the prescription in Appendix B, we thus get

$$I(\mathbf{k})=1+O(\epsilon^{s_c})\quad \text{for } any\ s_c.$$

Using this result, and also noting that the interactions are finite-ranged, we get three specialized forms of Eq. (59) (accurate to any finite order in $\epsilon$),

$$\frac{1}{2}(k_1^2+k_2^2+k_3^2)\mathcal{R}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}+\frac{1}{6}\int_{\mathbf{k}_1'\mathbf{k}_2'}U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}\mathcal{R}_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'} + \frac{1}{2}\int_{\mathbf{k}'}U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}'\mathbf{k}''}\mathcal{R}_{\mathbf{k}_3\mathbf{k}'\mathbf{k}''}+\cdots=E\mathcal{R}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}, \tag{66a}$$

$$(H\mathcal{S}^{\mathbf{q}})_{\mathbf{k}}+(3q^2/4-E)\mathcal{S}^{\mathbf{q}}_{\mathbf{k}}+I(\mathbf{q})\mathcal{W}^{\mathbf{q}}_{\mathbf{k}}=0, \tag{66b}$$

$$\left[\frac{1}{2}(q_1^2+q_2^2+q_3^2)-E\right]\mathcal{T}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}+\frac{1}{2}\sum_{i=1}^{3}I(\mathbf{q}_{i'})\int_{\mathbf{k}'}U_{\mathbf{p}_i\mathbf{k}'}\mathcal{S}^{\mathbf{q}_i}_{\mathbf{k}'} + \frac{1}{6}I(\mathbf{q}_1)I(\mathbf{q}_2)\int_{\mathbf{k}_1'\mathbf{k}_2'}U_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}\mathcal{R}_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}=0, \tag{66c}$$

$$\mathcal{W}^{\mathbf{q}}_{\mathbf{k}}\equiv\frac{1}{6}\int_{\mathbf{k}_1'\mathbf{k}_2'}U_{-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k},\mathbf{q},\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}\mathcal{R}_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'} + \left[\frac{1}{2}\int_{\mathbf{k}'}U_{-\mathbf{q}/2+\mathbf{k},\mathbf{q},\mathbf{k}'\mathbf{k}''}\mathcal{R}_{-\mathbf{q}/2-\mathbf{k},\mathbf{k}'\mathbf{k}''}+(\mathbf{q}\leftrightarrow-\mathbf{q})\right], \tag{67}$$

where $\mathcal{R}$, $\mathcal{S}$, and $\mathcal{T}$ are the sums of $\mathcal{R}^{(s)}$, $\mathcal{S}^{(s)}$, and $\mathcal{T}^{(s)}$, respectively, and in Eq. (66c), $1'=2, 2'=3, 3'=1$, and $\mathbf{p}_i$ is defined in Eq. (19).

The following *statement* is now true at $s_1=-6$:

***Statement*** $s_1$: The functions $\mathcal{T}^{(s)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ (for $s\leq s_1$), $\mathcal{S}^{(s)\mathbf{q}}_{\mathbf{k}}$ (for $s\leq s_1+2$), $\mathcal{R}^{(s)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ (for $s\leq s_1+5$), and $E^{(s)}$ (for $s\leq s_1+8$) have all been formally determined.

Now do the following expansions for $-6\leq s\leq s_1$:

$$\mathcal{T}^{(s)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}=\sum_n t'^{(n,s-n)}_{\mathbf{q},\mathbf{k}}, \tag{68a}$$

$$\mathcal{T}^{(s)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \sum_n t''^{(n,s-n)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}, \tag{68b}$$

where $\mathbf{q}/\epsilon$'s and $\mathbf{k}$'s are independent of $\epsilon$, $\mathbf{k}_i \sim k$, and $t'^{(n,s-n)}_{\mathbf{q},\mathbf{k}} \sim \epsilon^n k^{s-n}$, $t''^{(n,s-n)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} \sim \epsilon^n k^{s-n}$. For the same reason as Eq. (25a), we obtain the following asymptotic expansions at small $\mathbf{k}$'s:

$$\mathcal{S}^{(s_1+3)\mathbf{q}}_{\mathbf{k}} = \sum_{m=-s_1-9}^{-3} t'^{(s_1+3,m)}_{\mathbf{q},\mathbf{k}} + O(\epsilon^{s_1+3}k^{-2}), \tag{69a}$$

$$\mathcal{R}^{(s_1+6)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \sum_{m=-s_1-12}^{-6} t''^{(s_1+6,m)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + O(\epsilon^{s_1+6}k^{-5}). \tag{69b}$$

Extracting all the terms that scale like $\epsilon^{s_1+6}$ from Eq. (66a), we get

$$\frac{1}{2}(k_1^2+k_2^2+k_3^2)\mathcal{R}^{(s_1+6)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + \frac{1}{6}\int_{\mathbf{k}_1'\mathbf{k}_2'} U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}\mathcal{R}^{(s_1+6)}_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'} + \frac{1}{2}\int_{\mathbf{k}'} U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}'\mathbf{k}''}\mathcal{R}^{(s_1+6)}_{\mathbf{k}_3\mathbf{k}'\mathbf{k}''} + \cdots = \sum_{3\le n\le s_1+6} E^{(n)}\mathcal{R}^{(s_1+6-n)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}, \tag{70}$$

where the right-hand side is already known. This equation and Eq. (69b) [which expands $\mathcal{R}^{(s_1+6)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ to the order $k^{-6}$ at small $\mathbf{k}$'s] are sufficient to determine $\mathcal{R}^{(s_1+6)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$, due to the three-body version of the uniqueness theorem [analogous to Eq. (13)].

The above information for $\mathcal{S}^{\mathbf{q}}_{\mathbf{k}}$ and $\mathcal{R}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ is sufficient to determine each term in Eq. (66b), except the first term, to the order $\epsilon^{s_1+3}$ [note that $I(\mathbf{q})\sim\epsilon^0$], so $(H\mathcal{S}^{(s_1+3)\mathbf{q}})_{\mathbf{k}}$ is known; taking into account Eq. (69a), one can determine $\mathcal{S}^{(s_1+3)\mathbf{q}}_{\mathbf{k}}$.

The sum of all the interaction terms in Eq. (66c) can now be determined to the order $\epsilon^{s_1+3}$, with a result $c'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} + c_0\Pi_{i=1}^2(2\pi\epsilon)^3\delta(\mathbf{q}_i)$, where $c'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ vanishes at $\mathbf{q}_1=\mathbf{q}_2=\mathbf{0}$. Both $c'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ and $c_0$ are known up to the order $\epsilon^{s_1+3}$.

Because of Eq. (63), $\mathcal{T}'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} \equiv \mathcal{T}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} - \Pi_{i=1}^2(2\pi)^3\delta(\mathbf{q}_i)$ vanishes at $\mathbf{q}_1=\mathbf{q}_2=\mathbf{0}$. Solving Eq. (66c), we get $E=c_0\epsilon^6$ (so now $E$ is known to the order $\epsilon^{s_1+9}$) and

$$\mathcal{T}'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = G_{q_1q_2q_3}(E\mathcal{T}'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} - c'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}), \tag{71}$$

where $G_{q_1q_2q_3} \equiv 2/(q_1^2+q_2^2+q_3^2) \sim \epsilon^{-2}$. Because $E\sim\epsilon^3$, $\mathcal{T}'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} \sim \epsilon^x$, $x>-6$, and $E$ and $\mathcal{T}'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ are known to the orders $\epsilon^{s_1+9}$ and $\epsilon^{s_1}$, respectively, we know $E\mathcal{T}'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ to the order $\epsilon^{s_1+3}$. So from Eq. (71), we can now determine $\mathcal{T}'_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ (and thus $\mathcal{T}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$) to the order $\epsilon^{s_1+1}$.

The truth of *Statement* $(s_1+1)$ is now established.

Repeating the above routine, one can formally determine $A_{\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3}$ and $E$ to any orders in $\epsilon$. The following are the step-by-step results of this program.

***Step 1a***. $\mathcal{R}^{(0)}$, $\mathcal{R}^{(1)}$, and $\mathcal{R}^{(2)}$ satisfy the *zero*-energy Schrödinger equation [because of Eq. (70)]. They will all be determined in this paper. From Eq. (65), we get $t''^{(0,-6)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \Pi_{i=1}^2(2\pi)^3\delta(\mathbf{k}_i)$. So

$$\mathcal{R}^{(0)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}. \tag{72}$$

***Step 1b***. $t'^{(-3,-3)}_{\mathbf{q},\mathbf{k}} = (2\pi)^3\delta(\mathbf{q})(2\pi)^3\delta(\mathbf{k})$; $(H\mathcal{S}^{(-3)\mathbf{q}})_{\mathbf{k}}=0$. So

$$\mathcal{S}^{(-3)\mathbf{q}}_{\mathbf{k}} = (2\pi)^3\delta(\mathbf{q})\phi_{\mathbf{k}}. \tag{73}$$

***Step 2***. With the help of Eqs. (12), and noting that $\Sigma_{i=1}^3 \mathbf{q}_i \equiv \mathbf{0}$, we get

$$E = 12\pi a\epsilon^3 + o(\epsilon^3), \tag{74}$$

$$\mathcal{T}^{(-5)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \sum_{i=1}^3 -(4\pi a/p_i^2)J(\mathbf{p}_i)(2\pi)^3\delta(\mathbf{q}_i). \tag{75}$$

Using the method of Appendix B, we get

$$\begin{aligned}\mathcal{T}^{(-5)}_{-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k},\mathbf{q}} = {}& J(\mathbf{q})[-8\pi a/q^2 - \pi a(\hat{\mathbf{q}}\cdot\boldsymbol{\nabla}_k)^2 + O(\epsilon^2)]\\ &\times(2\pi)^3\delta(\mathbf{k}) + (2\pi)^3\delta(\mathbf{q})[-4\pi a/k^2\\ &-\alpha_1 a\epsilon(2\pi)^3\delta(\mathbf{k})/\pi + 2\pi a\epsilon^3\nabla_k^2(2\pi)^3\delta(\mathbf{k})/3\\ &+O(\epsilon^5)],\end{aligned} \tag{76a}$$

$$\mathcal{T}^{(-5)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \left(\sum_{i=1}^3 -(4\pi a/l_i^2)(2\pi)^3\delta(\mathbf{k}_i)\right) - (3\alpha_1 a\epsilon/\pi)(2\pi)^3\delta(\mathbf{k}_1) \times(2\pi)^3\delta(\mathbf{k}_2) + O(\epsilon^3), \tag{76b}$$

$$\mathbf{l}_1 \equiv (\mathbf{k}_2-\mathbf{k}_3)/2, \quad \text{and similarly for } \mathbf{l}_2,\mathbf{l}_3, \tag{77}$$

$$\alpha_s \equiv \lim_{\eta\to0^+}\sum_{\mathbf{n}\neq\mathbf{0}} \frac{e^{-\eta n}}{|\mathbf{n}|^{2s}} - \int d^3n \frac{e^{-\eta n}}{|\mathbf{n}|^{2s}} \; (s<3/2), \tag{78a}$$

$$\alpha_{1.5} \equiv \lim_{N\to\infty}\left[\left(\sum_{\mathbf{n}\neq\mathbf{0};n<N}|\mathbf{n}|^{-3}\right) - 4\pi\ln N\right], \tag{78b}$$

$$\alpha_s \equiv \sum_{\mathbf{n}\neq\mathbf{0}}|\mathbf{n}|^{-2s} \; (s>3/2). \tag{78c}$$

The above lattice sums are evaluated in Appendix C. One can easily extract $t'^{(j,-5-j)}_{\mathbf{q},\mathbf{k}}$ and $t''^{(j,-5-j)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ from Eqs. (76).

***Step 3a***. From $t''^{(1,-6)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ and Eq. (70), we get

$$\mathcal{R}^{(1)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = -(3\alpha_1 a\epsilon/\pi)\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}. \tag{79}$$

***Step 3b***. From $(H\mathcal{S}^{(-2)\mathbf{q}})_{\mathbf{k}}=0$, and $t''^{(-2,-3)}_{\mathbf{q},\mathbf{k}}$, we get

$$\mathcal{S}^{(-2)\mathbf{q}}_{\mathbf{k}} = [-(\alpha_1 a\epsilon/\pi)(2\pi)^3\delta(\mathbf{q}) - 8\pi aJ(\mathbf{q})/q^2]\phi_{\mathbf{k}}. \tag{80}$$

***Step 4***. This is similar to Step 2,

$$E = 12\pi a\epsilon^3(1-\alpha_1 a\epsilon/\pi) + O(\epsilon^5), \tag{81}$$

$$\mathcal{T}^{(-4)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = J_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}G_{n_1n_2n_3}\sum_{i=1}^3 2a^2/\pi^2\epsilon^4 n_i^2 + (a^2/\pi^2\epsilon) \times\sum_{i=1}^3(\alpha_1 m_i^{-2} + m_i^{-4})J(\mathbf{p}_i)(2\pi)^3\delta(\mathbf{q}_i), \tag{82}$$

$$J_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} \equiv \sum_{\mathbf{n}'_{1,2}\neq\mathbf{0},\mathbf{n}'_1+\mathbf{n}'_2\neq\mathbf{0}} \prod_{i=1}^{2} (2\pi\epsilon)^3 \delta(\mathbf{q}_i - 2\pi\epsilon\mathbf{n}'_i). \quad (83)$$

The three subscripts of $J_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ are always subject to the constraint $\Sigma_{i=1}^3 \mathbf{q}_i \equiv \mathbf{0}$. In Eq. (82) and in the following, $G_{n_1n_2n_3} \equiv 2/(n_1^2+n_2^2+n_3^2)$, and

$$\mathbf{n}_i \equiv \mathbf{q}_i/2\pi\epsilon, \quad \mathbf{n} \equiv \mathbf{q}/2\pi\epsilon, \quad \mathbf{m}_i \equiv \mathbf{p}_i/2\pi\epsilon. \quad (84)$$

$\mathcal{T}^{(-4)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}} = \Sigma_{j=-2}^{\infty} t'^{(j,-4-j)}_{\mathbf{q},\mathbf{k}}$, where

$$t'^{(-1,-3)}_{\mathbf{q},\mathbf{k}} = (a^2/\pi^2\epsilon)\{(\alpha_1^2+\alpha_2)(2\pi\epsilon)^3\delta(\mathbf{q})(2\pi)^3\delta(\mathbf{k}) + J(\mathbf{q}) \times[2\rho_{A1}(\mathbf{n}) + 2\alpha_1/n^2 - 6/n^4](2\pi)^3\delta(\mathbf{k})\}, \quad (85a)$$

$$t'^{(0,-4)}_{\mathbf{q},\mathbf{k}} = [16\pi^2a^2(2\pi\epsilon)^3\delta(\mathbf{q}) + 40\pi^2a^2J(\mathbf{q})]Z/k^4, \quad (85b)$$

$$t'^{(1,-5)}_{\mathbf{q},\mathbf{k}} = X^{(-4)}_{\mathbf{q},\mathbf{k}} J(\mathbf{q}). \quad (85c)$$

The actual formulas for $X^{(s)}_{\mathbf{q},\mathbf{k}}$ ($s=-4,-3,-2$; see Steps 6 and 8 below) are not needed in this paper. For $s \geqslant 1$,

$$\rho_{As}(\mathbf{n}) \equiv 2\theta_{As}(\mathbf{n}) + W_A(\mathbf{n})/n^{2s}, \quad (86a)$$

$$\theta_{As}(\mathbf{n}) \equiv \sum_{\mathbf{m}\neq\mathbf{0}} [(m^2+\mathbf{m}\cdot\mathbf{n}+n^2)m^{2s}]^{-1}, \quad (86b)$$

$$W_A(\mathbf{n}) \equiv \lim_{N\to\infty} \sum_{|\mathbf{m}|<N} (m^2+\mathbf{m}\cdot\mathbf{n}+n^2)^{-1} - 4\pi N, \quad (86c)$$

$$\mathcal{T}^{(-4)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = G_{k_1k_2k_3}\sum_{i=1}^{3} 32\pi^2a^2/k_i^2 + 12\alpha_1a^2\epsilon\sum_{i=1}^{3}(2\pi)^3\delta(\mathbf{k}_i)/l_i^2 + 3\pi^{-2}(2\beta_{1A}+\alpha_1^2-3\alpha_2)a^2\epsilon^2(2\pi)^6\delta(\mathbf{k}_1)\delta(\mathbf{k}_2) + O(\epsilon^3), \quad (87)$$

from which one can easily extract $t''^{(j,-4-j)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$. Here

$$\beta_{1A} \equiv \lim_{\eta\to0^+} \sum_{\mathbf{n}\neq\mathbf{0}} e^{-\eta n} W_A(\mathbf{n})/n^2 + 4\sqrt{3}\pi^3/\eta^2 \quad (88)$$

is evaluated in Eq. (C18).

