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

Shina Tan
Institute for Nuclear Theory, University of Washington, Seattle, Washington 98195-1550, USA
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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. An asymptotic expansion of this wave function at large interparticle distances is 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 interaction potentials, 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 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. Another key prediction is that there is a violation of the effective field theory (EFT) in the condensate fraction in dilute BECs, caused by short-range physics. EFT predictions for the ground state energy and few-body scattering amplitudes, however, are corroborated.

I. INTRODUCTION

The ground state energy per particle of a dilute Bose-Einstein condensate (BEC) is

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

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, by Bogoliubov [1], Lee, Huang, and Yang [2, 3], and Wu and others [4–6].

The \( \mathcal{E}_3' \) term has remained the least understood. It was known to Wu [4] that \( \mathcal{E}_3' \) is given by a parameter \( \mathcal{E}_3 \) for the ground state energy of 3 bosons in a periodic cubic volume [4], plus many-body corrections. Braaten and Nieto fully determined these many-body corrections using the effective field theory (EFT) [7] but, like Wu, they left undetermined a parameter \( g_3(\kappa) \) for the effective strength of the three-body force near the scattering threshold [7], which is related to Wu’s parameter \( \mathcal{E}_3 \) [4]. [The difference, \( g_3(\kappa) - g_3(\kappa') \), is known for any momentum scales \( \kappa \) and \( \kappa' \).]

For bosons with large scattering length, \( g_3(\kappa) \) was recently computed using the EFT [8]. For other model interactions, Braaten et al [9] used the Monte Carlo (MC) results of the energy density [10] to extract \( \mathcal{E}_3' \) but, because of statistical uncertainties of the MC data that are difficult to reduce, they did not obtain satisfying answers [9]. In summary, \( g_3(\kappa) \) remains unknown for almost all bosonic systems.

In this paper this three-body force and a few related properties of the \( N \)-body system are studied. Implications for dilute Bose-Einstein condensates are also explored.

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

\[
\phi_{q_1} = (2 \pi)^3 \delta(q) - 4 \pi a / q^2 + u_0 + O(q^2).
\]

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, \( \phi_{q_1 q_2 q_3}^{(3)} \). It is shown in this paper that this is indeed the case. For small momenta \( h q_i \sim h q (\sum_{i=1}^3 q_i = 0) \), it is found that

\[
\phi_{q_1 q_2 q_3}^{(3)} = (2 \pi)^6 \delta(q_1) \delta(q_2) + G_{q_1 q_2 q_3}
\]

\[
\times \left\{ \left[ \sum_{i=1}^3 -4 \pi a (2 \pi)^3 \delta(q_i) + 32 \pi^2 a^2 / q_i^2 - 16 \pi^2 w a^3 / q_i \right] - 64 \pi w a^4 \ln(q_i \! / |a|) \right\} - D + u_0 \sum_{i=1}^3 [(2 \pi)^3 \delta(q_i) - 8 \pi a / q_i^2]
\]

\[+ O(q^{-1}), \tag{3}
\]

where \( G_{q_1 q_2 q_3} \equiv 2 / (q_1^2 + q_2^2 + q_3^2) \), and that \( D \), named three-body scattering hypervolume (with dimension \( [\text{length}]^4 \)), is a suitable parameter for the three-boson interaction [11].

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 free space and matching the solution to Eq. (3) at small momenta or its Fourier transform at large relative distances.

In Sec. II of the present paper, \( \phi_{q_1 q_2 q_3}^{(3)} \) is expanded to the order \( q^4 \) at small momenta [Eqs. (40)] and, correspondingly, its Fourier transform 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 \( R^{-4} \), higher order corrections are determined, to facilitate much more accurate determinations of \( D \) from numerical solutions to 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 3-body Schrödinger equation numerically the author found

\[
D_{\text{HS}} \equiv (1761.5430 \pm 0.0004) a^4. \tag{4}
\]

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 [12] to the order \( L^{-7} \) (\( \hbar = m_{\text{boson}} = 1 \)):
\[
E = \frac{12\pi a}{L^3} \left[ 1 + 2.387 297 479 480 619 476 67 \frac{a}{L} + 9.725 330 808 459 240 057 \frac{a^2}{L^2} + \left( -39.307 830 355 480 219 057 \ln \frac{L}{a} \right) \right. \\
+ 95.852 723 604 821 230 29 \frac{a^3}{L^3} + 3 \pi a^2 r_s \frac{1}{L^3} + \left( -669.168 047 948 734 849 322 \ln \frac{L}{a} \right) + 810.053 286 803 649 420 \frac{a^4}{L^4} \\
+ 53.481 797 505 510 907 636 \frac{a^3 r_s}{L^4} \right] + \frac{D}{L^6} + 17.023 784 876 883 716 860 \frac{a D}{L^7} + O(L^{-8}),
\]

where \( r_s \) is the two-body effective range.

In Sec. IV B Wu’s parameter \( E_3 \) [4] is expressed in terms of \( D \); \( E_3 \) for hard-sphere bosons is then found [Eq. (109)].

In the rest of Sec. IV the \( N \)-boson energy and momentum distribution are found. The importance of the parameter \( u_0 \) [defined in Eq. (2)], which is absent in the effective field theory, is stressed. General formulas for the BEC energy and condensate depletion are obtained [Eqs. (118) and (119)].

In Sec. V the scattering amplitude of three bosons at low energy is computed [Eqs. (135)]. After a discrepancy between Ref. [7] and our result at \( r_s \neq 0 \) is resolved, \( g_s(\kappa) \) of Ref. [7] 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)].

\section{II. Asymptotics of \( \phi^{(3)} \) at Small Momenta or Large Relative Distances}

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 \( r_s \)). So the 2-body interaction \( \frac{1}{2} U_{k_1 k_2 k_3 k_4} \) conserves momentum, is invariant under rotation or any equal shift of \( k_i \)'s (1 \( \leq i \) \( \leq 4 \)), and is smooth. Also, because of Bose statistics, we can symmetrize \( U \) with respect to the incoming (outgoing) momenta without losing generality [13]:
\[
U_{k_1 k_2 k_3 k_4} = U_{k_2 k_1 k_3 k_4} = U_{k_3 k_1 k_2 k_4} = U_{k_4 k_1 k_2 k_3}.
\]

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

\begin{align}
\phi(r) &= 1 - a/r, \quad \text{(8a)} \\
f(r) &= -r^2/6 + a r/2 - a r_s/2, \quad \text{(8b)} \\
g(r) &= r^4/120 - a r^3/24 + a r_s r^2/12 - a r_s^2/24, \quad \text{(8c)} \\
\phi_n^{(d)}(r) &= (r^2/15 - 3a d/r^3) P_2(\hat{n} \cdot \hat{r}), \quad \text{(8d)} \\
f_n^{(d)}(r) &= (-r^4/210 - a d a d r^2/30 - a d^2/2r) P_2(\hat{n} \cdot \hat{r}), \quad \text{(8e)} \\
g_n^{(d)}(r) &= (r^4/945 - 105a d/r^5) P_4(\hat{n} \cdot \hat{r}), \quad \text{(8f)} \\
\phi_n^{(d)}(r) &= (r^6/135135 - 10395a d/r^7) P_6(\hat{n} \cdot \hat{r}), \quad \text{(8g)}
\end{align}

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

\[
k^{2l+1} \cot \delta_l(k) = -a_i^{-1} + r_k^2 k^2/2! + r_k^4 k^4/4! + O(k^6),
\]

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

\[
Q_n^{(l)}(k) \equiv k^l P_l(\hat{n} \cdot \hat{k}).
\]
\[ \phi_{nl}^{(l)} = \frac{i^l}{(2l+1)!!} Q_n^{(l)}(\nabla_k) (2\pi)^3 \delta(k) + \left[ -\frac{4\pi a_l}{i^l k^2} + \sum_{i=0}^{\infty} u_i^{(l)} k^{2i} \right] Q_n^{(l)}(k), \]

\[ f_{nl}^{(l)} = \left[ \frac{\nabla_k^2}{2!!(2l+3)!!} - \frac{a_l t_l}{2!!(2l+1)!!} \right] i^l Q_n^{(l)}(\nabla_k) (2\pi)^3 \delta(k) + \left[ -\frac{4\pi a_l Z}{i^l k^4} + \sum_{i=0}^{\infty} f_i^{(l)} k^{2i} \right] Q_n^{(l)}(k), \]

\[ g_{nl}^{(l)} = \left[ \frac{\nabla_k^4}{4!!(2l+5)!!} - \frac{a_l r_l \nabla_k^2}{2!!(2l+1)!!} - \frac{a_l r_l}{4!!(2l+2)!!} \right] i^l Q_n^{(l)}(\nabla_k) (2\pi)^3 \delta(k) + \left[ -\frac{4\pi a_l Z}{i^l k^6} + \sum_{i=0}^{\infty} g_i^{(l)} k^{2i} \right] Q_n^{(l)}(k), \]

(11a)

(11b)

(11c)

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

\[
\frac{Z}{k^4} = \frac{1}{k^3} (k > 0), \quad \int_{\mathbb{R}^3} \frac{Z}{k^4} \, dk = 0, \\
\frac{Z}{k^6} = \frac{1}{k^3} (k > 0), \quad \int_{\mathbb{R}^3} \frac{Z}{k^6} \, dk = \int_{\mathbb{R}^3} \frac{Z}{k^3} \, dk = 0.
\]

\( Z/k^4 \) and \( Z/k^6 \) have \( -\infty \) values at \( k = 0 \) to cancel certain integrals shown above. They inevitably arise from the Fourier transformation of functions such as \( \mathcal{F} \). 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 \( \phi_{nl}^{(l)}(r) \), \( f_{nl}^{(l)}(r) \), and \( g_{nl}^{(l)}(r) \) from Eqs. (8) at \( r < r_c \). Since \( r_c \rightarrow \infty \), these series are convergent.

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

\[
\frac{1}{2} \int \frac{d^3 k'}{(2\pi)^3} U_{kk'} \phi_{nl}^{(l)} = \left[ i^{-4\pi a_l} - \sum_{i=0}^{\infty} u_i^{(l)} k^{2i+2} \right] Q_n^{(l)}(k), \\
\frac{1}{2} \int \frac{d^3 k'}{(2\pi)^3} U_{kk'} f_{nl}^{(l)} = \sum_{i=0}^{\infty} \left[ u_i^{(l)} k^{2i} - f_i^{(l)} k^{2i+2} \right] Q_n^{(l)}(k), \\
\frac{1}{2} \int \frac{d^3 k'}{(2\pi)^3} U_{kk'} g_{nl}^{(l)} = \tilde{f}_0 + O(k^2).
\]

(12a)

(12b)

(12c)

For any unknown \( X_k \) we have the uniqueness theorem [15]:

\( (HX)_k \equiv 0 \) (all \( k \)) and \( X_k = o(k^{-3}) \) (small \( k \)) \( \Rightarrow \) \( X_k \equiv 0 \).

(13)

The following identity is needed in the analysis of the moment distribution of \( \mathcal{N} \) particles at low density (\( \mathbb{R} \) stands for the real part) [16]:

\[
\lim_{k_0 \to \infty} \int_{k > k_0} \frac{d^3 k}{(2\pi)^3} \left[ \left| \phi_k \right|^2 - \frac{\alpha_0^2 a^2}{k^4} \right] = -2\pi \alpha^2 r_s - 2\mathcal{R} u_0. \\
\]

(14)

B. Asymptotics of \( \phi_{k_1,k_2,k_3}^{(3)} \) at small momenta

From this point on, we let \( q_i \)'s be small momenta and \( q_i \)'s scale like \( q^3 \), while \( k \)'s be independent from \( q \)'s. We will derive the following asymptotic expansions:

\[
\phi_{q_1,q_2,q_3}^{(3)} = \sum_{s=-6}^{\infty} T_q^{(s)}(q),
\]

\[
\phi_k = \phi_{q_1,-q_2/2+k,-q_3/2-k}^{(3)} = \sum_{s=-3}^{\infty} S_k^{(s)q},
\]

(15)

(16)

where \( T^{(s)} \) and \( S_k^{(s)q} \) both scale like \( q^s \) (including possibly \( q^s \) \( \ln q_n \), \( n = 1, 2, \ldots \)). The minimum values of \( s \) in the above equations will be justified below.

The 3-body Schrödinger equation can be written in two special forms [17]:

\[
G_{q_1,q_2,q_3}^{-1} \phi_{q_1,q_2,q_3}^{(3)}(-q_1 - q_2 - q_3) = \left( \sum_{s=0}^{3} \frac{1}{2} \int_{k'} U_{p_1,k'} \phi_{q_1}^{(s)} \right) - U_{q_1,q_2,q_3}^{(3)} + \frac{1}{2} \int_{k'} U_{-q_1/2+k,k} \phi_{q_1}^{(s)}(q_1 \leftrightarrow q_2) + W_{q_1,q_2,q_3}^{(3)},
\]

(17)

\[
\int_{k'} \phi_{q_1,q_2,q_3}^{(3)}(q_1 \leftrightarrow q_2) + W_{q_1,q_2,q_3}^{(3)} = 0,
\]

(18)

\[ p_1 = (q_2 - q_3)/2, \text{ and similarly for } p_2, p_3, \]

(19)

\[
U_{q_1,q_2,q_3} = \frac{1}{6} \int_{k_1,k_2} U_{q_1,q_2,q_3,k_1,k_2}^{(3)}_{k_1,k_2},
\]

(20)

\[
W_{q_1,q_2,q_3} = \int_{k'} U_{q_1,q_2,q_3,k,k'} \phi_{q_1}^{(s)}(q_1 \leftrightarrow -q_3) + U_{-q_1/2+k,-q_2/2-k}^{(s)}(q_1 \leftrightarrow -q_2). \]

(21)

\[ \int_{k'} \text{ is the shorthand for } \int \frac{d^3 k'}{(2\pi)^3}, \text{ and } \int_{k'} \text{ stands for } \int \frac{d^3 k'}{(2\pi)^3}. \]

At small \( q \)'s we have Taylor expansions:

\[
U_{q_1,q_2,q_3} = \kappa_0 + \kappa_1 (q_1^2 + q_2^2 + q_3^2) + O(q^4),
\]

(22a)

\[
W_{q_1,q_2,q_3}^{(s)} = \sum_{q=0,2,4,\ldots} q^s W_{q_1,q_2,q_3}^{(s)}, \quad W_{q_1,q_2,q_3}^{(0)} = W_{q_1,q_2,q_3}^{(0)}. \]

(22b)

Now we fix the overall amplitude of \( \phi_{q_1,q_2,q_3}^{(3)}(\sum_{s=1}^{3} q_i = 0) \):

\[ \phi_{q_1,q_2,q_3}^{(3)} = (2\pi)^3 \delta(q_1) \delta(q_2) + \text{higher order terms}. \]

Because \( \delta(\Lambda q) = \lambda^{-3} \delta(q) \), \( \delta(q) \) scales like \( q^{-3} \). So \( s \geq -6 \) for \( T^{(s)} \), and

\[ T^{(-6)} = (2\pi)^6 \delta(q_1) \delta(q_2). \]

(23)
So \( T_{\chi_1\chi_2+k_1\chi_2-k}^{(-6)} = (2\pi)^3 \delta(q)(2\pi)^3 \delta(k) \sim q^{-3}k^{-3}, \)
indicating that \( s \geq -3 \) for \( S_{k}^{(3)}q \).

The following statement is now true at \( s_1 = -6 \):

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

We can then do the following expansions at small \( q \), for \(-6 \leq s \leq s_1 \):

\[
T^{(s)}_{\chi_1\chi_2+k_1\chi_2-k} = \sum_n i_{\chi_1\chi_2}^{(n,s-n)},
\]

(24)

where \( i_{\chi_1\chi_2}^{(n,s-n)} \) scales like \( q^n k^{s-n} \). Note also that \( S_{k}^{(-3)}q + S_{k}^{(-2)}q + \cdots = T^{(-6)}_{\chi_1\chi_2+k_1\chi_2-k} + T^{(-5)}_{\chi_1\chi_2+k_1\chi_2-k} + \cdots \)

\[= \phi^{(3)}_{\chi_1\chi_2+k_1\chi_2-k}. \]

Therefore, the asymptotic expansion of \( S_{k}^{(s+1)+3}q \) at small \( k \) has been determined to the order \( k^3 \):

\[S_{k}^{(s+1)+3}q = \sum_{m=-s_1}^{-9} i_{\chi_1\chi_2}^{(s+1)+3,m} + O(q^{s+1+k}k^2). \]

(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 \( q^{s+3} \) from Eq. (18), we get

\[HS^{(s+1)+3}q = -3q^2 c_{k}^{(s+1)+3}q/4 - W_{\chi_1\chi_2}^{(s+1)+3}q. \]

(25b)

If \( W_{\chi_1\chi_2}^{(s+1)+3} \neq 0 \) (ie, if \( s_1 + 3 = 0, 2, 4, \ldots \)), we take it as formal input. Solving Eqs. (25), with the help of (6) and (11), we thus determine \( c_{k}^{(s+1)+3}q \). The uniqueness of the solution is guaranteed by (13).