***Step 5a***. From $t''^{(2,-6)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$ and Eq. (70), we get

$$\mathcal{R}^{(2)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = 3\pi^{-2}(2\beta_{1A}+\alpha_1^2-3\alpha_2)a^2\epsilon^2\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}. \quad (89)$$

***Step 5b***. From $(H\mathcal{S}^{(-1)\mathbf{q}})_{\mathbf{k}}=0$, and $t'^{(-1,-3)}_{\mathbf{q},\mathbf{k}}$, we get

$$\mathcal{S}^{(-1)\mathbf{q}}_{\mathbf{k}} = (a^2/\pi^2\epsilon)\{(\alpha_1^2+\alpha_2)(2\pi\epsilon)^3\delta(\mathbf{q}) + [2\rho_{A1}(\mathbf{n}) + 2\alpha_1/n^2 - 6/n^4]J(\mathbf{q})\}\phi_{\mathbf{k}}. \quad (90)$$

***Step 6***. This is similar to Steps 2 and 4,

$$E = 12\pi a\epsilon^3[1-\alpha_1a\epsilon/\pi + (\alpha_1^2+\alpha_2)a^2\epsilon^2/\pi^2] + O(\epsilon^6), \quad (91)$$

$$\mathcal{T}^{(-3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \sum_{i=1}^{3}(6a^3/\pi^3\epsilon^3)J_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}G^2_{n_1n_2n_3}n_i^{-2} - (2a^3/\pi^3\epsilon^3)J_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}G_{n_1n_2n_3}[\rho_{A1}(\mathbf{n}_i) + \alpha_1/n_i^2 - 3/n_i^4] + \{[-4\rho_{A1}(\mathbf{m}_i)/m_i^2 - (\alpha_1^2+\alpha_2)/m_i^2 + 2\alpha_1/m_i^4 + 15/m_i^6]a^3/\pi^3 + u_0\}J(\mathbf{p}_i)(2\pi)^3\delta(\mathbf{q}_i). \quad (92)$$

In preparation for the subsequent steps, we derive

$$t'^{(0,-3)}_{\mathbf{q},\mathbf{k}} = \{-32\pi^2wa^3Z_{1/|a|}(k)/k^3 + [2u_0 + 16wa^3\ln(2\pi\epsilon|a|)] \times(2\pi)^3\delta(\mathbf{k}) + (2a^3/\pi^3)[-\rho_{AA1}(\mathbf{n}) - \alpha_1\rho_{A1}(\mathbf{n}) + 3\rho_{A2}(\mathbf{n}) + 3\rho_{B1}(\mathbf{n}) - (\alpha_1^2+\alpha_2)/n^2 + 6\alpha_1/n^4 - 9/n^6] \times(2\pi)^3\delta(\mathbf{k})\}J(\mathbf{q}) + \{-32\pi^2wa^3Z_{1/|a|}(k)/k^3 + [16wa^3\ln(2\pi\epsilon|a|) - u_0 + (15\alpha_3 + \alpha_1\alpha_2 - \alpha_1^3 - 4\alpha_{1A1})a^3/\pi^3](2\pi)^3\delta(\mathbf{k})\}(2\pi\epsilon)^3\delta(\mathbf{q}), \quad (93a)$$

$$t'^{(1,-4)}_{\mathbf{q},\mathbf{k}} = X^{(-3)}_{\mathbf{q},\mathbf{k}}J(\mathbf{q}) - (96\pi\alpha_1a^3\epsilon Z/k^4)(2\pi\epsilon)^3\delta(\mathbf{q}), \quad (93b)$$

where $\rho_{B1}(\mathbf{n})$, $\rho_{AA1}(\mathbf{n})$, and $\alpha_{1A1}$ are defined as follows.

For $s \geqslant 0$,

$$\rho_{Bs}(\mathbf{n}) \equiv 2\theta_{Bs}(\mathbf{n}) + W_B(\mathbf{n})n^{-2s}, \quad (94a)$$

$$\theta_{Bs}(\mathbf{n}) \equiv \sum_{\mathbf{m}\neq\mathbf{0}} [(m^2+\mathbf{m}\cdot\mathbf{n}+n^2)^2m^{2s}]^{-1}, \quad (94b)$$

$$W_B(\mathbf{n}) \equiv \sum_{\text{all } \mathbf{m}} (m^2+\mathbf{m}\cdot\mathbf{n}+n^2)^{-2}, \quad (94c)$$

$$\rho_{AA1}(\mathbf{n}) \equiv \lim_{N\to\infty}\left(2\sum_{\mathbf{m}\neq\mathbf{0};m<N}(m^2+\mathbf{m}\cdot\mathbf{n}+n^2)^{-1}\rho_{A1}(\mathbf{m}) - 8\pi^3w\ln N\right) + W_A(\mathbf{n})\rho_{A1}(\mathbf{n}). \quad (95)$$

It can be shown that at large $\mathbf{n}$,

$$\rho_{A1}(\mathbf{n}) = \pi^2w/n + 2\alpha_1/n^2 + O(n^{-4}),$$

$$\rho_{AA1}(\mathbf{n}) = -8\pi^3w\ln n - \pi^3w(7\pi/\sqrt{3}-8) + 2\pi^2w\alpha_1/n + O(n^{-2}).$$

We define some twofold lattice sums,

$$\alpha_{1A1} \equiv \lim_{N\to\infty}\left[\left(\sum_{\mathbf{n}\neq\mathbf{0};n<N} n^{-2}\rho_{A1}(\mathbf{n})\right) - 4\pi^3w\ln N\right], \quad (96a)$$

$$\alpha_{sAs'} \equiv \sum_{\mathbf{n}\neq\mathbf{0}} n^{-2s}\rho_{As'}(\mathbf{n}) \ (s+s' \geqslant 3), \quad (96b)$$

$$\alpha_{sBs'} \equiv \sum_{\mathbf{n}\neq\mathbf{0}} n^{-2s}\rho_{Bs'}(\mathbf{n}) \ (s+s' \geqslant 2). \quad (96c)$$

$\alpha_{1A1}$, $\alpha_{1A2}$, $\alpha_{2A1}$, and $\alpha_{1B1}$ are evaluated in Appendix C.

***Step 7***. From

$$(H\mathcal{S}^{(0)\mathbf{q}})_{\mathbf{k}} + (-6\pi a\phi_{\mathbf{k}} + W_{\mathbf{k}}^{(0)})J(\mathbf{q}) + (-12\pi a\phi_{\mathbf{k}} + W_{\mathbf{k}}^{(0)}) \times (2\pi\epsilon)^3\delta(\mathbf{q}) = 0 \quad (\text{all } \mathbf{k}),$$

$$\mathcal{S}_{\mathbf{k}}^{(0)\mathbf{q}} = \sum_{s=-5}^{-3} t'^{(0,s)}_{\mathbf{q},\mathbf{k}} + O(\epsilon^0 k^{-2}) \quad (\text{small } \mathbf{k}),$$

where $W_{\mathbf{k}}^{(0)}$ is defined in Eq. (22b), we get

$$\mathcal{S}_{\mathbf{k}}^{(0)\mathbf{q}} = \{[16wa^3\ln(\epsilon|a|) + 2a^3\tilde{\rho}_{AA1}(\mathbf{n})/\pi^3]\phi_{\mathbf{k}} + d_{\mathbf{k}} + 10\pi a\phi_{\mathbf{qk}}^{(d)}\}J(\mathbf{q}) + \{[16wa^3\ln(\epsilon|a|) + C_0a^3 + 3\pi a^2 r_s - 3u_0]\phi_{\mathbf{k}} + d_{\mathbf{k}} + 6\pi a f_{\mathbf{k}}\}(2\pi\epsilon)^3\delta(\mathbf{q}), \tag{97}$$

where $d_{\mathbf{k}}$ is defined in Eqs. (36),

$$C_0 \equiv 16w\ln(2\pi) + (15\alpha_3 + \alpha_1\alpha_2 - \alpha_1^3 - 4\alpha_{1A1})/\pi^3 - (14\pi/\sqrt{3} - 16)w = 95.852\,723\,604\,821\,230\,29, \tag{98}$$

and

$$\tilde{\rho}_{AA1}(\mathbf{n}) \equiv -\rho_{AA1}(\mathbf{n}) - \pi^3 w(7\pi/\sqrt{3} - 8) + 8\pi^3 w\ln(2\pi) - \alpha_1\rho_{A1}(\mathbf{n}) + 3\rho_{A2}(\mathbf{n}) + 3\rho_{B1}(\mathbf{n}) - (\alpha_1^2 + \alpha_2)/n^2 + 6\alpha_1/n^4 - 9/n^6. \tag{99}$$

See Appendix C for the evaluation of $C_0$ (and $C_1$ in Step 9).

***Step 8***. This is similar to Steps 2, 4, and 6. With the help of Eqs. (12) and (39), we get

$$E = 12\pi a\epsilon^3\{1 - \alpha_1 a\epsilon/\pi + (\alpha_1^2 + \alpha_2)a^2\epsilon^2/\pi^2 + [16wa^3\ln(\epsilon|a|) + C_0a^3 + 3\pi a^2 r_s]\epsilon^3\} + D\epsilon^6 + O(\epsilon^7), \tag{100}$$

$$\mathcal{T}^{(-2)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \sum_{i=1}^{3}\left[J(\mathbf{p}_i)(2\pi)^3\delta(\mathbf{q}_i)\mathcal{T}^{(-2\delta)}(\mathbf{m}_i) + J_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}\sum_{s=0}^{3}G^s_{\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3}\mathcal{T}_s^{(-2)}(\mathbf{n}_i)\right], \tag{101a}$$

$$\mathcal{T}^{(-2\delta)}(\mathbf{m}_i) \equiv -\alpha_1 a u_0\epsilon/\pi - au_0\epsilon/\pi m_i^2 - D\epsilon/4\pi^2 m_i^2 - 3a^3 r_s\epsilon/m_i^2 + \{-[4\tilde{\rho}_{AA1}(\mathbf{m}_i) + 48\pi^3 w\ln(\epsilon|a|) + \pi^3 C_0]/m_i^2 - [12\rho_{A1}(\mathbf{m}_i) + 9\alpha_1^2 + 6\alpha_2]/m_i^4 + 3\alpha_1/m_i^6 + 45/m_i^8\}a^4\epsilon/\pi^4, \tag{101b}$$

$$\mathcal{T}_0^{(-2)}(\mathbf{n}_i) \equiv -2au_0/\pi\epsilon^2 n_i^2, \tag{101c}$$

$$\mathcal{T}_1^{(-2)}(\mathbf{n}_i) \equiv -2[\tilde{\rho}_{AA1}(\mathbf{n}_i) + 8\pi^3 w\ln(\epsilon|a|)]a^4/\pi^4\epsilon^2 - D/12\pi^2\epsilon^2, \tag{101d}$$

$$\mathcal{T}_2^{(-2)}(\mathbf{n}_i) \equiv -6[\rho_{A1}(\mathbf{n}_i) + 2\alpha_1/n_i^2 - 3/n_i^4]a^4/\pi^4\epsilon^2, \tag{101e}$$

$$\mathcal{T}_3^{(-2)}(\mathbf{n}_i) \equiv 18a^4/\pi^4\epsilon^2 n_i^2. \tag{101f}$$

In preparation for the next step, we derive

$$t'^{(1,-3)}_{\mathbf{q},\mathbf{k}} = X^{(-2)}_{\mathbf{q},\mathbf{k}}J(\mathbf{q}) + \{96\pi w\alpha_1 a^4 Z_{1/|a|}(k)/k^3 + [-(96w\alpha_1/\pi)a^4\ln(\epsilon|a|) + C_1'a^4 - \alpha_1 D/4\pi^2 - 3\alpha_1 a^3 r_s](2\pi)^3\delta(\mathbf{k})\}\epsilon(2\pi\epsilon)^3\delta(\mathbf{q}), \tag{102}$$

$$C_1' \equiv \pi^{-4}[-4\tilde{\alpha}_{1AA1} - 48\pi^3 w\alpha_1\ln(2\pi) - \pi^3\alpha_1 C_0 - 12\alpha_{2A1} - 9\alpha_1^2\alpha_2 - 6\alpha_2^2 + 3\alpha_1\alpha_3 + 45\alpha_4], \tag{103}$$

where

$$\tilde{\alpha}_{1AA1} \equiv \lim_{N\to\infty}\left[\left(\sum_{\mathbf{m}\neq\mathbf{0};m<N} m^{-2}\tilde{\rho}_{AA1}(\mathbf{m})\right) - 32\pi^4 wN[\ln(2\pi N) - 1] + 12\pi^3 w\alpha_1\ln N\right] \tag{104}$$

is a threefold lattice sum (evaluated in Appendix C).