Once \( S^{(s+1)+3} \) is determined, the right-hand side of Eq. (17) can be determined up to the order \( q^{s+1}k^3 \), if the coefficients of the Taylor expansion of \( U^{(s)}_{\chi_1\chi_2q_3} \) [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 \( T^{(s+1)+3} \).

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.** \( S_{k}^{(s+1)+3}q = (2\pi)^3 \delta(q)(2\pi)^3 \delta(k) + O(q^{s+1+3}k^{-2}) \) at small \( k \), and \( (HS^{(s)+3})q = 0 \), so

\[S_{k}^{(s+1)+3}q = (2\pi)^3 \delta(q)\phi_k. \]

(26)

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

\[T^{(-5)}_{\chi_1\chi_2q_3} = \sum_{i=1}^{3} -i_{\chi_1\chi_2}^{(-5)}(4\pi a/\mu^2)(2\pi)^3 \delta(q_i). \]

(27)

Expanding \( T^{(-5)}_{\chi_1\chi_2q_3} \) at small \( q \), we get all the functions \( i_{\chi_1\chi_2}^{(n,m)} \) for \( n + m = -5 \); shown below are those in the range \(-2 \leq n \leq 3 \) (zeros are omitted):

\[
i_{\chi_1\chi_2}^{(-2,-3)} = -(8\pi a/q^2)(2\pi)^3 \delta(k), \]

(28a)

\[
i_{\chi_1\chi_2}^{(0,-5)} = -\pi a(\hat{q} \cdot \nabla k)^2/(2\pi)^3 \delta(k), \]

(28b)

\[
i_{\chi_1\chi_2}^{(2,-7)} = -(\pi a/4\hat{q})(\hat{q} \cdot \nabla k)^4/(2\pi)^3 \delta(k)q^2. \]

(28c)

**Step 3.** \( S_{k}^{(s)+3}q = i_{\chi_1\chi_2}^{(-2,-3)} + O(q^{s+2}k^{-2}) \) at small \( k \), and \( (HS^{(s)+3})q = 0 \), so

\[S_{k}^{(s)+3}q = -(8\pi a/q^{2})\phi_k. \]

(29)

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

\[T^{(-4)}_{\chi_1\chi_2q_3} = 32\pi^2 a^2 G_{q_1q_2q_3} \sum_{i=1}^{3} q_i^2. \]

(30)

At small \( q \) we have the following expansions (named “Z-\( \delta \) expansions”): see Appendix B for details:

\[
(2\pi)^3 \delta(k) = k^{-2} - \sqrt{3}(2\pi)^3 \delta(k)q/8\pi - 3q^2Z/4k^4
+ \sqrt{3}(2\pi)^3 \delta(k)q^3/64\pi + 9q^4 Z/16k^6
- 3\sqrt{3}(2\pi)^3 \delta(k)q^5/5120\pi + O(q^6), \]

(31a)

\[
(k + q/2)^{-2} + |k - q/2 (k^2 + 3q^2/4) = (2\pi)^3 \delta(k)/6q
+ 2Z/k^4 + [ -\nabla^2/48 + (1/24 - \sqrt{3}/16\pi)Q^{(d)}_k(\nabla) k] \times (2\pi)^3 \delta(k)q + \left(4ZQ^{(d)}_k(\nabla) k/3k^8 - 4Z/3k^6\right)^2
+ \left[\nabla^2/1280 - (1/448 - 3\sqrt{3}/896\pi)\nabla^2 Q^{(d)}_k(\nabla) k \right]
+ (19/10080 - 3\sqrt{3}/896\pi)Q^{(d)}_k(\nabla) k + 896\pi/k^4 \] \[
+ O(q^4), \]

(31b)

so \( T^{(-4)}_{\chi_1\chi_2+3}q_{\chi_1\chi_2-k} = \sum_{n=-\infty}^{n=-4} i_{\chi_1\chi_2}^{(-n,-4)} \), where

\[
i_{\chi_1\chi_2}^{(-2,-3)} = 32\pi^2 a^2/(2\pi)^2 k^2, \]

(32a)

\[
i_{\chi_1\chi_2}^{(0,-3)} = 4\pi awa(2\pi)^3 \delta(k)/q, \]

(32b)

\[
i_{\chi_1\chi_2}^{(0,-4)} = 4\pi awa^3 Z/k^4, \]

(32c)

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

**Step 5.** \( S_{k}^{(s)+3}q = i_{\chi_1\chi_2}^{(s)-3} + O(q^{s+2}k^{-2}) \) at small \( k \), and \( (HS^{(s)+3})q = 0 \), so

\[S_{k}^{(s)+3}q = (4\pi awa^3 q)/q). \]

(33)

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

\[T^{(-3)}_{\chi_1\chi_2q_3} = -16\pi^2 awa^3 G_{q_1q_2q_3} \sum_{i=1}^{3} q_i^{-1} + u_0 \sum_{i=1}^{3} (2\pi)^3 \delta(q_i). \]

(34)

Doing the \( Z-\delta \) expansion (Appendix B), one finds that \( T^{(-3)}_{\chi_1\chi_2+3}q_{\chi_1\chi_2-k} = \sum_{n=-\infty}^{n=-4} i_{\chi_1\chi_2}^{(-n,-4)} \). For brevity only one of the terms is shown here (to be used in the next step):

\[
i_{\chi_1\chi_2}^{(0,-3)} = \left[16awa^3 \ln(q/|a|) + 2u_0 + (14\pi/\sqrt{3} - 16wa^3) \right] \times (2\pi)^3 \delta(k) - 32\pi^2 awa^3 Z/k^4. \]

(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
\[(H S^{(0)}q)_{k} = 6\pi a\phi_k - W^{(0)}_k.\]
Because the right hand side does not depend on $k$ or $q$, we can introduce a single function $d_k$, which is independent of $k$ and satisfies
\[(H d)_{k} = 6\pi a\phi_k - W^{(0)}_k,\] (36a)
and get $S^{(0)}_{k} = d_k + (\text{linear combination of } \phi^{(l)}_{k q})$. Equation (36a) does not completely determine $d_k$, since $d_k + \eta\phi$ satisfies the same equation. At small $k$ [Eq. (25a)],
\[S^{(0)}_{k} = \left[ -2\pi a Q^{(d)}_{k q} (\nabla q)^{2}/3 + 16\pi a^3 \ln(q|a|) \right] (2\pi)^3 \delta(k) + d_a(k) + O(k^{-2}),\] (36b)
does not depend on $k$ or $q$. Noting Eq. (11a), we can now complete our definition of $d_k$ [18] and determine $S^{(0)}_{k}$:
\[d_k = d_a(k) + O(k^{-2})\] at small $k$. (36c)

\[S^{(0)}_{k} = 16\pi a^3 \ln(q|a|) \phi_k + 10\pi a \phi^{(d)}_{k q} + d_k.\] (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
\[T^{(-2)}_{a_{1}a_{2}q_{3}} = G_{a_{1}a_{2}q_{3}} \left[ -64\pi a^4 \ln(q)a_{3}|a|^3 - D \right] - \sum_{i=1}^{3} 8\pi a u_0 / q_i^2,\] (38)
\[D = \frac{3}{2} \int_{k'} U_{0,1,k'} d_{k'} + \frac{1}{6} \int_{k_1k_2} U_{0,0,0,k'_1k'_2k'_3} \phi^{(d)}_{k'_1k'_2k'_3} - 18\pi a u_0.\] (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:

\[
\phi^{(3)}_{-q/2+k,-q/2-k,q} = \left[ (2\pi)^3 \delta(q) - \frac{8\pi a}{q^2} + \frac{4\pi a^2}{q} + 16\pi a^3 \ln(q|a|) + 24\sqrt{3}\pi a^4 \ln(q|a|) + \frac{32\sqrt{3}\pi a^5}{\pi} q^2 \ln(n|a|) - \xi_2 q^2 \ln(q|a|) - \xi_3 q^3 \ln(q|a|) + \xi_4 q^4 \right] \phi_k + \left[ -3\pi a^2 q - 12\pi a^3 \ln(q|a|) - 18\sqrt{3}\pi a^4 \ln(q|a|) - \frac{3\xi_1}{4} q^3 \right] \sum_{i=1}^{3} \sqrt{\pi a} \ln(q_i) + \frac{9\pi w}{4} a^2 q^3 g_k + \left[ 10\pi a - 10\pi (2\pi - 3\sqrt{3}) a^2 q - 4\pi a^3 \ln(q|a|) + \xi_3 q^3 \right] \phi^{(d)}_{k q} + \frac{15\pi}{2} (2\pi - 3\sqrt{3}) a^2 q^3 f^{(d)}_{k q} + \left[ -\frac{9\pi}{2} a q^2 + \frac{3\pi}{4} (76\pi - 135\sqrt{3}) a^2 q^3 \right] \phi^{(g)}_{k q} + d_k + q^2 d^{(2)}_{k q} + O(q^4),\] (40a)

\[
\phi^{(3)}_{q_1q_2q_3} = (2\pi)^3 \delta(q_1) (2\pi)^3 \delta(q_2) [2 q_1 + q_2 + q_3 + 3 \sum_{i=1}^{3} \left[ -4\pi a (2\pi)^3 \delta(q_i) + \frac{32\pi a^2}{q_i^2} - 16\pi a^3 \ln(q_i|a|) - D \right] - 96\sqrt{3}\pi a^5 q_i \ln(q_i|a|) - 4\pi a \xi_1 q_i + 128\sqrt{3}\pi a^6 q_i^2 \ln(q_i|a|) + 4\pi a \xi_2 q_i^2 \ln(q_i|a|) + 40\pi a \xi_3 q_i^3 \ln(q_i|a|) - 4\pi a \xi_4 q_i^4 - 40\pi (2\pi - 3\sqrt{3}) a^2 a q_i \xi^{(d)}_{q_i} (a_i) + \sum_{i=1}^{3} \left[ A q_i^3 \delta(q_i) (u_0 + u_1 p_i^2 + u_2 p_i^4) - 8\pi a q_i^3 u_0 (u_0 + u_1 p_i^2 + u_2 p_i^4) + 4\pi w q_i^2 (u_0 + u_1 p_i^2 + u_2 p_i^4) + 16\pi a^3 \ln(q_i|a|) u_0 + 24\sqrt{3}\pi a^4 q_i \ln(q_i|a|) u_0 + \xi_3 q_i u_0 - 3\pi a^2 q_i f_0 \right] + \chi_0 + O(q^2),\] (40b)

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

\[
\xi^{(d)}_{3} \equiv 5(9\sqrt{3} - 4\pi) a^4/3 + 15\pi (2\pi - 3\sqrt{3}) a^2 a d r_d 4,\] (41c)

\[
\xi_{3} \equiv (24/\pi + 16/\sqrt{3}) a^6 + 9\sqrt{3} a^5 r_s,\] (41d)
\( \xi_1 \equiv -\left[ (1/8\pi^2 + 1/12\sqrt{3}\pi) a + 3\sqrt{3} r_s / 64\pi \right] aD \\
+ \left( 17\sqrt{3}/2 + 22/\pi + 353\pi/27 \right) w a^6 \\
+ \left( 11\sqrt{3}/4 - \pi/6 \right) w a^5 r_s + 9 w a^4 r_s^2 / 16 \\
+ 3 w a^3 r_s^3 / 32 + (10\pi^2 - 45\sqrt{3}\pi/4) a a_d, \)  
(41e)

\[ \chi_0 = 9 \pi a u_1 - 3 \omega_1 / 2 - 2 \kappa_1 - \int_{k'} U_{0k'} \phi_{qk}^{(2)} \, d k'. \]  
(42)

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

\[ \frac{1}{2} \int_{k'} U_{kk'} d k' = \omega_0 + \omega_1 k^2 + O(k^4). \]  
(43)

The other symbols in Eqs. (40) are defined previously: \( a, r_s, r'_s, a_d, \) and \( r_d \) in Eq. (9). \( \phi_k, \hat{f}_k, g_k, \phi_{qk}^{(d)}, f_{qk}^{(d)}, \) and \( \phi_{qk}^{(g)} \) in Eqs. (6) and (11), \( u_i \), and \( f_{ik} \) in Eqs. (11) with \( l = 0, w = 4\pi / 3 - \sqrt{3}, \sum_1 q_i \equiv 0, \) \( p_i \) in Eq. (19), \( Q^{(d)} \) in Eq. (10) with \( l = 2, \) and \( d_k \) in Eqs. (36).

At the order \( q^2 \) in the expansion of \( \phi_{q_1 q_2 q_3}^{(3)} \), one will encounter another 3-body parameter, \( D' \), in the term \( -D' G_{q_1 q_2 q_3} \sum_{i=1}^3 q_i^4 \). [Another contribution at the same order, \( \chi_1 (q_1^4 + q_2^4 + q_3^4) \), 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 \( \phi_{q_1 q_2 q_3}^{(3)} \) to the order \( q^m \), one will encounter a total of exactly

\[ N_3(m) = \text{round}(m^2 / 48 + m' / 3 + 89 / 72) \]  
(44)

independent 3-body parameters that contribute to the Fourier transform of \( \phi_{q_1 q_2 q_3}^{(3)} \) at large relative distances, where \( m' = m \) (if \( m \) is even), \( m' = m - 1 \) (if \( m \) is odd), and “round” rounds to the nearest integer.

C. Asymptotics of \( \phi_{q_1 q_2 q_3}^{(3)}(r_1 r_2 r_3) \) at large relative distances

\( \phi_{q_1 q_2 q_3}^{(3)}(r_1 r_2 r_3) \equiv \int \frac{d^3 k_1}{(2\pi)^3} \frac{d^3 k_2}{(2\pi)^3} \phi_{q_1 k_1} \phi_{q_2 k_2} \phi_{q_3 k_3} \exp \left( \sum_{i=1}^3 i k_i \cdot r_i \right), \)

where \( \sum_{i=1}^3 k_i \equiv 0. \) We consider the asymptotic expansions of \( \phi_{q_1 q_2 q_3}^{(3)}(r_1 r_2 r_3) \) in two different limits: 1) the distance \( r \) between two bosons is fixed, but the distance between their center of mass and the third boson, \( R, \) is large, or 2) all three interparticle distances, \( s_1, s_2, \) and \( s_3, \) are large but their ratio is fixed. These two expansions are respectively

\[ \phi_{q_1 q_2 q_3}^{(3)}(r_1 r_2 r_3) = 1 + \sum_{t=1}^3 \left[ \frac{36 w a^3 (2t - 3) \sin \theta_t - 2 \theta_t \cos \theta_t - \sqrt{3} a \xi_1 \sin \theta_t - 96 w a^6 \left[ 3 \theta_t^2 \sin 4 \theta_t + (6t - 11) \theta_t \sin 2 \theta_t + 2 \theta_t \cos 2 \theta_t \right] - \frac{3 \sqrt{3} D}{8 \pi D} \right] B^3 \sin^2 2 \theta_t, \]  
(45a)

\[ \phi_{q_1 q_2 q_3}^{(3)}(r_1 r_2 r_3) = 1 + \sum_{t=1}^3 \left[ \frac{3 \sqrt{3} a \xi_1 \cos \theta_t \cos 4 \theta_t + 45 \sqrt{3} a a_d (24 \theta_t - 8 \sin \theta_t + \sin 8 \theta_t) P_2(\hat{R}_t \cdot \hat{s}_t) + \frac{3 \sqrt{3} a \xi_1 \cos \theta_t \cos 4 \theta_t}{8 \pi B^3 \sin^2 2 \theta_t} \right] + O(B^{-8}). \]  
(45b)
where $\tau = \ln(\tilde{\gamma}R/|a|)$, $t \equiv \ln(\tilde{\gamma}B/|a|)$, $\tilde{\gamma} \equiv e^7 = 1.78107 \cdots$, $\gamma$ is Euler’s constant, and

$$s_1 = r_2 - r_3, \quad s_2 = r_3 - r_1, \quad s_3 = r_1 - r_2, \quad (46)$$

$$R_1 = r_1 - (r_2 + r_3)/2, \text{ and similarly for } R_2 \text{ and } R_3,$$

$$B = \sqrt{(s_1^2 + s_2^2 + s_3^2)/2}, \quad \theta_1 = \arctan(2R_1/\sqrt{3}s_1).$$