***Step 9***. From

$$(H\mathcal{S}^{(1)\mathbf{q}})_{\mathbf{k}} + (24\alpha_1 a^2\epsilon^4\phi_{\mathbf{k}} - 3\alpha_1 a\epsilon^4 W_{\mathbf{k}}^{(0)}/\pi)(2\pi)^3\delta(\mathbf{q}) + \{6[n^2\rho_{A1}(\mathbf{n}) + \alpha_1 + n^{-2}]a^2\epsilon\phi_{\mathbf{k}} - 3\alpha_1 a\epsilon W_{\mathbf{k}}^{(0)}/\pi\}J(\mathbf{q}) = 0$$

and [note that $t'^{(1,-7)}_{\mathbf{q},\mathbf{k}} = t'^{(1,-6)}_{\mathbf{q},\mathbf{k}} = 0$]

$$\mathcal{S}_{\mathbf{k}}^{(1)\mathbf{q}} = \sum_{s=-5}^{-3} t'^{(1,s)}_{\mathbf{q},\mathbf{k}} + O(\epsilon^1 k^{-2}) \quad (\text{for small } \mathbf{k}),$$

we get

$$\mathcal{S}_{\mathbf{k}}^{(1)\mathbf{q}} = \{[-(96w\alpha_1/\pi)a^4\ln(\epsilon|a|) + C_1a^4 - \alpha_1 D/4\pi^2 - 6\alpha_1 a^3 r_s + 6\alpha_1 a u_0/\pi]\phi_{\mathbf{k}} - 6\alpha_1 a^2 f_{\mathbf{k}} - 3\alpha_1 a d_{\mathbf{k}}/\pi\} \times \epsilon(2\pi\epsilon)^3\delta(\mathbf{q}) + Y(\mathbf{q},\mathbf{k})J(\mathbf{q}), \tag{105}$$

where

$$C_1 \equiv C_1' + 6w\alpha_1(7/\sqrt{3} - 8/\pi) = 810.053\,286\,803\,649\,420, \tag{106}$$

and the actual formula for $Y(\mathbf{q},\mathbf{k})$ is not needed in this paper.

***Step 10***. Substituting the latest results for $\mathcal{S}_{\mathbf{k}}^{\mathbf{q}}$ and $\mathcal{R}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ into Eq. (66c), extracting all the terms that contain the factor $(2\pi)^6\delta(\mathbf{q}_1)\delta(\mathbf{q}_2)$ from this equation, noting that $\mathcal{T}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} - (2\pi)^6\delta(\mathbf{q}_1)\delta(\mathbf{q}_2)$ vanishes at $\mathbf{q}_1 = \mathbf{q}_2 = \mathbf{0}$, and using Eqs. (12) and (39) to simplify the result, we get

$$E = 12\pi a\epsilon^3\{1 - \alpha_1 a\epsilon/\pi + (\alpha_1^2 + \alpha_2)a^2\epsilon^2/\pi^2 + [16wa^3\ln(\epsilon|a|) + C_0a^3 + 3\pi a^2 r_s]\epsilon^3 + [-(96w\alpha_1/\pi)a^4\ln(\epsilon|a|) + C_1a^4 - 6\alpha_1 a^3 r_s]\epsilon^4\} + (\epsilon^6 - 6\alpha_1 a\epsilon^7/\pi)D + O(\epsilon^8). \tag{107}$$

Substituting the numerical values of the lattice sums (see Appendix C) to the above equation, we get Eq. (5).

We will not proceed to determine $\mathcal{T}^{(-1)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ in this paper.

### B. Wu's parameter $\mathcal{E}_3$

Wu computed the three-boson energy in the large periodic cubic volume to order $L^{-6}$, and he left an unknown parameter

$\mathcal{E}_3$ for the three-boson interaction strength at low energy [5]. $\mathcal{E}_3$ is needed to determine the full order-$\rho^2$ correction to the many-body energy [5].

Comparing our Eq. (100) with Wu's result, Eq. (5.29) of Ref. [5] (note that the unit of mass in [5] is $2m_{\rm boson}=1$), we find that Huang and Yang's constant [22] $C=-\alpha_1/\pi=2.837\ldots$, [23] different from the number 2.37 which was first provided in Ref. [22] and then adopted by [5]; the symbols $\xi_s$ in Ref. [5] equal $\alpha_s/\pi^s$; the symbol $\mathcal{E}_3$ in Ref. [5] is now expressed in terms of $D$ of the present paper,

$$\mathcal{E}_3 = D/12\pi a^4 + 3\pi r_s/a - 4\alpha_{1A1}/\pi^3 + 16w\ln(2\pi) - (14\pi/\sqrt{3} - 16)w = D/12\pi a^4 + 3\pi r_s/a + 73.699\,808\,371\,935\,4035. \quad (108)$$

For hard-sphere bosons, $D$ is given by Eq. (4) and $r_s=2a/3$, so

$$\mathcal{E}_3 = 126.709\,37 \pm 0.000\,06 \text{ (for hard spheres)}. \quad (109)$$

### C. Results for the three-body ground-state wave function

There are six expansion formulas for $A_{\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3}$, each of which is valid in a subregion of the discrete momentum configuration space,

$$A_{000} \equiv L^6, \quad (110a)$$

$$\begin{aligned}A_{0,\mathbf{n},-\mathbf{n}} = {}& -aL^5/\pi n^2 + (\alpha_1/n^2 + 1/n^4)a^2L^4/\pi^2 + \{-[\alpha_1^2+\alpha_2 + 4\rho_{A1}(\mathbf{n})]/n^2 + 2\alpha_1/n^4 + 15/n^6\}a^3L^3/\pi^3 + u_0L^3 \\ &+ \{[-4\tilde\rho_{AA1}(\mathbf{n})/n^2 + 48\pi^3 w n^{-2}\ln(L/|a|) - \pi^3 C_0/n^2 - (9\alpha_1^2+6\alpha_2)/n^4 - 12\rho_{A1}(\mathbf{n})/n^4 + 3\alpha_1/n^6 \\ &+ 48/n^8]a^4/\pi^4 - (\alpha_1 + n^{-2})au_0/\pi - D/4\pi^2n^2 - 3a^3r_s/n^2\}L^2 + O(L^1), \quad (110b)\end{aligned}$$

$$\begin{aligned}A_{\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3} = {}& \sum_{i=1}^{3}\{2a^2L^4/\pi^2n_i^2 - 2[\rho_{A1}(\mathbf{n}_i) + \alpha_1/n_i^2 - 3/n_i^4]a^3L^3/\pi^3 - DL^2/12\pi^2 + 2[8\pi^3 w\ln(L/|a|) - \tilde\rho_{AA1}(\mathbf{n}_i)]a^4L^2/\pi^4\} \\ &\times G_{n_1n_2n_3} + \{6a^3L^3/\pi^3n_i^2 - 6[\rho_{A1}(\mathbf{n}_i) + 2\alpha_1/n_i^2 - 3/n_i^4]a^4L^2/\pi^4\}G^2_{n_1n_2n_3} + 18a^4L^2G^3_{n_1n_2n_3}/\pi^4n_i^2 \\ &- 2au_0L^2/\pi n_i^2 + O(L^1), \quad (110c)\end{aligned}$$

$$\begin{aligned}A_{0,\mathbf{N},-\mathbf{N}} = {}& \{L^3 - \alpha_1 aL^2/\pi + (\alpha_1^2+\alpha_2)a^2L/\pi^2 - 16wa^3\ln(L/|a|) + C_0a^3 + 3\pi a^2r_s - 3u_0 + [(96w\alpha_1/\pi)a^4\ln(L/|a|) \\ &+ C_1a^4 - \alpha_1 D/4\pi^2 - 6\alpha_1 a^3 r_s + 6\alpha_1 au_0/\pi]L^{-1}\}\phi_{\mathbf{k}} + (1-3\alpha_1 a/\pi L)d_{\mathbf{k}} + (6\pi a - 6\alpha_1 a^2/L)f_{\mathbf{k}} + O(L^{-2}), \quad (110d)\end{aligned}$$

$$\begin{aligned}A_{\mathbf{n},-\mathbf{n}/2+\mathbf{N},-\mathbf{n}/2-\mathbf{N}} = {}& \{-2aL^2/\pi n^2 + [2\rho_{A1}(\mathbf{n}) + 2\alpha_1/n^2 - 6/n^4]a^2L/\pi^2 - 16wa^3\ln(L/|a|) \\ &+ 2a^3\tilde\rho_{AA1}(\mathbf{n})/\pi^3\}\phi_{\mathbf{k}} + 10\pi a\phi^{(d)}_{\hat{\mathbf{n}}\mathbf{k}} + d_{\mathbf{k}} + O(L^{-1}), \quad (110e)\end{aligned}$$

$$A_{\mathbf{N}_1\mathbf{N}_2\mathbf{N}_3} = [1 - 3\alpha_1 a/\pi L + 3(2\beta_{1A} + \alpha_1^2 - 3\alpha_2)a^2/\pi^2L^2]\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + O(L^{-3}), \quad (110f)$$

where $\mathbf{n}$'s are *nonzero* vectors of order unity, $\mathbf{N}$'s are large vectors of order $L/\max(r_e,|a|)$ ($r_e$ is the range of the interaction), $\mathbf{k}\equiv 2\pi\mathbf{N}/L$, $\mathbf{k}_i\equiv 2\pi\mathbf{N}_i/L$, and $G_{n_1n_2n_3}\equiv 2/(n_1^2+n_2^2+n_3^2)$. The formulas for $A_{0,0,0}$, $A_{0,\mathbf{n},-\mathbf{n}}$, and $A_{\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3}$ are extracted from the above results for $\mathcal{T}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$; those for $A_{0,\mathbf{N},-\mathbf{N}}$ and $A_{\mathbf{n},-\mathbf{n}/2+\mathbf{N},-\mathbf{n}/2-\mathbf{N}}$ are extracted from $\mathcal{S}^{\mathbf{q}}_{\mathbf{k}}$; the formula for $A_{\mathbf{N}_1\mathbf{N}_2\mathbf{N}_3}$ results from the expansion of $\mathcal{R}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$. The numerical constants in the above formulas are computed in Appendix C.

### D. Momentum distribution

The expectation value of the number of bosons with momentum $2\pi\mathbf{n}/L$ is $\mathcal{N}_{\mathbf{n}}=c\Sigma_{\text{all }\mathbf{n}'}|A_{\mathbf{n},\mathbf{n}',-\mathbf{n}-\mathbf{n}'}|^2$ for some constant $c$ such that $\Sigma_{\text{all }\mathbf{n}}\mathcal{N}_{\mathbf{n}}=3$.

For any nonzero integral vector $\mathbf{n}$ of order unity and any large integral vector $\mathbf{N}$ of order $L/\max(r_e,|a|)$, we have

$$\mathcal{N}_0 = c|A_{000}|^2 + c\sum_{0<n'\le N_c}|A_{0,\mathbf{n}',-\mathbf{n}'}|^2 + c\sum_{N'>N_c}|A_{0,\mathbf{N}',-\mathbf{N}'}|^2, \quad (111a)$$

$$\mathcal{N}_{\mathbf{n}} = 2c|A_{0,\mathbf{n},-\mathbf{n}}|^2 + c\sum_{\mathbf{n}'\neq\pm\mathbf{n}/2,n'\le N_c}|A_{\mathbf{n},-\mathbf{n}/2+\mathbf{n}',-\mathbf{n}/2-\mathbf{n}'}|^2 + c\sum_{N'>N_c}|A_{\mathbf{n},-\mathbf{n}/2+\mathbf{N}',-\mathbf{n}/2-\mathbf{N}'}|^2, \quad (111b)$$

$$\mathcal{N}_{\mathbf{N}} = 2c|A_{0,\mathbf{N},-\mathbf{N}}|^2 + 2c\sum_{\mathbf{n}'\neq 0,n'\le N_c}|A_{\mathbf{n}',\mathbf{N},-\mathbf{n}'-\mathbf{N}}|^2 + c\sum_{N'>N_c,|\mathbf{N}'+\mathbf{N}|>N_c}|A_{\mathbf{N}',\mathbf{N},-\mathbf{N}'-\mathbf{N}}|^2, \quad (111c)$$

where $N_c$ satisfies $1\ll N_c\ll L/\max(r_e,|a|)$; in Eq. (111b), $\mathbf{n}'\pm\mathbf{n}/2$ and $\mathbf{N}'\pm\mathbf{n}/2$ have integral Cartesian components. Substituting Eqs. (110) and using Eq. (14), we get

$$\mathcal{N}_0/c = L^{12} + \alpha_2 a^2L^{10}/\pi^2 - 2(\alpha_1\alpha_2+\alpha_3)a^3L^9/\pi^3 - 2\,\mathrm{Re}\,u_0L^9 - 2\pi a^2r_sL^9 + O(L^8),$$

$$\mathcal{N}_{\mathbf{n}}/c = 2a^2L^{10}/\pi^2n^4 - 4(\alpha_1/n^4 + 1/n^6)a^3L^9/\pi^3 + O(L^8),$$

$$\mathcal{N}_{\mathbf{N}}/c = 2L^6(1 - 2\alpha_1 a/\pi L)|\phi_{2\pi\mathbf{N}/L}|^2 + O(L^4).$$

Solving $\Sigma_{\text{all }\mathbf{n}}\mathcal{N}_{\mathbf{n}}=3$ [using Eq. (14) again], we get

$$c = 3L^{-12}[1 - 3\alpha_2a^2/\pi^2L^2 + 6(\alpha_1\alpha_2+\alpha_3)a^3/\pi^3L^3 + 6\,\mathrm{Re}\,u_0/L^3 + 6\pi a^2r_s/L^3 + O(L^{-4})] \quad (112)$$

and

$$\mathcal{N}_0/3 = 1 - 2\alpha_2 a^2/\pi^2 L^2 + 4(\alpha_1\alpha_2 + \alpha_3)a^3/\pi^3 L^3 + (4\,\mathrm{Re}\,u_0 + 4\pi a^2 r_s)/L^3 + O(L^{-4}) = 1 - 3.350\,147\,643 a^2/L^2 + (4\,\mathrm{Re}\,u_0 + 4\pi a^2 r_s - 17.926\,831\,164 a^3)/L^3 + O(L^{-4}), \tag{113a}$$

$$\mathcal{N}_{\mathbf{n}} = 6a^2/\pi^2 L^2 n^4 - (12a^3/\pi^3 L^3)(\alpha_1/n^4 + 1/n^6) + O(L^{-4}) = (0.607\,927\,102/n^4)(a/L)^2 + (3.449\,740\,068/n^4 - 0.387\,018\,413/n^6)(a/L)^3 + O(L^{-4}), \tag{113b}$$

$$\mathcal{N}_{\mathbf{N}} = 6L^{-6}(1 - 2\alpha_1 a/\pi L)|\phi_{2\pi\mathbf{N}/L}|^2 + O(L^{-8}) = 6L^{-6}(1 + 5.674\,594\,959 a/L)|\phi_{2\pi\mathbf{N}/L}|^2 + O(L^{-8}). \tag{113c}$$

One can derive higher-order results for $\mathcal{N}$'s from Eqs. (110).