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

$$\xi_4 \equiv [1/10\pi^3 + 1/15\sqrt{3}\pi^2]a - 7\sqrt{3}r_\omega/80\pi^2a^2D$$

$$- (536/25\pi^2 + 124/27 - 86/25\sqrt{3}\pi)\omega^7$$

$$+ (65/3 + 309\sqrt{3}/25\pi)\omega^5 r_\omega - 6\omega^5 r_\omega^2/5$$

$$- 60\pi - 87\sqrt{3}a^2d - 9\omega a^4 r_\omega/20, \quad (47b)$$

$$\zeta_4^{(d)} \equiv \sqrt{3}\omega^6 D/28\pi^2 - (416/21 - 8384\sqrt{3}/245\pi)\omega^5$$

$$- 3\omega^4 r_\omega/7 - 3\omega^3 a d r_\omega/2. \quad (47c)$$

$$R_i = B \sin \theta_i, \quad s_i = \frac{a}{\sqrt{3}}B \cos \theta_i, \text{ and } \sum_{i=1}^3 \cos 2\theta_i = 0.$$

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

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

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

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

**III. LOW-ENERGY EFFECTIVE INTERACTION OF 3 HARD-SPHERE BOSONS**

In this section, we consider the hard-sphere (HS) interaction. The 2-body potential $V(r) = 0$ $(r > 1)$, $V(r) = +\infty$ $(r < 1)$ ($a = 1$ in this section), and there is no 3-body potential. We numerically solve Schrödinger equation at zero energy in the coordinate representation, in conjunction with Eq. (45a) at large $R$, to determine $D$.[19]

For 3-body configurations excluded by the repulsive interaction, $\phi^{(3)}$ vanishes; for allowed configurations, $\phi^{(3)}$ satisfies the free Schrödinger equation. So $\sum_{i=1}^3 \nabla_i^2\phi^{(3)}(r_1, r_2, r_3)$ is nonzero on the boundary $B$ between these two regions only (in fact, it has a $\delta$-function singularity on $B$). Thus

$$\phi^{(3)}(r_1, r_2 r_3) = 1 - 4\sqrt{3}/\pi \int_0^1 dc' \int_{R_{\min}}^{\infty} dR' F(R', c')R'^2 dR'$$

$$\times \left\{ G[s_1, s_2, s_3; 1, s_-(R', c'), s_+(R', c')] + G[s_1, s_2, s_3; s_-(R', c'), 1, s_+(R', c')] + G[s_1, s_2, s_3; s_-(R', c'), s_+(R', c'), 1] \right\}. \quad (49)$$

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

$$G(s_1 s_2 s_3; s_1' s_2' s_3') = \left\{ \left[ \left( s_1^2 + s_2^2 + s_3^2 + s_1'^2 + s_2'^2 + s_3'^2 \right)^2 \right. \right.$$

$$\left. - 2 \left( 5 s_1^2 s_2'^2 - s_1 s_2'^2 - s_1'^2 s_2 - s_2'^2 s_2 - s_1^2 s_2'^2 + s_2'^2 s_2 - s_2^2 s_3 - s_1^2 s_3 - s_2^2 s_3 \right) \right.$$

$$\left. - s_1^2 s_3'^2 - s_2' s_3'^2 \right] \right\} - 36 \left( 8 s_1 s_2 s_3 + s_1 s_2'^2 + s_2 s_3'^2 + s_3 s_1'^2 \right.$$}

$$\left. \times \left( 2 s_1'^2 s_2 + 2 s_2'^2 s_3 + 2 s_3'^2 s_1 - s_1'^4 - s_2'^4 - s_3'^4 \right) \right\} ^{-1/2} \quad (51a)$$

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

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

Because $\phi^{(3)}(r_1 r_2 r_3)$ vanishes on $B$, the unknown function $F(R', c')$ in Eq. (49) satisfies an integral equation:

$$\phi^{(3)}(r_1 r_2 r_3) = 0 \text{ at } s_1 = 1, s_2 = s_3 = s_\pm(R, c), \quad (52)$$

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

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

$$\left( \nabla_i^2 + 3\nabla_R^2/4 \right) \phi^{(3)}(r/2, -r/2, R) = F(R, c)\delta(r-1) \quad (53)$$

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

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

The 2-boson special functions satisfy Eqs. (8) at $r \geq 1$ and vanish at $r \leq 1$, so

$$a = 1, \quad r_s = 2/3, \quad r_s' = 8/15, \quad a_d = 1/45, \quad a_d = -150/7, \quad a_g = 1/99225, \quad a_i = 1/1404728325.$$

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

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

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

\[ D = 48\pi^2 Q - 192\pi w(1 - \gamma) - 12\pi^2 \]
\[ = 473.741 011 252 289 Q - 744.946 799 290 500. \quad (55) \]

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

\[ Q = \lim_{R \to \infty} \int_0^1 \int_{R_{\text{min}}(c')} dR' \frac{F(R', c')}{R'^2} \left[ R^2 - (R^2/3 + 2wR/\pi - (4w/\pi) \ln R) \right]. \quad (56) \]

Solving Eqs. (52) and (56) for $F(R, c)$ and $Q$ numerically, 
[using $F_a^{(1)}(R', c') + Q F_a^{(2)}(R', c')$ 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

\[ Q = 5.290 844 \pm 0.000 005. \]

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

IV. GROUND STATE OF 3 BOSONS IN A PERIODIC CUBIC VOLUME

In this section we return to the general interactions considered in Sec. II. The 3 bosons are now placed in a large periodic cubic volume of side $L$, and

\[ \epsilon \equiv 1/L \quad (57) \]

is the small parameter.

A. Ground state wave function and energy

Let $A_{n_1 n_2 n_3}$ ($\sum_{i=1}^3 n_i \leq 0$) be proportional to the probability amplitude that the bosons have momenta $2\pi c n_i$ ($i = 1, 2, 3$). We shall call $n_i$ an integral vector, since its Cartesian components (along the sides of the cubic volume) are integers.

\[ F_a^{(1)}(R, c) = 1 - \frac{2}{R} + \frac{2w}{\pi R^2} - \frac{4w}{R^3} + \frac{24\sqrt{3}w}{\pi^2} \ln R + \frac{12}{\pi^2} \left( 8/\sqrt{3} \pi \right)^4 R^{-4} + \left( 96\sqrt{3}w/\pi^2 \right) R^{-5} + \left( 105/\pi^2 - 8/\sqrt{3} \pi \right) R^{-6} + \left( 64(7\sqrt{3} \pi - 9)w/\pi^3 \right) R^{-15} \]
\[ + \frac{120\sqrt{3}w}{\pi^2} \ln R \]
\[ = 6\sqrt{3}/\pi R^4 \left( 24\sqrt{3}/\pi R^6 - (72/\pi^2 + 43\sqrt{3}/\pi) R^{10} - \left( 144/\pi^2 - 112\sqrt{3}/\pi + 30\sqrt{3} P_2(c)/\pi \right) R^{-7} \right), \quad (58) \]

Schrödinger equation ($\hbar = m_{\text{boson}} = 1$)

\[ [2\pi^2 c^2 (n_1^2 + n_2^2 + n_3^2) - E] A_{n_1 n_2 n_3} \]
\[ + \frac{1}{2 L^2} U_{2\pi c n_1, 2\pi c n_2, 2\pi c n_3} A_{n'_1 n'_2 n'_3} \]
\[ + \frac{1}{2 L^2} U_{2\pi c n_1, 2\pi c n_2, 2\pi c n_3} A_{n_1 n_2 n_3} \]
\[ = 0, \quad (59) \]

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

\[ \left[ (k_1^2 + k_2^2 + k_3^2)/2 - E \right] \psi_{k_1 k_2 k_3} \]
\[ + \frac{1}{6} L_{(k_1)} L_{(k_2)} \int_{k_1 k_2} U_{k_1 k_2 k_3} \psi_{k_1 k_2 k_3} \psi_{k_1 k_2 k_3} \]
\[ + \frac{1}{2} L_{(k_1)} \int_{k_1} U_{k_1 k_2 k_3} \psi_{k_1 k_2 k_3} + \cdots = 0, \quad (60) \]

\[ \psi_{k_1 k_2 k_3} = \sum_{n_1 n_2 n_3} A_{n_1 n_2 n_3} \prod_{i=1}^3 (2\pi)^3 \delta(k_i - 2\pi c n_i), \]

where $\sum_{i=1}^3 k_i = 0$, $\int_{k_1 k_2} \equiv \int \frac{d^3 k_1'}{(2\pi)^3}$, $\int_{k_1 k_2} \equiv \int \frac{d^3 k_1' d^3 k_2'}{(2\pi)^6}$, and

\[ L_{(k)} \equiv \sum_n (2\pi)^3 \delta(k - 2\pi c n), \quad J_{(k)} \equiv \sum_{n \neq 0} (2\pi)^3 \delta(k - 2\pi c n). \quad (61) \]

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

Let

\[ A_{0,0,0} \equiv L^6, \quad (63) \]

so $\psi_{q_1 q_2 q_3} = \prod_{i=1}^3 (2\pi)^3 \delta(q_i) + o(\epsilon^{-6})$. 