Equation (113a) shows that the population of the zero-momentum state depends on the parameter $u_0$.

### E. The parameter $u_0$ and the condensate fraction

Given the two-body potential $\frac{1}{2}U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}$, one can solve the Schrödinger equation for the two-body $s$-wave scattering wave function at zero energy, $\phi(\mathbf{r})$. From $\phi(\mathbf{r})$, one can compute $u_0$ and $r_s$,

$$u_0 = \int [\phi(\mathbf{r}) - (1 - a/r)]\mathrm{d}^3 r, \tag{114a}$$

$$-2\pi a^2 r_s = \int [|\phi(\mathbf{r})|^2 - (1 - a/r)^2]\mathrm{d}^3 r. \tag{114b}$$

Because $\phi(\mathbf{r}) = 1 - a/r$ outside of the range of the interaction, the integrands are nonzero within the range only. Because there exists a two-body potential $V(\mathbf{r}) = \phi^{-1}(\mathbf{r})\nabla^2\phi(\mathbf{r})$ for any function $\phi(\mathbf{r})$, Eqs. (114) indicate that $u_0$ is in general *independent* from $a$ and $r_s$.

In fact, by making a short-range unitary similarity transformation of the two-body Hamiltonian [24], one can keep all the two-body effective-range expansion parameters [namely those in Eq. (9)] unchanged, but change the two-body potential [24], the function $\phi(\mathbf{r})$, and the integral $u_0$ in Eq. (114a). This transformation changes the momentum distribution and, in particular, the "condensate fraction" in Eq. (113a), which depends on $u_0$. One may thus ask whether the momentum distribution is an observable at all, a question that was first raised in Ref. [25], where it was shown that certain quantum field redefinitions also leave scattering data and energy spectra unchanged but modify the momentum distribution.

Despite this issue, the author believes that the results for momentum distributions in this paper *are* useful, for a few reasons. First, for atomic systems, there is a well-defined convention for the effective potentials between atomic nuclei, based on the Born-Oppenheimer approximation and the Coulomb interaction. Secondly, for certain systems such as superfluid $^4$He, one can cleanly extract the momentum distribution from deep inelastic neutron-scattering data, using the impulse approximation. Perhaps this neutron-scattering technique can also be applied to a dilute metastable gas of $^4$He at ultracold temperatures. Thirdly, it is the results in this paper that show explicitly how the ambiguity in the two-body potential propagates to the condensate fraction—the ambiguity in the latter quantity is dominated by $u_0$ at low density, and $u_0$, in turn, is directly determined by the potential.

We will show in Sec. IV F 2 how $u_0$ affects the condensate fraction in the many-body state.

### F. Generalization to $\mathcal{N}$ bosons

#### 1. Results

To understand the ground-state energy and momentum distribution of dilute Bose-Einstein condensates (BECs), the author generalized the above calculations of the energy and momentum distribution to $\mathcal{N}$ bosons ($\mathcal{N}=1,2,3,4,\ldots$).

Solving the $\mathcal{N}$-boson Schrödinger equation perturbatively in powers of $1/L$, using the same *finite-range* interactions as above, the author obtained the volume expansion for $E$ up to the order $L^{-6}$, and found that it exactly agrees with the Beane, Detmold, and Savage result for $E$ [26], which was derived with zero-range pseudopotentials [26], if the three-boson contact interaction parameter $\eta_3(\mu)$ in Ref. [26] satisfies

$$\eta_3(|a|^{-1}) - 48a^4(4\mathcal{Q} + 2\mathcal{R})/\pi^2 = D + 12\pi^2 a^3 r_s - 48a^4\alpha_{1A1}/\pi^2 + 24\pi w a^4[8\ln(2\pi) - (7\pi/\sqrt{3} - 8)] = D + 12\pi^2 a^3 r_s + 2778.417\,318\,626\,973\,645 a^4, \tag{115}$$

where $4\mathcal{Q}+2\mathcal{R}$ is a number defined in Ref. [26]. It is the combination $\eta_3(\mu) - 48a^4(4\mathcal{Q}+2\mathcal{R})/\pi^2$ that appears in their formula [26] for $E$. In summary,

$$E = P(1/L; a, \mathcal{N}) - \frac{192\pi w a^4}{L^6}\binom{\mathcal{N}}{3}\ln\frac{L}{|a|} + \binom{\mathcal{N}}{3}\frac{D + 12\pi^2 a^3 r_s}{L^6} + \binom{\mathcal{N}}{2}\frac{8\pi^2 a^3 r_s}{L^6} + O(L^{-7}), \tag{116}$$

where $P$ is a well-determined [26] power series in $1/L$ with $a$ and $\mathcal{N}$ as the only parameters, and $\binom{n}{i} = \frac{n!}{i!(n-i)!}$.

In addition to the energy, the present author obtained the following results for the momentum distribution:

$$x \equiv \mathcal{N}_0/\mathcal{N} = 1 - (\mathcal{N}-1)\alpha_2(a/\pi L)^2 + 2(\mathcal{N}-1)(\mathrm{Re}\,u_0 + \pi a^2 r_s)/L^3 + 2(\mathcal{N}-1)[\alpha_1\alpha_2 + (2\mathcal{N}-5)\alpha_3](a/\pi L)^3 + O(L^{-4}), \tag{117a}$$

$$\mathcal{N}_{\mathbf{n}} = \mathcal{N}(\mathcal{N}-1)n^{-4}(a/\pi L)^2 - 2\mathcal{N}(\mathcal{N}-1)[\alpha_1/n^4 + (2\mathcal{N}-5)/n^6] \times (a/\pi L)^3 + O(L^{-4}), \tag{117b}$$

$$\mathcal{N}_{\mathbf{N}} = \mathcal{N}(\mathcal{N}-1)L^{-6}(1 - 2\alpha_1 a/\pi L)|\phi_{2\pi\mathbf{N}/L}|^2 + O(L^{-8}). \tag{117c}$$

#### 2. Implications for dilute Bose-Einstein condensates in the thermodynamic limit

Let $a>0$. Let $\rho=\mathcal{N}/L^3$. At large $\mathcal{N}$, there are two different low-density regimes (and an intermediate regime between the two), depending on the box size $L$:

(i) $L \gg \mathcal{N}a$, so that $L$ is *small* compared to the BEC healing length $\xi\sim(\rho a)^{-1/2}$.

(ii) $\mathcal{N}^{1/3}a \ll L \ll \mathcal{N}a$, and the system is a dilute BEC near the thermodynamic limit ($L\gg\xi$).

The $1/L$ expansions for the energy and the momentum distribution are valid in the first regime only. In the second regime, they diverge like $\sum_{i=0}^{\infty} c_i(a\mathcal{N}/L)^i$. Nevertheless, one can infer many properties of the BEC in the second regime.

Now we tentatively take the thermodynamic limit ($\rho$ fixed, $\mathcal{N}$ and $L$ large) of the $1/L$ expansions of the energy per particle $E_0=E/\mathcal{N}$ and the condensate fraction $x=\mathcal{N}_0/\mathcal{N}$ [see Eq. (117a)]. Each term that remains finite is retained; each term that diverges must be rendered finite by a resummation [3] that includes all similar but higher-order (and increasingly more divergent) contributions [3].

Thus the mean-field energy term for $E_0$ is reproduced. The logarithmic term $\approx -32\pi w a^4\rho^2 \ln(L/a)$ is rendered finite by a resummation that changes $L$ to $O(\xi)$, yielding precisely the same logarithmic term as in Eq. (1). The leading nonuniversal terms (in the sense that parameters other than $a$ contribute) become $\rho^2(D/6+2\pi^2a^3r_s)$. Comparing these findings with Eq. (1), we deduce that

$$E_0 = 2\pi\rho a[1 + (128/15\sqrt{\pi})(\rho a^3)^{1/2} + 8w\rho a^3 \ln(\rho a^3) + (D/12\pi a^4 + \pi r_s/a + C^E)\rho a^3] \tag{118}$$

plus higher-order terms in density $\rho$, where $C^E$ is a universal constant that remains the same for all Bose gases. Because $E_0$ was computed by Braaten and Nieto [8], a comparison will be made between Eq. (118) and Ref. [8] (in Sec. V D).

The corrections to $x$ that depend on $a$ only are divergent in the thermodynamic limit. After a resummation that includes higher-order terms in $\mathcal{N}a/L$ [analogous to Eq. (55) of Ref. [3]], they must reproduce Bogoliubov's well-known formula $x=1-\frac{8}{3\sqrt{\pi}}\sqrt{\rho a^3}+\cdots$. The leading nonuniversal term becomes $\rho(2\,\mathrm{Re}\,u_0+2\pi a^2 r_s)$; because this term comes from the short-range behavior in two-body collisions, it must extend into the thermodynamic limit. Combining these observations with an EFT prediction of the condensate fraction [10] (which should be valid through order $\rho^1$ at $u_0=a^2r_s=0$, at the very least), we find that the condensate fraction is

$$x = 1 - \frac{8}{3\sqrt{\pi}}\sqrt{\rho a^3} + \rho(2\,\mathrm{Re}\,u_0 + 2\pi a^2 r_s) + C^x\rho a^3 \tag{119}$$

plus higher-order terms in $\rho$, where $C^x$ is another universal numerical constant. Thus the nonuniversal effect in the condensate fraction is larger than the prediction of Ref. [10] by a factor of order $(\rho a^3)^{-1/2}$ at low density, if $u_0^{1/3}\sim r_s\sim a$. This disagreement is entirely caused by the fact that the momentum distribution at $k\sim 1/r_e \gg (\rho a)^{1/2}$ is approximately $\rho^2|\phi_{\mathbf{k}}|^2$, rather than a structureless function $\approx 16\pi^2a^2\rho^2/k^4$.

As discussed in Sec. IV E, however, short-range unitary transformations [24] or quantum field redefinitions [25] can alter the momentum distribution without affecting many observables [25]. Thus, whether the above disagreement is physically relevant is an open question. The present author, however, believes that it is at least relevant in certain situations (see Sec. IV E).

According to Eq. (119), the condensate fraction of a dilute Bose gas of hard spheres (for which $2u_0+2\pi a^2r_s=\frac{8\pi}{3}a^3$) is slightly *greater* than that of a Bose gas with $r_e\ll a$ (for which $|2u_0+2\pi a^2r_s|\ll a^3$) by about $\frac{8\pi}{3}\rho a^3$ at zero temperature, if the two gases have the same number density and scattering length.

## V. LOW-ENERGY THREE-BODY SCATTERING AMPLITUDES AND IMPLICATIONS FOR THE MANY-BODY PHYSICS

In this section, we compute the T-matrix elements of three identical bosons at low energy (where $a$ can have any sign) and discuss their implications for the many-body BEC physics (where $a\geq 0$). The interactions are the same as in Sec. II. The T-matrix is denoted with roman type T below, since the italic $T$ is already used for the wave-function components.

In Sec. V A, we compute the two-body T-matrix elements at low energy. In Sec. V B, we expand the three-body T-matrix elements at low energy. In Sec. V C, we compare our results in Sec. V B with those in Ref. [8] to establish the relation between the parameter $D$ in the present paper and the three-body coupling constant $g_3(\kappa)$ in Ref. [8]. In Sec. V D, we express the BEC ground-state energy in terms of $D$, taking advantage of the above relation. Implications for the nonuniversal effects are discussed.

### A. Two-boson scattering amplitude

The two-boson T-matrix can be expressed in terms of the scattering phase shifts [27] ($\hbar=m_{\mathrm{boson}}=1$),

$$\mathrm{T}(b,\hat{\mathbf{b}}\cdot\hat{\mathbf{q}}) = (4\pi/\mathrm{i}q)\sum_{l=0,2,4,\ldots}(\mathrm{e}^{2\mathrm{i}\delta_l(q)}-1)(2l+1)P_l(\hat{\mathbf{b}}\cdot\hat{\mathbf{q}}), \tag{120}$$

where $\pm\mathbf{b}$ and $\pm\mathbf{q}$ are the momenta of the two bosons before and after the scattering, respectively, and $q=b$.

At small $q$, we apply Eq. (9) to the above formula and get

$$\mathrm{T}(b,\hat{\mathbf{b}}\cdot\hat{\mathbf{q}}) = -8\pi a + \mathrm{i}8\pi a^2 q + 8\pi a^2(a-r_s/2)q^2 - \mathrm{i}8\pi a^3(a - r_s)q^3 + O(q^4). \tag{121}$$

The first two terms in this expansion agree with Ref. [8], and all higher-order corrections disagree, since the effective range $r_s$ is not included in [8]. Equation (121) agrees with Ref. [10] where $r_s$ is taken into account.

### B. Three-boson scattering amplitude

Equation (121) can be alternatively derived from a systematic perturbative solution to the two-body Schrödinger equation at incoming momenta $\pm\mathbf{b}$ and energy $E=b^2$,

$$\Psi_{\mathbf{q}} = \frac{1}{2}(2\pi)^3[\delta(\mathbf{q}+\mathbf{b})+\delta(\mathbf{q}-\mathbf{b})] + \frac{\mathrm{T}(b,\hat{\mathbf{b}}\cdot\hat{\mathbf{q}})}{2(q^2-E-\mathrm{i}\eta)} + (\text{terms that are regular at } q^2=E),$$

where $-\mathrm{i}\eta$ specifies an outgoing wave ($\eta\to 0^+$).

Similarly, from the stationary wave function $\Psi_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ describing the scattering of three bosons with incoming momenta $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$, and energy

$$E=(b_1^2+b_2^2+b_3^2)/2, \tag{122}$$

one can extract the three-boson T-matrix elements,

$$\Psi_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \frac{(2\pi)^6}{6}\sum_P \delta(\mathbf{q}_1-\mathbf{b}_{P1})\delta(\mathbf{q}_2-\mathbf{b}_{P2}) + \frac{1}{6}G^E_{q_1q_2q_3}\left[\mathrm{T}(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3;\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3) + \sum_{i,j=1}^{3}\mathrm{T}(h_i,\hat{\mathbf{h}}_i\cdot\hat{\mathbf{p}}_j)\times(2\pi)^3\delta(\mathbf{q}_j-\mathbf{b}_i)\right] + [\text{terms that are regular at } (q_1^2+q_2^2+q_3^2)/2=E]. \tag{123}$$

Here $P$ refers to all six permutations of "123," $\Sigma_{i=1}^3 \mathbf{b}_i \equiv \Sigma_{i=1}^3 \mathbf{q}_i \equiv 0$, $\mathbf{p}_i$ is defined in Eq. (19), and

$$G^E_{q_1q_2q_3} = [(q_1^2+q_2^2+q_3^2)/2-E-\mathrm{i}\eta]^{-1}, \tag{124}$$

$$\mathbf{h}_1=(\mathbf{b}_2-\mathbf{b}_3)/2, \text{ and similarly for } \mathbf{h}_2,\mathbf{h}_3. \tag{125}$$

Let $b_i\sim q_i\sim q$ be small. We determine $\Psi$ perturbatively next.