The following expansions will be found:

$$\psi_{k_1 k_2 k_3} = \sum_{s \geq 0} \mathcal{R}^{(s)}_{k_1 k_2 k_3},$$ (64a)

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

$$\psi_{q_1 q_2 q_3} = \sum_{s \geq -6} \mathcal{T}^{(s)}_{q_1 q_2 q_3},$$ (64c)

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

where \(\mathcal{R}^{(s)}_{k_1 k_2 k_3}, \mathcal{S}^{(s)q}_k, \mathcal{T}^{(s)}_{q_1 q_2 q_3},\) 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 \(\psi_{k_1 k_2 k_3}\) within a large but fixed spatial region in powers of \(\epsilon\), and then transform the result back to the \(k_i\)-space term by term, to obtain \(\sum_s \mathcal{R}^{(s)}_{k_1 k_2 k_3}\). Equation (64b) is similar: we expand the partial Fourier transform, \(\int_k \psi_{q,-q/2+k,-q/2-k} \exp(\text{i}k \cdot r)\), within a large but fixed region of the \(r\)-space, for fixed \(q/\epsilon\), in powers of \(\epsilon\), and then transform the result back to the \(k\)-space term by term, to obtain \(\sum_s \mathcal{S}^{(s)q}_k\).

Obviously

$$\mathcal{T}^{(-6)}_{q_1 q_2 q_3} = (2\pi)^3 \delta(q_1)(2\pi)^3 \delta(q_2).$$ (65)

Therefore

$$\mathcal{T}^{(-6)}_{k_1 k_2 k_3} = (2\pi)^3 \delta(k_1)(2\pi)^3 \delta(k_2)$$ and

$$\mathcal{T}^{(-6)}_{q,-q/2+k,-q/2-k} = (2\pi)^3 \delta(q)(2\pi)^3 \delta(k),$$ indicating that the minimum values of \(s\) for \(\mathcal{R}^{(s)}_{k_1 k_2 k_3}\) and \(\mathcal{S}^{(s)q}_k\) are 0 and \(-3\), respectively. Since the energy is dominated by pairwise mean-field interactions, \(E \sim \epsilon^3\).

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

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

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 \(\epsilon\)):

$$\frac{1}{2}(k_1^2 + k_2^2 + k_3^2)\mathcal{R}_{k_1 k_2 k_3} + \frac{1}{6} \int_{k_1 k_2 k_3} U_{k_1 k_2 k_3 k_1' k_2' k_3'} \mathcal{R}_{k_1' k_2' k_3'} \equiv \mathcal{H} \mathcal{S}_k^0 + I(q) \mathcal{W}_k \equiv 0,$$ (66a)

$$\left(\mathcal{H} \mathcal{S}_k^0 + (3q^2/4 - E)\mathcal{S}_k^0 + I(q)\mathcal{W}_k\right) = 0,$$ (66b)

$$\left[\frac{1}{2}(q_1^2 + q_2^2 + q_3^2) - E\right] T_{q_1 q_2 q_3} + \frac{1}{2} \sum_{i=1}^3 I(q_i) \int_{k_i} U_{k_i k_i} \mathcal{S}_k^0 + \frac{1}{6} I(q_1) I(q_2) \int_{k_1 k_2} U_{q_1 q_2 k_1 k_2 k_3} \mathcal{R}_{k_1 k_1 k_2} \mathcal{R}_{k_2 k_3} = 0,$$ (66c)

\[ \mathcal{W}_k^q = \frac{1}{6} \int_{k_1 k_2 k_3} U_{-q/2+k_1,-q/2+k_2,q} \mathcal{R}_{k_1 k_2 k_3} + \left(\frac{1}{2} \int_{k_1' k_2' k_3'} U_{-q/2+k_1' k_2' k_3'} \mathcal{R}_{k_1' k_2' k_3'} \right) + \mathcal{T}_{q,-q/2+k,-q/2-k} + (q \leftrightarrow -q), \] (67)

where \(\mathcal{R}, \mathcal{S}, \text{ and } \mathcal{T}\) are the sums of \(\mathcal{R}^{(s)}_{k_1 k_2 k_3}, \mathcal{S}^{(s)q}_k, \text{ and } \mathcal{T}^{(s)}_{q_1 q_2 q_3}\), respectively, and in Eq. (66c), \(1' = 2, 2' = 3, 3' = 1, \text{ and } p_j\) is defined in Eq. (19).

The following statement is now true at \(s_1 = -6\):

**Statement s1:** The functions \(T^{(s)}_{q_1 q_2 q_3}\) (for \(s \leq s_1\)), \(S^{(s)q}_k\) (for \(s \leq s_1 + 2\)), \(R^{(s)}_{k_1 k_2 k_3}\) (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 \(-6 \leq s \leq s_1\):

$$T^{(s)}_{q_1 q_2 q_3} = \sum_n n^{(n,s-n)}_{q_1 q_2 q_3},$$ (68a)

$$R^{(s_1+6)}_{k_1 k_2 k_3} = \sum_{m=-s_1-12}^n m^{(m,s_1+6,m)}_{k_1 k_2 k_3} + O(\epsilon^{s_1+6} k^{-5}).$$ (68b)

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

$$\frac{1}{2}(k_1^2 + k_2^2 + k_3^2)\mathcal{R}_{k_1 k_2 k_3} + \frac{1}{6} \int_{k_1 k_2 k_3} U_{k_1 k_2 k_3 k_1' k_2' k_3'} \mathcal{R}_{k_1' k_2' k_3'} + \frac{1}{2} \int_{k_1} U_{k_1 k_2 k_3 k_1' k_2' k_3'} \mathcal{R}_{k_1' k_2' k_3'} + \cdots = \sum_{3 \leq \kappa \leq s_1+6} \mathcal{S}^{(s_1+6_\kappa)}_{k_1 k_2 k_3},$$ (70)

where the right-hand side is already known. This equation and Eq. (69b) [which expands \(\mathcal{R}^{(s_1+6)}_{k_1 k_2 k_3}\) to the order \(\epsilon^{s_1+6}\) at small \(k\)-s] are sufficient to determine \(\mathcal{R}^{(s_1+6)}_{k_1 k_2 k_3}\), due to the 3-body version of the uniqueness theorem [analogous to Eq. (13)].

The above information for \(\mathcal{S}^{(r)}_{k_1 k_2 k_3}\) and \(\mathcal{R}^{(s_1+6)}_{k_1 k_2 k_3}\) is sufficient to determine each term in Eq. (66b), except the first term, to the order \(\epsilon^{s_1+3}\) [note that \(I(q) \sim 0\)], so \(\mathcal{H} \mathcal{S}^{(s_1+3)}_{k_1 k_2 k_3}\) is known; taking into account Eq. (69a), one can determine \(\mathcal{S}^{(s_1+3)}_{k_1 k_2 k_3}\).

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_0^{(q_1 q_2 q_3)} + c_0 \sum_{i=1}^3 I(q_i)\int_{k_1} U_{k_1} \mathcal{S}^{(r)}_{k_1 k_1 k_1} + \frac{1}{6} I(q_1) I(q_2) \int_{k_1 k_2} U_{q_1 q_2 k_1 k_1 k_2} \mathcal{R}_{k_1 k_1 k_2} \mathcal{R}_{q_1 k_1 k_2} = 0,$$ (66c)

$$C_{q_1 q_2 q_3} = G_{q_1 q_2 q_3} (ET'_{q_1 q_2 q_3} - c'_{q_1 q_2 q_3}),$$ (71)
where \( G_{q_1 q_2 q_3} = 2/(q_1^2 + q_2^2 + q_3^2) \sim \epsilon^{-2} \). Because \( \epsilon \sim \epsilon^4 \), \( T'_{q_1 q_2 q_3} \sim \epsilon^4 \), \( x > -6 \), and \( E \) and \( T'_{q_1 q_2 q_3} \) are known to the orders \( \epsilon^{i+9} \) and \( \epsilon^{i+1} \), respectively, we know \( E T'_{q_1 q_2 q_3} \) to the order \( \epsilon^{i+3} \). So from Eq. (71), we can now determine \( T'_{q_1 q_2 q_3} \) (and thus \( T_{q_1 q_2 q_3} \)) to the order \( \epsilon^{i+1} \).