The equations for $\Psi$ here are formally identical with Eqs. (66) in Sec. IV, except for three differences: (i) the box size $L=\infty$ here, so $I(\mathbf{q})\equiv 1$, (ii) $E\sim q^2$ here, instead of $1/L^3$ in Sec. IV, and (iii) the leading contribution to $\Psi_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ is

$$T^{(-6)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \frac{(2\pi)^6}{6}\sum_P \delta(\mathbf{q}_1-\mathbf{b}_{P1})\delta(\mathbf{q}_2-\mathbf{b}_{P2}). \tag{126}$$

Naturally, $\Psi_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}\to\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ in the limit $E$, $b_i\to 0$, and the calculation here will be a generalization of Sec. II to nonzero incoming momenta. So we use the same symbols $T$ ($\neq\mathrm{T}$) and $S$ as in Sec. II, in the asymptotic expansions

$$\Psi_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \sum_{s=-6}^{\infty} T^{(s)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}, \tag{127}$$

$$\Psi^{\mathbf{q}}_{\mathbf{k}} \equiv \Psi_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}} = \sum_{s=-3}^{\infty} S^{(s)\mathbf{q}}_{\mathbf{k}}, \tag{128}$$

where $T^{(s)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}$ and $S^{(s)\mathbf{q}}_{\mathbf{k}}$ scale like $q^s$ (not excluding $q^s\ln^m q$). When $E$, $b_i\to 0$ but $\mathbf{q}$'s and $\mathbf{k}$ are fixed, the (complicated) results for $T^{(s)}$ and $S^{(s)}$ in this section will reduce to the much simpler ones in Sec. II.

When the three bosons all come to a region of size $\sim r_e$ (radius of interaction), effects due to a nonzero $E$ are small. So at momenta $k_i\sim 1/r_e \gg \sqrt{E}$ [28],

$$\Psi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + O(\sqrt{E}). \tag{129}$$

Employing the same systematic expansion method as in Secs. II and IV, we obtain the following results (listed in the same order as they were obtained):

$$S^{(-3)\mathbf{q}}_{\mathbf{k}} = \frac{1}{3}\sum_{i=1}^{3}(2\pi)^3\delta(\mathbf{q}-\mathbf{b}_i)\phi_{\mathbf{k}}, \tag{130a}$$

$$T^{(-5)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = -\frac{4\pi a}{3}G^E_{q_1q_2q_3}\sum_{i,j=1}^{3}(2\pi)^3\delta(\mathbf{q}_j-\mathbf{b}_i), \tag{130b}$$

$$S^{(-2)\mathbf{q}}_{\mathbf{k}} = -\frac{1}{3}\sum_{i=1}^{3}[8\pi a G^E_{\mathbf{q}\mathbf{b}_i} + \mathrm{i}ah_i(2\pi)^3\delta(\mathbf{q}-\mathbf{b}_i)]\phi_{\mathbf{k}}, \tag{130c}$$

$$T^{(-4)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \frac{16\pi^2a^2}{3}G^E_{q_1q_2q_3}\sum_{i,j=1}^{3}\left(2G^E_{\mathbf{q}_j\mathbf{b}_i} + \frac{\mathrm{i}h_i}{4\pi}(2\pi)^3\delta(\mathbf{q}_j-\mathbf{b}_i)\right), \tag{130d}$$

$$S^{(-1)\mathbf{q}}_{\mathbf{k}} = \frac{1}{3}\sum_{i=1}^{3}\{[8\pi a^2(\mathrm{i}h_i-\sqrt{3q^2/4-E-\mathrm{i}\eta})G^E_{\mathbf{q}\mathbf{b}_i} + 64\pi^2a^2c_1^E(\mathbf{q},\mathbf{b}_i)]\phi_{\mathbf{k}} + h_i^2(2\pi)^3\delta(\mathbf{q}-\mathbf{b}_i)[f_{\mathbf{k}} - a(a-r_s/2)\phi_{\mathbf{k}} - 5\phi^{(d)}_{\hat{\mathbf{h}}_i\mathbf{k}}]\}, \tag{130e}$$

$$T^{(-3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \frac{1}{3}G^E_{q_1q_2q_3}\sum_{i,j=1}^{3}[32\pi^2a^3(\sqrt{3q_j^2/4-E-\mathrm{i}\eta}-\mathrm{i}h_i)G^E_{\mathbf{q}_j\mathbf{b}_i} - 256\pi^3a^3c_1^E(\mathbf{q}_j,\mathbf{b}_i) + 4\pi a^2(a-r_s/2)h_i^2(2\pi)^3\delta(\mathbf{q}_j-\mathbf{b}_i)] + \frac{u_0}{3}\sum_{i,j=1}^{3}(2\pi)^3\delta(\mathbf{q}_j-\mathbf{b}_i), \tag{130f}$$

$$S^{(0)\mathbf{q}}_{\mathbf{k}} = d_{\mathbf{k}} - \frac{1}{3}\sum_{i=1}^{3}[6\pi a + 2\pi a(4E-3q^2)G^E_{\mathbf{q}\mathbf{b}_i} + \mathrm{i}ah_i^3(2\pi)^3\delta(\mathbf{q}-\mathbf{b}_i)]f_{\mathbf{k}} + \frac{10\pi a}{3}\sum_{i=1}^{3}q_i'^2G^E_{\mathbf{q}\mathbf{b}_i}\phi^{(d)}_{\hat{\mathbf{q}}_i'\mathbf{k}} + \frac{1}{3}\sum_{i=1}^{3}[64\pi^2a^3(\sqrt{3q^2/4-E-\mathrm{i}\eta}-\mathrm{i}h_i)c_1^E(\mathbf{q},\mathbf{b}_i) - 256\pi^3a^3c_2^E(\mathbf{q},\mathbf{b}_i,|a|^{-1}) + 8\pi a^2(a-r_s/2)(E-3q^2/4+h_i^2)G^E_{\mathbf{q}\mathbf{b}_i} + \mathrm{i}8\pi a^3h_i\sqrt{3q^2/4-E-\mathrm{i}\eta}\,G^E_{\mathbf{q}\mathbf{b}_i} - 3\pi a^2r_s - (14\pi/\sqrt{3}-16)wa^3 + \mathrm{i}a^2(a-r_s)h_i^3(2\pi)^3\delta(\mathbf{q}-\mathbf{b}_i)]\phi_{\mathbf{k}}, \tag{130g}$$

$$T^{(-2)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = G^E_{q_1q_2q_3}\Bigg\{-D - \frac{4\pi a}{3}\sum_{i,j=1}^{3}[64\pi^2a^3(\sqrt{3q_j^2/4-E-\mathrm{i}\eta} - \mathrm{i}h_i)c_1^E(\mathbf{q}_j,\mathbf{b}_i) - 256\pi^3a^3c_2^E(\mathbf{q}_j,\mathbf{b}_i,|a|^{-1}) + 8\pi a^2(a - r_s/2)(E-3q_j^2/4+h_i^2)G^E_{\mathbf{q}_j\mathbf{b}_i} + \mathrm{i}8\pi a^3 h_i\sqrt{3q_j^2/4-E-\mathrm{i}\eta}G^E_{\mathbf{q}_j\mathbf{b}_i} - 3\pi a^2 r_s - (14\pi/\sqrt{3} - 16)wa^3 + \mathrm{i}a^2(a-r_s)h_i^3(2\pi)^3\delta(\mathbf{q}_j-\mathbf{b}_i)]\Bigg\} + \frac{u_0}{3}\sum_{i,j=1}^{3}[-8\pi a G^E_{\mathbf{q}_j\mathbf{b}_i} - \mathrm{i}ah_i(2\pi)^3\delta(\mathbf{q}_j-\mathbf{b}_i)], \tag{130h}$$

where $\mathrm{i}=\sqrt{-1}\neq i$, $\mathbf{q}'_i\equiv\mathbf{q}+2\mathbf{b}_i$ (*not* the outgoing momenta), $\sqrt{z}$ is defined with a branch cut along the negative real $z$ axis, and

$$G^E_{\mathbf{qb}} \equiv (q^2+\mathbf{q}\cdot\mathbf{b}+b^2-E-\mathrm{i}\eta)^{-1}, \tag{131}$$

$$c_1^E(\mathbf{q},\mathbf{b}) \equiv \int\frac{d^3k}{(2\pi)^3}G^E_{\mathbf{qk}}G^E_{\mathbf{kb}}, \tag{132}$$

$$c_2^E(\mathbf{q},\mathbf{b},\kappa) \equiv \lim_{K\to\infty} -\frac{w}{16\pi^3}\ln\frac{K}{\kappa} + \int_{k<K}\frac{d^3k}{(2\pi)^3}G^E_{\mathbf{qk}}\left(2c_1^E(\mathbf{k},\mathbf{b}) - \frac{\sqrt{3k^2/4-E-\mathrm{i}\eta}}{4\pi}G^E_{\mathbf{kb}}\right). \tag{133}$$

The loop integrals $c_1^E$ and $c_2^E$ emerge from the $Z$-$\delta$ expansions (Appendix B) of $T^{(-4)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}$ and $T^{(-3)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}$, respectively.

Remarkably, $c_2^E$ (or any loop integral or lattice sum encountered in the present paper) is free from uncontrolled ultraviolet divergence; this finiteness follows naturally from the rules of the $Z$-$\delta$ expansion (as can be easily understood from a similar but simpler problem, Example 2 in Appendix B).

Comparing the above results for $\Psi_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3}(=\Sigma_s T^{(s)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3})$ with Eq. (123), we find the same result for the two-boson T-matrix as Eq. (121), and the first three terms in the low-energy expansion of the three-boson T-matrix,

$$\mathrm{T}(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3;\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3) = \sum_{s=-2}^{\infty}\mathrm{T}^{(s)}(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3;\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3), \tag{134}$$

where $\mathrm{T}^{(s)}(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3;\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3)\sim E^{s/2}$ (*not* excluding $E^{s/2}\ln^m E$),

$$\mathrm{T}^{(-2)}(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3;\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3) = 64\pi^2a^2\sum_{i,j=1}^{3}G^E_{\mathbf{q}_j\mathbf{b}_i}, \tag{135a}$$

$$\mathrm{T}^{(-1)}(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3;\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3) = \sum_{i,j=1}^{3}[-512\pi^3a^3c_1^E(\mathbf{q}_j,\mathbf{b}_i) - \mathrm{i}64\pi^2a^3(p_j+h_i)G^E_{\mathbf{q}_j\mathbf{b}_i}], \tag{135b}$$

$$\mathrm{T}^{(0)}(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3;\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3) = -6[D-24\pi w(7\pi/\sqrt{3}-8)a^4 - 36\pi^2a^3r_s] + 64\pi^2a^3\sum_{i,j=1}^{3}[32\pi^2ac_2^E(\mathbf{q}_j,\mathbf{b}_i,|a|^{-1}) + (r_s/2-a)(p_j^2+h_i^2)G^E_{\mathbf{q}_j\mathbf{b}_i} - ap_jh_iG^E_{\mathbf{q}_j\mathbf{b}_i} + \mathrm{i}8\pi a(p_j+h_i)c_1^E(\mathbf{q}_j,\mathbf{b}_i)]. \tag{135c}$$

The momenta $\mathbf{q}_i$'s satisfy the constraint $\Sigma_{i=1}^3 q_i^2/2=E$, in addition to $\Sigma_{i=1}^3\mathbf{q}_i=\Sigma_{i=1}^3\mathbf{b}_i=\mathbf{0}$, in Eqs. (135).

The two lowest-order contributions to the three-boson T-matrix, as well as the logarithmic dependence on energy at the third order [in $a^4c_2^E(\mathbf{q}_j,\mathbf{b}_i,|a|^{-1})$], are universal in the sense that they depend on the scattering length $a$ only, in agreement with Ref. [29]. The leading nonuniversal contributions are

$$-6(D-36\pi^2a^3r_s) + 32\pi^2a^3r_s\sum_{i,j=1}^{3}(p_j^2+h_i^2)G^E_{\mathbf{q}_j\mathbf{b}_i}.$$

The momentum-independent term in this expression is proportional to $D-36\pi^2a^3r_s$, while the leading nonuniversal contribution to the BEC energy [in Eq. (118)] is proportional to $D+12\pi^2a^3r_s$. We conclude that they *cannot* be absorbed into a single three-body contact interaction parameter $g_3$, *unless* the two-body effective range $r_s=0$. This disagrees with the effective field theory (EFT) prediction of Ref. [8].

### C. Comparison with Ref. [8]

If $r_s=0$, Eqs. (135) then agree with Ref. [8]. To see this, we use the power series for the two-boson T-matrix to expand the last term in Eq. (77) of [8] (note that $q_{12}$ in [8] is twice $h_3$ here), and get all four terms in Eqs. (135) of the present paper that contain $G^E_{\mathbf{q}_j\mathbf{b}_i}$. The quantity $\mathcal{T}_1^{\mathrm{1PI}}$ of [8] corresponds to the first term on the right-hand side of Eq. (135b) above; the finite contribution to $\mathcal{T}_2^{\mathrm{1PI}}$ in Eq. (80) of [8] corresponds to the last term of Eq. (135c) above. The sum of the divergent [8], but dimensionally regularized [8], terms in $\mathcal{T}_2^{\mathrm{1PI}}$ and the three-body term $-[g_3(\kappa)+\delta g_3(\kappa)]$ [8] can be expressed in terms of $c_2^E$ defined above,

$$\frac{(8\pi a)^4}{2}\left(c_{\mathrm{MS}} + \sum_{i,j=1}^{3}c_2^E(\mathbf{k}_i,\mathbf{k}'_j,\kappa)\right) - g_3(\kappa),$$

where

$$c_{\mathrm{MS}} = \frac{18w[\ln(2\pi)+1-\gamma]+\sqrt{3}[2\delta'+9\ln 3-18]}{64\pi^3} = 0.055\,571\,793\,27.$$

Here $\delta'=\Sigma_{n=0}^{\infty}[(1/3+n)^{-2}-(2/3+n)^{-2}]$. The momentum-dependent terms in Eqs. (135) thus completely agree with Ref. [8] at $r_s=0$. Further matching the constant terms, we find the relation between the three-body parameter $g_3(\kappa)$ of Ref. [8] and the scattering hypervolume $D$ defined in the present paper at $r_s=0$,

$$g_3(|a|^{-1}) = 6[D - 24\pi w(7\pi/\sqrt{3} - 8)a^4] + \frac{(8\pi a)^4}{2} c_{\mathrm{MS}}$$
$$= 6(D + 977.736\,695 a^4).$$

At $r_s \neq 0$, the discrepancy between the EFT prediction of Ref. [8] and our result, Eqs. (135), disappears if $r_s$ is included in the EFT. The two-boson EFT interaction vertex becomes [10]

$$\mathrm{i}(-8\pi a - 2\pi a^2 r_s k^2 - 2\pi a^2 r_s k'^2),$$

where $\mathbf{k}_c/2 \pm \mathbf{k}$ and $\mathbf{k}_c/2 \pm \mathbf{k}'$ are the momenta of the two bosons before and after the interaction, respectively. $k \neq k'$ if a virtual particle is involved. The tree diagram contribution to the three-boson T-matrix, Fig. 5.(a) of Ref. [8], is modified as

$$\sum_{i,j=1}^{3} G^E_{\mathbf{q}_j \mathbf{b}_i}[8\pi a + 2\pi a^2 r_s p_j^2 + 2\pi a^2 r_s(\mathbf{b}_i + \mathbf{q}_j/2)^2][8\pi a + 2\pi a^2 r_s h_i^2 + 2\pi a^2 r_s(\mathbf{q}_j + \mathbf{b}_i/2)^2] = \left[64\pi^2 a^2 \sum_{i,j=1}^{3} G^E_{\mathbf{q}_j \mathbf{b}_i} + 32\pi^2 a^3 r_s \sum_{i,j=1}^{3}(p_j^2 + h_i^2) G^E_{\mathbf{q}_j \mathbf{b}_i}\right] + 288\pi^2 a^3 r_s + O(E^1).$$

$r_s$ corrections to all other diagrams are $O(E^s)$, $s \geq 1/2$. Comparing the modified EFT results with Eqs. (135), we find

$$g_3(|a|^{-1}) = \frac{6\hbar^2}{m_{\mathrm{boson}}}(D + 12\pi^2 a^3 r_s + 977.736\,695 a^4), \tag{136}$$

where the SI units have been restored.

### D. Implications for the BEC energy and other properties

The BEC energy per particle at zero temperature was computed to order $\rho^2$ by Braaten and Nieto [8]. The result, Eq. (96) of Ref. [8], is expressed in terms of $g_3(\kappa)$.

Although the three-boson scattering amplitude receives $r_s$ corrections as shown above, the BEC energy per particle does not suffer from $r_s$ corrections at order $\rho^2$ in the thermodynamic limit, if it is expressed in terms of $g_3(\kappa)$ [10].

Using Eq. (136), we can now express Braaten and Nieto's result for the BEC energy [8] in terms of the scattering hypervolume $D$ defined in Eq. (3). The outcome agrees with Eq. (118) precisely, and $C^E$ in Eq. (118) is found,

$$C^E = 977.736695/12\pi + 8w[\ln(16\pi) + 0.80 \pm 0.005]$$
$$= 118.65 \pm 0.10. \tag{137}$$

The present author did an independent calculation of $C^E$, using finite-range interactions (details to appear elsewhere), and found

$$C^E = 118.498\,920\,346\,444 \text{ (exactly rounded)}, \tag{138}$$

which is nearly the same as Eq. (137).

For a dilute Bose gas of hard spheres, using Eqs. (4), (118), and (138), and $r_s = 2a/3$, we obtain the following result for the constant defined in Eq. (1):

$$\mathcal{E}_3' = 167.319\,69 \pm 0.000\,06. \tag{139}$$

This completes our calculation of the ground-state energy per particle of a dilute Bose gas of hard spheres, through order $\rho^2$.

For a dilute Bose gas with $a \gg r_e$ ($r_e$ is the range of interparticle forces), Braaten, Hammer, and Mehen found that $\mathcal{E}_3'$ is near 141 [9] and has a small imaginary part associated with three-body recombination [9]. In comparison to this system, a hard-sphere Bose gas with the same scattering length $a$, number density $\rho$, and boson mass has an energy density that is larger by a relative fraction $\approx 26\rho a^3$, a pressure that is larger by a fraction $\approx 52\rho a^3$, a speed of sound that is faster by a fraction $\approx \frac{3}{2} \times 26\rho a^3 = 39\rho a^3$, and a specific heat that is *smaller* by a fraction $\approx \frac{9}{2} \times 26\rho a^3 = 117\rho a^3$. Here the specific heats are compared at the same temperature $T \ll \rho^{1/3} a T_c$, where they are dominated by phonons with wavelengths $\gg 1/\sqrt{\rho a}$. ($T_c$ is the critical temperature).

These differences, i.e., nonuniversal effects, must extend to finite temperatures, including both $T < T_c$ and $T \geq T_c$. (Their magnitudes will change when $T$ is raised.) The reason is that for $T/T_c \sim O(1)$ and $\rho a^3, \rho r_e^3 \ll 1$, the thermal de Broglie wavelength greatly exceeds $r_e$ and $a$, and the interaction is well described by the constants $a$, $r_s$, $D$, etc.

The nonuniversal corrections to $T_c$, as an extension of the many calculations reviewed in Ref. [30], are of particular interest. Is the *leading-order* nonuniversal correction determined by $r_s$, or $D$, or both? The present author speculates that it is perhaps by $r_s$ alone, and is of the form $c' \rho a^2 r_s T_c^0$, where $T_c^0$ is the critical temperature of the noninteracting Bose gas, and $c'$ is a universal numerical constant.

## VI. SUMMARY

We have shown that the effective three-body force near the scattering threshold can be predicted in a way very similar to the two-body force, i.e., by solving the Schrödinger equation at zero energy and matching the solution to the asymptotic formula for the wave function at large relative distances. This approach is applicable to the $n$-body force as well.

Although in this paper the three-body parameter $D$ is explicitly determined for the hard-sphere potential only, one can apply the general formulas, Eqs. (45), to many other finite-range potentials to determine the effective three-body forces. The unknown wave function has three independent variables only, because of the translational and rotational symmetry, and is not very difficult to study on a present-day computer.

The author believes that the asymptotics of the three-boson wave function at large relative distances found in this paper is also applicable to *composite* bosons. For weakly bound dimers of fermionic atoms with equal mass, the two-dimer scattering length and effective range are, respectively, $a^{(dd)} \approx 0.6 a^{(ff)}$ [31] and $r_s^{(dd)} \approx 0.2 a^{(dd)}$ [32], where $a^{(ff)}$ is the atomic scattering length, but the three-dimer scattering hypervolume $D$ is still unknown. To determine the equation of state of many such dimers at low density ($\rho a^{(dd)3} \ll 1$) [31,33,34] more accurately, one must compute $D$ (by solving the three-dimer, or six-fermion, problem).

We have expanded the ground-state energy of three bosons in a large periodic volume to the order $L^{-7}$, using a perturbation procedure that resembles the derivation of the small-momentum structure of $\phi^{(3)}$. One may combine the result, Eq. (5), with Monte Carlo simulations (for nonrelativistic particles) or lattice QCD simulations (for low-energy pions or kaons) to extract values of $D$.

Equation (5) suggests that, to determine $D$ accurately, the box size $L$ should greatly exceed $17a$ in these simulations, or the higher-order corrections from $D$ can overwhelm the lowest-order correction.

For pions, the Compton wavelength is comparable to $a$ and $r_s$; whether the relativistic corrections modify the *form* of Eq. (5) is a question of interest.

To extract $D$ from $\mathcal{N}$-body simulations in volumes of modest sizes, one may find it helpful to derive a systematic expansion of $E$ at large $L$, but fixed $\mathcal{N}a/L$, corresponding to the *intermediate regime* discussed in Sec. IV F 2.

We have computed the scattering amplitude of three bosons at low energy to $O(E^0)$, using finite-range interactions. Our result, Eqs. (135), disagrees with an EFT prediction [8] at $r_s \neq 0$. If $r_s$ corrections are included in the EFT, however, the discrepancy disappears completely. The resultant relation between $g_3(\kappa)$ and $D$, combined with the many-body energy formula of Ref. [8], and the three-body force computed in the present paper [Eq. (4)], solves a long-standing problem in the literature [5,10], namely the complete second-order correction to the ground-state energy of a dilute Bose gas of hard spheres. The result shows small observable differences between this system and a dilute Bose gas with large scattering length considered by Ref. [9].

We have studied the energies and momentum distributions of $\mathcal{N}$ bosons in a large volume, from which we have deduced the energies and condensate fractions of dilute homogeneous BECs. The result for the energy, Eq. (118), agrees with an EFT calculation, but the condensate fraction, Eq. (119), disagrees. Our result suggests that even the population of the *zero*-momentum state, or the off-diagonal *long*-range order [35], is affected by short-range two-body physics. However, quantum field redefinitions [25] or short-range unitary transformations [24] can alter the momentum distribution but leave many observables unchanged [25]. One thus has reason to question whether the above disagreement is physically relevant (the present author, however, believes it is at least sometimes relevant, as discussed in Sec. IV E).

Although the three-body force is usually a small perturbation to properties of dilute BECs, dramatic effects may be obtained near a three-body resonance [9,36]. Alternatively, one may reduce the two-body force by tuning the scattering length to a zero crossing [37]. At $a=0$, the BEC ground-state energy density $\approx \hbar^2 D\rho^3/6m$ instead of $2\pi\hbar^2 a\rho^2/m$; this will lead to a *qualitative* change of the familiar Gross-Pitaevskii equation and many observable consequences.

The author would like to draw the readers' attention to a few mathematical techniques. The $Z$ functions and $Z$-$\delta$ expansions (Appendixes A and B), an extension of the familiar $\delta$-function method, facilitate the derivation of the small-momentum and the large-volume expansions. The method of tail-singularity separation, as described in Appendix C, enables us to evaluate many lattice sums with virtually arbitrary precision. The utility of these methods is certainly *not* limited to the present work.

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## APPENDIX A: THE Z FUNCTIONS

We define generalized functions $Z/k^{2n}$ and $Z_b(k)/k^{2n+1}$ ($n=1,2,3,\ldots$, and $b>0$ is a constant),

$$\frac{Z}{k^{2n}} = \frac{1}{k^{2n}}\ (k>0), \quad \frac{Z_b(k)}{k^{2n+1}} = \frac{1}{k^{2n+1}}\ (k>0), \tag{A1}$$

$$\int_{\text{all }\mathbf{k}} \mathrm{d}^3k \frac{Z}{k^{2n}} p^{(s)}(\mathbf{k}) = 0\ (s \leq 2n-4), \tag{A2}$$

$$\int_{|\mathbf{k}|<k_0} \mathrm{d}^3k \frac{Z}{k^{2n}} p^{(2n-3)}(\mathbf{k}) = 0\ (k_0>0 \text{ and } n \geq 2), \tag{A3}$$

$$\int_{\text{all }\mathbf{k}} \mathrm{d}^3k \frac{Z_b(k)}{k^{2n+1}} p^{(s)}(\mathbf{k}) = 0\ (s \leq 2n-3), \tag{A4}$$

$$\int_{|\mathbf{k}|<b} \mathrm{d}^3k \frac{Z_b(k)}{k^{2n+1}} p^{(2n-2)}(\mathbf{k}) = 0, \tag{A5}$$

where $p^{(s)}(\mathbf{k})$ is any homogeneous polynomial of $\mathbf{k}$ with degree $s$ ($=0,1,2,\ldots$). $Z/k^2$ can be identified with $1/k^2$.

We can use ordinary functions to approach the $Z$ functions. For instance, $(k^2-3\eta^2)/(k^2+\eta^2)^3 \to Z/k^4$ when $\eta \to 0^+$.

The $Z$ functions, like the $\delta$ function, are merely Fourier transforms of some ordinary functions ($n=1,2,3,\ldots$),

$$\int \frac{\mathrm{d}^3k}{(2\pi)^3} \frac{Z}{k^{2n}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = \frac{(-1)^{n+1} r^{2n-3}}{4\pi(2n-2)!}, \tag{A6}$$

$$\lim_{\eta\to 0^+} \int \mathrm{d}^3r \frac{(-1)^{n+1} r^{2n-3}}{4\pi(2n-2)!} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}-\eta r} = \frac{Z}{k^{2n}}, \tag{A7}$$

$$\int \frac{\mathrm{d}^3k}{(2\pi)^3} \frac{Z_b(k)}{k^{2n+1}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = F_b^{(n)}(r), \tag{A8}$$

$$\lim_{\eta\to 0^+} \int \mathrm{d}^3r F_b^{(n)}(r) \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}-\eta r} = \frac{Z_b(k)}{k^{2n+1}},$$

$$F_b^{(n)}(r) \equiv \frac{(-1)^n r^{2n-2}}{2\pi^2(2n-1)!}\left(\ln(br) + \gamma - \sum_{i=1}^{2n-1} \frac{1}{i}\right), \tag{A9}$$

where $\gamma=0.5772\ldots$ is Euler's constant.

$Z_b(k)/k^{2n+1}$ has the following properties:

$$\frac{Z_b(k)}{k^{2n+1}} - \frac{Z_{b'}(k)}{k^{2n+1}} = \frac{4\pi \ln(b'/b)}{(2n-1)!}\nabla_k^{2n-2}\delta(\mathbf{k}), \tag{A10}$$

$$\frac{Z_b(ck)}{(ck)^{2n+1}} = \frac{1}{c^{2n+1}}\frac{Z_{b/c}(k)}{k^{2n+1}} \text{ (constant } c>0). \tag{A11}$$

## APPENDIX B: $Z$-$\delta$ EXPANSIONS

*Example 1*. Consider the expansion of $(|\mathbf{k}|^2+3q^2/4)^{-1}$ at small $q$. Naively, it is $1/k^2-3q^2/(4k^4)+O(q^4)$. But this series fails around $\mathbf{k}=\mathbf{0}$. In particular, $R_0(\mathbf{k},\mathbf{q})=(k^2+3q^2/4)^{-1}-1/k^2$ has a *finite* integral over all $\mathbf{k}$: $\int\frac{d^3k}{(2\pi)^3}R_0(\mathbf{k},\mathbf{q})=-\frac{\sqrt{3}}{8\pi}q$, but the integral of $-3q^2/(4k^4)$ over all $\mathbf{k}$ is *infinite*.

Now subtract $-\frac{\sqrt{3}}{8\pi}q(2\pi)^3\delta(\mathbf{k})$ from $R_0(\mathbf{k},\mathbf{q})$ to obtain $R_1(\mathbf{k},\mathbf{q})$. Clearly $R_1(\mathbf{k},\mathbf{q})\approx -3q^2/(4k^4)$ at $k>0$ and $q\to 0$, but $\int R_1(\mathbf{k},\mathbf{q})d^3k=0$, so actually

$$R_1(\mathbf{k},\mathbf{q}) \approx -\frac{3q^2}{4}\frac{Z}{k^4},$$

where $Z/k^4$ is defined in Appendix A. Further subtracting $-3q^2Z/(4k^4)$ from $R_1(\mathbf{k},\mathbf{q})$, we get a remainder $\approx(\sqrt{3}/64\pi)q^3\nabla_k^2(2\pi)^3\delta(\mathbf{k})$. Continuing this subtraction procedure to higher orders in $q$, we get Eq. (31a).