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

Repeating the above routine, one can formally determine \( A_{n_1 n_2 n_3} \) and \( E \) to any orders in \( \epsilon \). The following are the step-by-step results of this program.

**Step 1a.** \( R^{(0)}(0) \), \( R^{(1)}(1) \), and \( R^{(2)}(2) \) satisfy the zero-energy Schrödinger equation [because of Eq. (70)]. They will all be determined in this paper. From Eq. (65) we get 
\[
\phi^{(0,-6)}_{k_1 k_2 k_3} = \prod_{i=1}^{3}(2\pi)^3 \delta(k_i).
\]
So 
\[
R^{(0)}_{k_1 k_2 k_3} = \phi^{(3)}_{k_1 k_2 k_3}.
\]

**Step 1b.** \( t^{(-3,-3)}_{q k} = (2\pi)^3 \delta(q)(2\pi)^3 \delta(k) \); \( (H S^{(-3)}q)_{k} = 0 \).

So 
\[
S^{(-3)}_{k} = (2\pi)^3 \delta(q) \phi_{k}.
\]

**Step 2.** With the help of Eqs. (12), and noting that \( \sum_{i=1}^{3} q_i = 0 \), we get 
\[
E = 12\pi a e^3 + o(e^3),
\]
\[
T^{(-5)}_{q_1 q_2 q_3} = \sum_{i=1}^{3} \left[-(4\pi a/\eta_i^2)J(\eta_i)(2\pi)^3 \delta(q_i)\right].
\]
Using the method of Appendix B, we get 
\[
T^{(-5)}_{q_1 k_1 q_2 k_2 k_3} = \sum_{i=1}^{3} \left[-(4\pi a/\eta_i^2)(2\pi)^3 \delta(k_i)\right]
\]
\[
= (3\alpha_1 e/\pi)(2\pi)^3 \delta(k_1)(2\pi)^3 \delta(k_2) + O(e^3),
\]
where 
\[
T^{(-5)}_{q_1 k_2 k_3} = \sum_{i=1}^{3} \left[-(4\pi a/\eta_i^2)(2\pi)^3 \delta(k_i)\right]
\]
\[
= (3\alpha_1 e/\pi)(2\pi)^3 \delta(k_i)(2\pi)^3 \delta(k_j) + O(e^3),
\]
and similarly for \( l_2 \) and \( l_3 \). 

**Step 3a.** From \( t^{(1,-6)}_{k_1 k_2 k_3} \) and Eq. (70), we get 
\[
R^{(1)}_{k_1 k_2 k_3} = -(\alpha_1 e/\pi)\phi^{(3)}_{k_1 k_2 k_3}.
\]

**Step 3b.** From \( (H S^{(-2)}q)_{q} = 0 \), and \( t^{(2,-3)}_{q k} \), we get 
\[
S^{(-2)}_{q} = [-((\alpha_1 e/\pi)(2\pi)^3 \delta(q) - 8\pi a J(q)/q^2)] \phi_{q}.
\]

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

\[
E = 12\pi a e^3 (1 - \alpha_1 e/\pi) + O(e^5),
\]
\[
T^{(-4)}_{q_1 q_2 q_3} = J_{q_1 q_2 q_3} G_{n_1 n_2 n_3} \sum_{i=1}^{3} 2\alpha^2/\pi^2 e^4 n_i^2
\]
\[
+ (a^2/\pi^2 e) \sum_{i=1}^{3} (\alpha_1 m_i - m_i^4) J(p_i)(2\pi)^3 \delta(q_i),
\]
\[
J_{q_1 q_2 q_3} = \sum_{n_i, j \neq 0} \prod_{i=1}^{3}(2\pi)^3 \delta(q_i - 2\pi n_i).
\]

The three subscripts of \( J_{q_1 q_2 q_3} \), are always subject to the constraint \( \sum_{i=1}^{3} q_i = 0 \). In Eq. (82) and in the following, \( G_{n_1 n_2 n_3} = 2/(n_1^2 + n_2^2 + n_3^2) \), and 
\[
\eta_i = q_i/2\epsilon, \quad n_i = q_i/2\epsilon, \quad m_i = p_i/2\epsilon,
\]
\[
T^{(-4)}_{q_1 q_2 + k, q_2 - k} = \sum_{j=2} T^{(j,-3-j)}_{q_1 k},
\]
where 
\[
t^{(-4)}_{q k, l} = (a^2/\pi^2 e) \left\{ (a_2 + \alpha_3)(2\pi)^3 \delta(q)(2\pi)^3 \delta(k) \right\}
\]
\[
+ J(q) \left\{ (\alpha_4 - \alpha_5)(2\pi)^3 \delta(q)(2\pi)^3 \delta(k) \right\},
\]
\[
t^{(0,-4)}_{q k, l} = [16\pi^2 a^2 (2\pi)^3 \delta(q) + 40\pi^2 a^2 J(q)] Z/k^4,
\]
\[
t^{(1,-5)}_{q k, l} = X^{(-4)}_{q k} J(q).
\]
The actual formulas for \( X^{(s)}_{q k} \) \((s = -4, -3, -2)\); see Steps 6 and 8 below) are not needed in this paper. For \( s \geq 1 \), 
\[
\rho_A(n) = 2\theta_A(n) + W_A(n)/n^{2s},
\]
\[
\theta_A(n) = \sum_{m \neq 0} \left\{ (m^2 + m \cdot n + n^2) m^{2s} \right\}^{-1},
\]
\[
W_A(n) = \lim_{N \to \infty} \sum_{|m| < N} (m^2 + m \cdot n + n^2)^{-1} - 4\pi N.
\]

The above lattice sums are evaluated in Appendix C. One can easily extract \( t^{(j,-5-j)}_{q k} \) and \( R^{(j,-5-j)}_{k_1 k_2 k_3} \) from Eqs. (76).
where one can easily extract \( t_{k,k_2,k_3}^{(j,-j)} \). Here

\[
\beta_{1A} \equiv \lim_{\eta \to 0} \sum_{n \neq 0} e^{-\eta n} W_A(n)/n^2 + 4\sqrt{3} \pi^3/\eta^2
\]

(88)

is evaluated in Eq. (C18).

**Step 5a.** From \( t_{k,k_2,k_3}^{(n,2,0)} \) and Eq. (70), we get

\[
R^{(2)}_{k,k_2,k_3} = 3\pi^{-27} (2\beta_{1A} + \alpha^2_1 - 3\alpha_2) \alpha^2 \phi_{k,k_2,k_3}.
\]

(89)

**Step 5b.** From \((HS^{(-1)}q)_k = 0, \) and \( t_{q,k}^{(-1,-3)} \), we get

\[
S^{(-1)}_k = (a^2/\pi^2 \epsilon) \{ (a_1^2 + a_2^2/(2\pi \epsilon)^3 \delta(q) + [2\rho_{A1}(n) + 2\alpha_1/n^2 - 6/n^4J(q)] \} \phi_k.
\]

(90)

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

\[
E = 12\pi a^3 \left[ 1 - \alpha_1 a \epsilon/\pi + (\alpha_1^2 + \alpha_2^2) a^2 \epsilon^2/\pi^2 \right] + O(\epsilon^6),
\]

(91)

\[
T^{(-3)}_{q_1,q_2,q_3} = \frac{3}{6} \left( 6a^3/\pi^3 \epsilon^3 \right) J_{q_1,q_2,q_3} G_{n_1 n_2 n_3}^{-1} n_i^{-2}
\]

\[
- (2a^2/\pi^2 \epsilon) J_{q_1,q_2,q_3} G_{n_1 n_2 n_3} \left[ \rho_{A1}(n_1) + \alpha_1/n_2^2 - 3/n_3^2 \right] + \left\{ -4 \rho_{A1}(m_1/m_2^{-\alpha_1^2 + \alpha_2^2/m_2^2 + 2a_1/m_4^4 + 15/m_4^6} \times a^3/\pi^3 + u_0 \right\} J(p\epsilon)(2\pi)^3 \delta(q).
\]

(92)