The second method to derive the $Z$-$\delta$ expansion of $(k^2+3q^2/4)^{-1}$ is as follows: first Fourier transform it for fixed $\mathbf{q}$ to obtain $\exp(-\sqrt{3}qr/2)/(4\pi r)$, then expand it in powers of $\mathbf{q}$,

$$\frac{1}{4\pi r} - \frac{\sqrt{3}q}{8\pi} + \frac{3q^2}{32\pi}r - \frac{\sqrt{3}q^3}{64\pi}r^2 + \frac{3q^4}{512\pi}r^3 - \frac{3\sqrt{3}q^5}{5120\pi}r^4 + O(q^6),$$

and finally transform the series back to the $\mathbf{k}$ space term by term. With the help of Eq. (A7), one gets Eq. (31a).

Although the above two methods are equally valid, the first one is more useful, because the Fourier transforms of most functions of $\mathbf{k}$ in this paper cannot be found analytically.

*Example 2* [needed in deriving Eq. (35)]. At small $\mathbf{q}$,

$$(|\mathbf{k}+\mathbf{q}/2|^{-1}+|\mathbf{k}-\mathbf{q}/2|^{-1})/(k^2+3q^2/4) = 2Z_\kappa(k)/k^3 + [8\pi - 4\pi^2/\sqrt{3} - 8\pi\ln(q/\kappa)]\delta(\mathbf{k}) + O(q^2),$$

where $\kappa>0$ is arbitrary. Higher-order corrections may easily be obtained as well (see the general rules below).

*Generics*. Consider a function $F(\mathbf{k},o)$ (where $o$ are a set of variables), with a finite integral over any finite region of the $\mathbf{k}$ space for $o\neq 0$, and a unique singularity at $\mathbf{k}=\mathbf{0}$ for $o\to 0$. The $Z$-$\delta$ expansion is of the form $F(\mathbf{k},o)=F_Z(\mathbf{k},o)+F_\delta(\mathbf{k},o)$, where $F_Z$ is a series including ordinary and/or $Z$ functions of $\mathbf{k}$ and may be directly inferred from the Taylor expansion of $F(\mathbf{k},o)$ at small $o$, and

$$F_\delta(\mathbf{k},o) = \sum_{mj} c_{mj}(o)\nabla_k^{2m}Q^{(j)}(\nabla_k)(2\pi)^3\delta(\mathbf{k}), \tag{B1a}$$

$$c_{mj}(o) = (-1)^{l_j}\{\nabla_k^{2m}Q^{(j)}(\nabla_k)[k^{2m}Q^{(j)}(\mathbf{k})]\}^{-1} \times \int \frac{d^3k}{(2\pi)^3}k^{2m}Q^{(j)}(\mathbf{k})[F(\mathbf{k},o)-F_Z(\mathbf{k},o)]. \tag{B1b}$$

Here $Q^{(j)}$ are all the independent homogeneous harmonic polynomials, satisfying $\int Q^{(j)}(\hat{\mathbf{k}})Q^{(j')}(\hat{\mathbf{k}})d^2\hat{\mathbf{k}}=0$ for $j\neq j'$. The degree of $Q^{(j)}$ is $l_j$.

If $F(\mathbf{k},o)$ is rotationally invariant around an axis $\hat{\mathbf{q}}$, only $Q_{\hat{\mathbf{q}}}^{(l)}$ are needed above, and the coefficient before the integral sign in Eq. (B1b) becomes $\frac{(-1)^l(2l+1)}{(2m)!!(2m+2l+1)!!}$.

If $F(\mathbf{k},o)$ is a completely symmetric and even function of $k_x$, $k_y$, and $k_z$, only those harmonic polynomials with the $A_1^+$ symmetry are needed: $Q^{(j)}(\mathbf{k})=1$, $Q^{(g)}(\mathbf{k})$, $Q^{(i)}(\mathbf{k})$, $Q^{(8)}(\mathbf{k}),\ldots$, where

$$Q^{(g)}(\mathbf{v}) \equiv v_x^4+v_y^4+v_z^4-3(v_x^2v_y^2+v_y^2v_z^2+v_z^2v_x^2), \tag{B2a}$$

$$Q^{(i)}(\mathbf{v}) \equiv v_x^6+v_y^6+v_z^6-(15/2)(v_x^4v_y^2+v_y^4v_z^2+v_z^4v_x^2+v_x^2v_y^4 + v_y^2v_z^4+v_z^2v_x^4)+90v_x^2v_y^2v_z^2, \tag{B2b}$$

$$Q^{(8)}(\mathbf{v}) \equiv v_x^8+v_y^8+v_z^8-14(v_x^6v_y^2+v_y^6v_z^2+v_z^6v_x^2+v_x^2v_y^6+v_y^2v_z^6 + v_z^2v_x^6)+35(v_x^4v_y^4+v_y^4v_z^4+v_z^4v_x^4). \tag{B2c}$$

## APPENDIX C: LATTICE SUMS

The following methods are used to evaluate lattice sums: *tail-singularity separation*, Poisson summation formula, and convergence acceleration (based on the large-$\mathbf{n}$ asymptotics of the summands).

To evaluate a lattice sum $\Sigma_{\mathbf{n}}X(\mathbf{n})$ (sum over 3-vectors of integers), where $X(\mathbf{n})$, as a continuous function, has both singularity in the real-$\mathbf{n}$ space and a power-law tail at large $\mathbf{n}$, we sometimes break $X(\mathbf{n})$ in two pieces: $X(\mathbf{n})=X_1(\mathbf{n})+X_2(\mathbf{n})$, such that $X_1(\mathbf{n})$ has singularity but no power-law tail (i.e., it decays much more rapidly at large $n$), while $X_2(\mathbf{n})$ has a power-law tail but is sufficiently smooth. $\Sigma_{\mathbf{n}}X_1(\mathbf{n})$ is done directly, while $\Sigma_{\text{all }\mathbf{n}}X_2(\mathbf{n})$ is approximated by $\int d^3nX_2(\mathbf{n})$ to a very high precision. We call this method *tail-singularity separation* (TSS).

For instance, to compute $\alpha_s$ ($s=1,2,3,\ldots$), we write $n^{-2s}=\Sigma_{i=0}^{s-1}\frac{(\eta n^2)^i}{i!}\frac{\exp(-\eta n^2)}{n^{2s}}+X_2(\mathbf{n})$, where $\eta>0$ is small. $X_2(\mathbf{n})$ is very smooth, so $\Sigma_{\text{all }\mathbf{n}}X_2(\mathbf{n})$ is approximated by an integral. Straightforward algebra yields

$$\alpha_s = c_s\pi^{3/2}\eta^{s-3/2} - \frac{\eta^s}{s!} + \sum_{\mathbf{n}\neq\mathbf{0}}\sum_{i=0}^{s-1}\frac{(\eta n^2)^i}{i!}\frac{e^{-\eta n^2}}{n^{2s}} + O(e^{-\pi^2/\eta}), \tag{C1}$$

where $c_1=-2$, $c_2=2$, $c_3=1/3$, $c_4=1/15$, $c_5=1/84$, $c_6=1/540,\ldots$, and the error $\sim O(e^{-\pi^2/\eta})$ results from the approximation $\Sigma_{\text{all }\mathbf{n}}X_2(\mathbf{n})\approx\int d^3nX_2(\mathbf{n})$ [38]. Equation (C1) applies to both $s=1$ and $s=2,3,\ldots$. At $\eta=1/10$, one already gets about 43-digit precision for $\alpha_s$.

The TSS is *not* an arbitrary exponential accelaration method. For example, $\Sigma_{\mathbf{n}\neq 0}n^{-3}$ is not sufficiently accelerated by $\Sigma_{\mathbf{n}\neq 0}\exp(-\eta n^3)n^{-3}$, because $[1-\exp(-\eta n^3)]n^{-3}$ is *not* smooth enough: it contains a term $\sim|\mathbf{n}|^3$ at small $\mathbf{n}$ that is singular. Inspired by Takahasi and Mori's quadrature method [39], we obtain a proper TSS formula,

$$1/n^3-\pi\eta/2n^2=2/[1+\exp(\pi\sinh\eta n)]n^3+S(\mathbf{n}),$$

where $S(\mathbf{n})$ is smooth. We then easily derive (all the lattice sums below, except $\beta_{1A}$, are used in computing $C_0$ and $C_1$)

$$\alpha_{1.5}=j_1+4\pi\ln\eta+\pi\alpha_1\eta/2+\pi(\pi^2-2)\eta^3/24+\sum_{\mathbf{n}\neq\mathbf{0}}2/[1+\exp(\pi\sinh\eta n)]n^3+O(\mathrm{e}^{-\pi^2/\eta}),$$

$$j_1\equiv\lim_{R\to\infty}4\pi\int_0^R x^{-1}\tanh\left(\frac{\pi}{2}\sinh x\right)\mathrm{d}x-4\pi\ln R$$
$$=16.489\,380\,548\,112\,915\,838\,168\,866\,783\,965\,159\,811. \tag{C2a}$$

Similarly,

$$\alpha_{2.5}=\pi\alpha_2\eta/2+j_2\eta^2-\pi(\pi^2-2)\alpha_1\eta^3/24-\pi(\pi^4-5\pi^2+1)\eta^5/240+\sum_{\mathbf{n}\neq\mathbf{0}}2/[1+\exp(\pi\sinh\eta n)]n^5+O(\mathrm{e}^{-\pi^2/\eta}),$$

$$j_2\equiv 4\pi\int_0^\infty\left[x^{-3}\tanh\left(\frac{\pi}{2}\sinh x\right)-\pi/2x^2\right]\mathrm{d}x$$
$$=-24.436\,776\,868\,803\,521\,072\,197\,485\,676\,562\,043\,398. \tag{C2b}$$

Let

$$\alpha_s^{(g)}\equiv\lim_{\eta\to 0^+}\sum_{\mathbf{n}\neq\mathbf{0}}\mathrm{e}^{-\eta n}Q^{(g)}(\mathbf{n})/n^{2s}, \tag{C3}$$

and similarly for $\alpha_s^{(i)}$ and $\alpha_s^{(8)}$. Here $Q^{(g)}$, $Q^{(i)}$, and $Q^{(8)}$ are defined in Eqs. (B2).

For any *integer* $s\geq 1$, we derive a TSS formula,

$$\alpha_s^{(g)}=\sum_{\mathbf{n}\neq\mathbf{0}}\frac{Q^{(g)}(\mathbf{n})}{n^{2s}}\sum_{i=0}^{s-1}\frac{(\eta n^2)^i}{i!}\mathrm{e}^{-\eta n^2}+O(\mathrm{e}^{-\pi^2/\eta}), \tag{C4}$$

and similarly for $\alpha_s^{(i)}$ and $\alpha_s^{(8)}$.

Using the Poisson summation formula and the TSS method, we get

$$\alpha_{5.5}^{(g)}=-(2^6\pi^5/9!!)\sum_{\mathbf{n}\neq\mathbf{0}}Q^{(g)}(\mathbf{n})\tilde{l}(\eta n)+O(\mathrm{e}^{-\pi^2/\eta}), \tag{C5a}$$

$$\alpha_{7.5}^{(i)}=(2^8\pi^7/13!!)\sum_{\mathbf{n}\neq\mathbf{0}}Q^{(i)}(\mathbf{n})\tilde{l}(\eta n)+O(\mathrm{e}^{-\pi^2/\eta}), \tag{C5b}$$

$$\alpha_{9.5}^{(8)}=-(2^{10}\pi^9/17!!)\sum_{\mathbf{n}\neq\mathbf{0}}Q^{(8)}(\mathbf{n})\tilde{l}(\eta n)+O(\mathrm{e}^{-\pi^2/\eta}), \tag{C5c}$$

where $\tilde{l}(x)\equiv\ln[\tanh(\frac{\pi}{2}\sinh x)]$.

Using the Poisson summation formula, we get

$$W_A(\mathbf{n})=-\sqrt{3}\pi^2 n+\pi\sum_{\mathbf{m}\neq\mathbf{0}}\mathrm{e}^{-\sqrt{3}\pi mn-\mathrm{i}\pi\mathbf{m}\cdot\mathbf{n}}/m, \tag{C6a}$$

$$W_B(\mathbf{n})=(2\pi^2/\sqrt{3}n)\sum_{\text{all }\mathbf{m}}\mathrm{e}^{-\sqrt{3}\pi mn-\mathrm{i}\pi\mathbf{m}\cdot\mathbf{n}}. \tag{C6b}$$

We derive TSS formulas

$$\theta_{A1}(\mathbf{n})=-\eta(1-\mathrm{e}^{-\eta n^2})/n^2+2\pi\int_0^\infty\mathrm{d}m\int_{-1}^1\mathrm{d}c(1-\mathrm{e}^{-\eta S_{nmc}})(1-\mathrm{e}^{-\eta m^2})/S_{nmc}+\sum_{\mathbf{m}\neq\mathbf{0}}S_{\mathbf{nm}}^{-1}m^{-2}(\mathrm{e}^{-\eta S_{\mathbf{nm}}}+\mathrm{e}^{-\eta m^2}-\mathrm{e}^{-\eta S_{\mathbf{nm}}-\eta m^2})+O(\mathrm{e}^{-\pi^2/2\eta}), \tag{C6c}$$

$$\theta_{B1}(\mathbf{n})=\eta[(1+\eta n^2)\mathrm{e}^{-\eta n^2}-1]/n^4+2\pi\int_0^\infty\mathrm{d}m\int_{-1}^1\mathrm{d}c[1-(1+\eta S_{nmc})\mathrm{e}^{-\eta S_{nmc}}](1-\mathrm{e}^{-\eta m^2})/S_{nmc}^2+\sum_{\mathbf{m}\neq\mathbf{0}}S_{\mathbf{nm}}^{-2}m^{-2}[(1+\eta S_{\mathbf{nm}})\mathrm{e}^{-\eta S_{\mathbf{nm}}}(1-\mathrm{e}^{-\eta m^2})+\mathrm{e}^{-\eta m^2}]+O(\mathrm{e}^{-\pi^2/2\eta}), \tag{C6d}$$

where $S_{\mathbf{nm}}\equiv n^2+\mathbf{n}\cdot\mathbf{m}+m^2$, and $S_{nmc}\equiv n^2+nmc+m^2$. With Eqs. (C6), $\rho_{A1}(\mathbf{n})$ and $\rho_{B1}(\mathbf{n})$ [Eqs. (86a) and (94a)] are evaluated very accurately for any *finite* 3-vector of integers $\mathbf{n}\neq\mathbf{0}$.

In addition, at *large* $\mathbf{n}$ we derive asymptotic formulas

$$\rho_{A1}(\mathbf{n})=\rho_{A1}^{(11)}(\mathbf{n})+O(n^{-12}),$$

$$\rho_{A1}^{(11)}(\mathbf{n})\equiv\pi^2 w/n+2\alpha_1/n^2+4/3n^4+4\alpha_1^{(g)}Q^{(g)}(\mathbf{n})/15n^{10}+4\alpha_1^{(i)}Q^{(i)}(\mathbf{n})/231n^{14}+4\alpha_1^{(8)}Q^{(8)}(\mathbf{n})/195n^{18}, \tag{C7a}$$

$$\rho_{B1}(\mathbf{n})=\rho_{B1}^{(13)}(\mathbf{n})+O(n^{-14}),$$

$$\rho_{B1}^{(13)}(\mathbf{n})\equiv 2\sqrt{3}\pi^2/n^3+2\alpha_1/n^4+2/n^6+4\alpha_1^{(g)}Q^{(g)}(\mathbf{n})/3n^{12}+4\alpha_1^{(i)}Q^{(i)}(\mathbf{n})/33n^{16}+12\alpha_1^{(8)}Q^{(8)}(\mathbf{n})/65n^{20}. \tag{C7b}$$

For $\alpha_{1A1}$, $\alpha_{2A1}$, and $\alpha_{1B1}$, we thus have

$$\alpha_{sA1}=\pi^2 w\alpha_{0.5+s}+2\alpha_1\alpha_{1+s}+4\alpha_{2+s}/3+4\alpha_1^{(g)}\alpha_{5+s}^{(g)}/15+4\alpha_1^{(i)}\alpha_{7+s}^{(i)}/231+4\alpha_1^{(8)}\alpha_{9+s}^{(8)}/195+\sum_{\mathbf{n}\neq\mathbf{0}}n^{-2s}[\rho_{A1}(\mathbf{n})-\rho_{A1}^{(11)}(\mathbf{n})], \tag{C8a}$$

$$\alpha_{1B1} = 2\sqrt{3}\pi^2\alpha_{2.5} + 2\alpha_1\alpha_3 + 2\alpha_4 + 4\alpha_1^{(g)}\alpha_7^{(g)}/3 + 4\alpha_1^{(i)}\alpha_9^{(i)}/33 + 12\alpha_1^{(8)}\alpha_{11}^{(8)}/65 + \sum_{\mathbf{n}\neq\mathbf{0}} n^{-2}[\rho_{B1}(\mathbf{n}) - \rho_{B1}^{(13)}(\mathbf{n})], \quad \text{(C8b)}$$

and the sums over $\mathbf{n}$ are truncated at $|n_x|,|n_y|,|n_z| \leq 15$ to yield results for $\alpha_{1A1}$, $\alpha_{2A1}$, and $\alpha_{1B1}$ with more than 18-digit precision.

From Eq. (99), we deduce

$$\tilde{\alpha}_{1AA1} = -\alpha_{1AA1} - \pi^3 w(7\pi/\sqrt{3} - 8)\alpha_1 + 8\pi^3 w\alpha_1 \ln(2\pi) - \alpha_1\alpha_{1A1} + 3\alpha_{1A2} + 3\alpha_{1B1} - (\alpha_1^2 + \alpha_2)\alpha_2 + 6\alpha_1\alpha_3 - 9\alpha_4, \quad \text{(C9)}$$

$$\alpha_{1AA1} \equiv \lim_{N\to\infty} \sum_{\mathbf{n}\neq\mathbf{0};\ n<N} n^{-2}\rho_{AA1}(\mathbf{n}) - 8\pi^3 w\alpha_1 \ln N + 4\pi^4 wN(8\ln N - 16 + 7\pi/\sqrt{3}). \quad \text{(C10)}$$

It can be shown that $\alpha_{1A2} = \alpha_{2A1}$, and

$$\alpha_{1AA1} = \lim_{N\to\infty} \sum_{\mathbf{n}\neq\mathbf{0};\ n<N} \rho_{A1}^2(\mathbf{n}) - 4\pi^5 w^2 N - 16\pi^3 w\alpha_1 \ln N. \quad \text{(C11)}$$

At large $\mathbf{n}$, we derive from Eq. (C7a)

$$\rho_{A1}^2(\mathbf{n}) = K^{(12)}(\mathbf{n}) + O(n^{-13}), \quad \text{(C12)}$$

$$K^{(12)}(\mathbf{n}) \equiv \pi^4 w^2/n^2 + 4\pi^2 w\alpha_1/n^3 + 4\alpha_1^2/n^4 + 8\pi^2 w/3n^5 + 16\alpha_1/3n^6 + 8\pi^2 w\alpha_1^{(g)}Q^{(g)}(\mathbf{n})/15n^{11} + [16/9n^8 + 16\alpha_1\alpha_1^{(g)}Q^{(g)}(\mathbf{n})/15n^{12}] + 8\pi^2 w\alpha_1^{(i)}Q^{(i)}(\mathbf{n})/231n^{15} + [32\alpha_1^{(g)}Q^{(g)}(\mathbf{n})/45n^{14} + 16\alpha_1\alpha_1^{(i)}Q^{(i)}(\mathbf{n})/231n^{16}] + 8\pi^2 w\alpha_1^{(8)}Q^{(8)}(\mathbf{n})/195n^{19} + [64\alpha_1^{(g)2}/4725n^{12} + 64\alpha_1^{(g)2}Q^{(g)}(\mathbf{n})/3575n^{16} + (128\alpha_1^{(g)2}/10395 + 32\alpha_1^{(i)}/693)Q^{(i)}(\mathbf{n})/n^{18} + (16\alpha_1^{(g)2}/585 + 16\alpha_1\alpha_1^{(8)}/195)Q^{(8)}(\mathbf{n})/n^{20}]. \quad \text{(C13)}$$

So

$$\alpha_{1AA1} = \pi^4 w^2\alpha_1 + 4\pi^2 w\alpha_1\alpha_{1.5} + 4\alpha_1^2\alpha_2 + 8\pi^2 w\alpha_{2.5}/3 + 16\alpha_1\alpha_3/3 + 8\pi^2 w\alpha_1^{(g)}\alpha_{5.5}^{(g)}/15 + 16\alpha_4/9 + 16\alpha_1\alpha_1^{(g)}\alpha_6^{(g)}/15 + 8\pi^2 w\alpha_1^{(i)}\alpha_{7.5}^{(i)}/231 + 32\alpha_1^{(g)}\alpha_7^{(g)}/45 + 16\alpha_1\alpha_1^{(i)}\alpha_8^{(i)}/231 + 8\pi^2 w\alpha_1^{(8)}\alpha_{9.5}^{(8)}/195 + 64\alpha_1^{(g)2}\alpha_6/4725 + 64\alpha_1^{(g)2}\alpha_8^{(g)}/3575 + (128\alpha_1^{(g)2}/10395 + 32\alpha_1^{(i)}/693)\alpha_9^{(i)} + (16\alpha_1^{(g)2}/585 + 16\alpha_1\alpha_1^{(8)}/195)\alpha_{10}^{(8)} + \sum_{\mathbf{n}\neq\mathbf{0}}[\rho_{A1}^2(\mathbf{n}) - K^{(12)}(\mathbf{n})], \quad \text{(C14)}$$

where the sum over $\mathbf{n}$ converges very rapidly; truncating it at $|n_x|,|n_y|,|n_z| \leq 15$, we obtain the result for $\alpha_{1AA1}$ with 18-digit precision.

The results for the above lattice sums are listed below. They determine $C_0$ and $C_1$.

Onefold lattice sums (rounded to fit the two-column format),

$$\alpha_1 = -8.913\,632\,917\,585\,151\,272\,687\,120\,136, \quad \text{(C15a)}$$

$$\alpha_{1.5} = 3.821\,923\,503\,940\,635\,799\,730\,123\,034, \quad \text{(C15b)}$$

$$\alpha_2 = 16.532\,315\,959\,761\,669\,643\,892\,704\,593, \quad \text{(C15c)}$$

$$\alpha_{2.5} = 10.377\,524\,830\,847\,083\,864\,728\,948\,355, \quad \text{(C15d)}$$

$$\alpha_3 = 8.401\,923\,974\,827\,539\,993\,146\,138\,987, \quad \text{(C15e)}$$

$$\alpha_4 = 6.945\,807\,927\,226\,369\,624\,170\,778\,023, \quad \text{(C15f)}$$

$$\alpha_6 = 6.202\,149\,045\,047\,518\,551\,930\,416\,392, \quad \text{(C15g)}$$

$$\alpha_1^{(g)} = 1.127\,757\,148\,686\,792\,075\,014\,583\,731, \quad \text{(C15h)}$$

$$\alpha_{5.5}^{(g)} = 5.672\,605\,625\,422\,259\,129\,524\,572\,370, \quad \text{(C15i)}$$

$$\alpha_6^{(g)} = 5.772\,772\,158\,341\,296\,181\,095\,291\,055, \quad \text{(C15j)}$$

$$\alpha_7^{(g)} = 5.890\,866\,300\,404\,517\,457\,312\,864\,285, \quad \text{(C15k)}$$

$$\alpha_8^{(g)} = 5.947\,443\,615\,615\,246\,912\,541\,646\,623, \quad \text{(C15l)}$$

$$\alpha_1^{(i)} = -2.434\,385\,049\,385\,522\,287\,574\,679\,853, \quad \text{(C15m)}$$

$$\alpha_{7.5}^{(i)} = 5.242\,702\,841\,443\,828\,214\,862\,689\,624, \quad \text{(C15n)}$$

$$\alpha_8^{(i)} = 5.451\,072\,910\,162\,494\,576\,739\,294\,958, \quad \text{(C15o)}$$

$$\alpha_9^{(i)} = 5.715\,464\,651\,152\,249\,495\,454\,861\,607, \quad \text{(C15p)}$$

$$\alpha_1^{(8)} = 16.571\,410\,717\,493\,131\,178\,469\,668\,510, \tag{C15q}$$

$$\alpha_{9.5}^{(8)} = 6.156\,579\,477\,795\,506\,959\,879\,789\,010, \tag{C15r}$$

$$\alpha_{10}^{(8)} = 6.109\,685\,927\,989\,065\,132\,252\,619\,095, \tag{C15s}$$

$$\alpha_{11}^{(8)} = 6.054\,088\,533\,916\,337\,242\,283\,438\,742. \tag{C15t}$$

Twofold lattice sums,

$$\alpha_{1A1} = -190.172\,897\,984\,865\,754\,8, \tag{C16a}$$

$$\alpha_{1A2} = \alpha_{2A1} = 111.807\,832\,628\,721\,133\,609, \tag{C16b}$$

$$\alpha_{1B1} = 221.523\,005\,657\,695\,107\,22. \tag{C16c}$$

Threefold lattice sums,

$$\alpha_{1AA1} = -2996.889\,395\,378\,764\,86, \tag{C17a}$$

$$\tilde{\alpha}_{1AA1} = -6591.229\,842\,103\,439\,89. \tag{C17b}$$

Finally, from Eq. (C6a) we get

$$\beta_{1A} = -\sqrt{3}\pi^2\alpha_{0.5} + \pi \sum_{\mathbf{n},\mathbf{m}\neq 0} \mathrm{e}^{-\sqrt{3}\pi mn - \mathrm{i}\pi\mathbf{m}\cdot\mathbf{n}}/n^2 m$$
$$= 48.614\,754\,175\,227\,821\,038\,934\,419\,912. \tag{C18}$$

(One can show that $\alpha_{0.5} = \alpha_1/\pi$.) $\beta_{1A}$ is needed in Eq. (110f).

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[12] This paper is not about the physical nature of three-body interaction potentials, but about the *effective* three-body coupling constant, which may even arise from purely two-body potentials [5], although a true three-body potential will certainly affect this effective coupling [as is evident in Eq. (39)].
[13] The $|a|$ in $\ln(q_i|a|)$ ensures that Eq. (3) is also valid for $a<0$.
[14] The first term in this expansion was first found by P. Price, thesis, Cambridge University, Cambridge, 1951 (unpublished); the second and third terms were found by Huang and Yang for $\mathcal{N}$ particles [22], although numerical coefficients were inexact; the term $\propto L^{-6}\ln L$ was discovered by Wu [5]. $O(L^{-6})$ corrections were recently computed independently by Beane, Detmold, and Savage [26] for $\mathcal{N}$ particles.
[15] For any two-body potential $V(r)$, $U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} = \frac{1}{2}\Sigma_{i=1}^2\Sigma_{j=3}^4\tilde{V}_{\mathbf{k}_i-\mathbf{k}_j}$, where $\mathbf{k}_1+\mathbf{k}_2 \equiv \mathbf{k}_3+\mathbf{k}_4$, and $\tilde{V}_{\mathbf{k}} \equiv \int \mathrm{d}^3 r V(r)\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$.
[16] These functions can be obtained from the wave function of the two-body $l$-wave scattering state at energy $E\to 0$: $\phi_{\hat{\mathbf{n}}\mathbf{k}}^{(l,E)} = \phi_{\hat{\mathbf{n}}\mathbf{k}}^{(l)} + Ef_{\hat{\mathbf{n}}\mathbf{k}}^{(l)} + E^2 g_{\hat{\mathbf{n}}\mathbf{k}}^{(l)} + O(E^3)$, whose amplitude is defined by $\int\frac{\mathrm{d}^3k}{(2\pi)^3}\phi_{\hat{\mathbf{n}}\mathbf{k}}^{(l,E)}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = (-1)^{l+1}a_l Q_{\hat{\mathbf{n}}}^{(l)}(\nabla_r)[\sin(\sqrt{E}r+\delta_l)/r\sin\delta_l]$ for $r$ greater than the range of the interaction. Expanding the latter expression in powers of $E$, and using Eq. (9), one can derive Eqs. (8). Here $Q_{\hat{\mathbf{n}}}^{(l)}$ is defined by Eq. (10).
[17] Note that $Q_{\hat{\mathbf{n}}}^{(l)}(\nabla_k)(2\pi)^3\delta(\mathbf{k})$ scales with $k$ like $k^{-3-l}$.
[18] It can be shown that $a$ and $r_s$ are real.
[19] The vector sum of the three subscripts of $\phi^{(3)}$ is fixed as zero.
[20] Using the expansion formulas for $\phi_{\mathbf{k}}$ and $\phi^{(3)}_{-\mathbf{k},\mathbf{k}/2+\mathbf{k}',\mathbf{k}/2-\mathbf{k}'}$ at small $\mathbf{k}$, and noting that $U^{\phi}_{\mathbf{k},-\mathbf{k},0}$ and $\int_{\mathbf{k}'}U_{\mathbf{k}\mathbf{k}'}d_{\mathbf{k}'}$ are smooth functions of $\mathbf{k}$, one can readily verify that Eqs. (36a) and (36c) are compatible.
[21] Although $U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}$ is divergent for the hard-sphere interaction, one can use a soft-sphere interaction to derive Eqs. (45), and then take the hard-sphere limit, in which the two-body special functions and parameters and the parameter $D$ are modified, but the *form* of Eqs. (45) remains unchanged.
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