In preparation for the subsequent steps, we derive

\[
t_{q,k}^{(0,-3)} = \left\{ -32\pi^2 a^3/\pi^3 \epsilon Z_{1,1,1}(k)/k^3 + \left[ \frac{2u_0 + 16a^3 \ln(2\pi a)}{2\pi^3 \epsilon} + (2a^2/\pi^3) \right] \delta(k) + (2a^2/\pi^3) \times \left[ -\rho_{A1}(n_1) + \rho_{A1}(n_1) + 3\rho_{A2}(n_1) + 3\rho_{B1}(n_1) - (\alpha_1^2 + \alpha_2^2)/n_1^2 + 6\alpha_1/n_1^4 - 9/n_1^6 \right] \right\} \delta(k) \}
\]

\[
+ \left\{ -32\pi^2 a^3/\pi^3 \epsilon Z_{1,1,1}(k)/k^3 + \left[ 16\pi a^3 \ln(2\pi a) - u_0 \right] + \left[ 15\alpha_3 + \alpha_1 \alpha_2 - \alpha_3^2 - 4\alpha_1 a_3^3/\pi^3 \right] \right\} \delta(k) \}
\]

(93a)

\[
t_{q,k}^{(1,-1)} = \frac{X_{q,k}}{a^3/\pi^3} J(q) - 96\pi a_3^2 Z_k^4/\pi^3(2\pi)^3 \delta(q),
\]

(93b)

where \( \rho_{B1}(n), \rho_{A1}(n), \) and \( \alpha_{A1} \) are defined as follows. For \( s \geq 0, \)

\[
\rho_{B1}(n) \equiv 2\theta_{B1}(n) + W_B(n)n^{-2s},
\]

(94a)

\[
\theta_{B1}(n) \equiv \sum_{m \neq 0} \left\{ \left[ (m^2 + m \cdot n + n^2) \right] m^2 s^{-1} \right\},
\]

(94b)

\[
W_B(n) \equiv \sum_{m \neq 0} \left[ (m^2 + m \cdot n + n^2)^{-2} \right].
\]

(94c)

\[
\rho_{A1}(n) \equiv \lim_{N \to \infty} \left( \frac{2}{\pi^3} \right) \sum_{m \neq 0; m < N} \left\{ -8\pi^3 \ln(n) + W_A(n) \rho_{A1}(n) \right\}.
\]

(95)

It can be shown that at large \( n \)

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

\[
\rho_{A2}(n) = -8\pi^3 w n - \pi^3 w(7\pi/\sqrt{3} - 8) + 2\pi^2 w a_1/n + O(n^{-2}).
\]

We define some 2-fold lattice sums:

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

(96a)

\[
\alpha_{sA_i} \equiv \sum_{n \neq 0} n^{-2s} \rho_{A_i}(n) \quad (s + s' \geq 3),
\]

(96b)

\[
\alpha_{sB_i} \equiv \sum_{n \neq 0} n^{-2s} \rho_{B_i}(n) \quad (s + s' \geq 2).
\]

(96c)

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

**Step 7.** From

\[
(HS^{(0)}q)_k + (-6\pi a \phi_k + W_k^{(0)})(2\pi)^3 \delta(q) = 0 \quad (\text{all } k),
\]

(97)

where \( W_k^{(0)} \) is defined in Eq. (22b), we get

\[
S^{(0)}_k = \sum_{s=-5}^{3} t_{q,k}^{(0,s)} + O(\epsilon^0 k^{-2}) \quad \text{(small } k),
\]

where \( \phi_k \) is defined in Eqs. (36),

\[
C_0 \equiv 16\pi a \ln(2\pi) + (15\alpha_3 + \alpha_1 \alpha_2 - \alpha_3^2 - 4\alpha_{1A1})/\pi^3
\]

\[
- (14\pi/\sqrt{3} - 16) w
\]

\[
= 95.852 \, 723 \, 604 \, 821 \, 230 \, 29,
\]

(98)

and

\[
\tilde{\rho}_{A1}(n) \equiv -\rho_{A1}(n) - \pi^3 w(7\pi/\sqrt{3} - 8) + 8\pi^3 w \ln(2\pi)
\]

\[
- \alpha_1 \rho_{A1}(n) + 3\rho_{A2}(n) + 3\rho_{B1}(n)
\]

\[
- (\alpha_1^2 + \alpha_2)/n^2 + 6\alpha_1/n^4 - 9/n^6.
\]

(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

\[
E = 12\pi a^3 \left( 1 - \alpha_1 a \epsilon/\pi + (\alpha_1^2 + \alpha_2^2) a^2 \epsilon^2/\pi^2 \right)
\]

\[
+ [16\pi a^3 \ln(\epsilon |a|) + C_0 a^3 + 3\pi a^2 r_s]^3 \epsilon^3 + D \epsilon^6 + O(\epsilon^7).
\]

(100)
\[ T_{q_1,q_2}(\mathbf{q}) = \sum_{i=1}^{3} [J(\mathbf{p})(2\pi)^3 \delta(\mathbf{q}_i) T^{(-25)}(\mathbf{m}_i) + J_{q_1,q_2,q_3} \sum_{s=0}^{3} C_{n_1,n_2,n_3} T^{(-2)}(\mathbf{n}_i)], \quad (101a) \]

\[ T^{(-28)}(\mathbf{m}_i) \equiv -\alpha_1 \omega_0 e^{-\pi} - \alpha_0 \omega_0 e^{-m_i} - 6\epsilon/4\pi^2 m_i^2 \]

\[ - 3\alpha_0^2 r_3 m_i^2 + \{ -4\rho_{AA}(\mathbf{m}_i) + 48\pi^3 w \ln(\epsilon|a|) \}

\[ + \pi^3 C_0/m_i^2 - [12\rho_{A1}(\mathbf{m}_i) + 9\alpha_2^2 + 6\alpha_2]/m_i^4 + 3\alpha_1/m_i^3 + 45/m_i^3 \} a^4/\pi^4, \quad (101b) \]

\[ T_0^{(-2)}(\mathbf{n}_i) \equiv -2\alpha_0/\pi^2 n_i^2, \quad (101c) \]

\[ T_1^{(-2)}(\mathbf{n}_i) \equiv -2[\rho_{AA}(\mathbf{n}_i) + 8\pi^3 w \ln(\epsilon|a|)] a^4/\pi^4, \]

\[ - D/12\pi^2 e^2, \quad (101d) \]

\[ T_2^{(-2)}(\mathbf{n}_i) \equiv -6[\rho_{A1}(\mathbf{n}_i) + 2\alpha_1/n_i^2 - 3/n_i^2] a^4/\pi^4 e^2, \quad (101e) \]

\[ T_3^{(-2)}(\mathbf{n}_i) \equiv 18 a^4/\pi^4 e^2 n_i^2. \quad (101f) \]

In preparation for the next step, we derive

\[ t^{(1,-3)}_{q,k} = X^{(-2)}_{q,k} J(\mathbf{q}) + \{ 96\pi w a_1^4 Z_{1/a}(k)/k^3 \}

\[ + \left[ - (96\omega_1/\pi) a^4 \ln(\epsilon|a|) + C_1 a^4 - \alpha_1 D/4\pi^2 \right. \]

\[ - 3\alpha_0^2 r_3 \} (2\pi)^3 \delta(\mathbf{k}) \} \epsilon(2\pi)^3 \delta(\mathbf{q}), \quad (102) \]

\[ C_1 \equiv \pi^2 \left[ -4\rho_{AA1} - 48\pi^3 w_1 \ln(2\pi) - \pi^2 \right. \alpha_1 C_0 \]

\[ - 12\alpha_2 A_1 - 9\alpha_2^2 - 6\alpha_2 + 3\alpha_1 \alpha_3 + 45\alpha_4 \}, \quad (103) \]

where

\[ \bar{\alpha}_{1,AA1} \equiv \lim_{N \to \infty} \left\{ \sum_{m \neq 0, m < N} m^{-2} \rho_{AA}(\mathbf{m}) \right. \]

\[ - 32\pi^4 w N \left[ \ln(2\pi N) - 1 \right] + 12\pi^3 w_1 \ln N \} \quad (104) \]

is a 3-fold lattice sum (evaluated in Appendix C).

**Step 9.** From

\[ (H^{(1)})_{q,k} = \left[ 24\alpha_1 a^2 \epsilon \phi_k - 3\alpha_1 a^4 W^{(0)}_{k}/\pi \right] (2\pi)^3 \delta(\mathbf{q}) \]

\[ + \left[ 6\rho_{A1}(\mathbf{n}) + \alpha_1 + n_2 \right] a^2 \epsilon \phi_k - 3\alpha_1 a^4 W^{(0)}_{k}/\pi \} J(\mathbf{q}) \]

and [note that \( t^{(1,-7)}_{q,k} = t^{(1,-6)}_{q,k} = 0 \)]

\[ S_k^{(1)} = \sum_{s=-5}^{-3} t^{(1,s)}_{q,k} + O(\epsilon k^2) \quad \text{(for small k)}, \]

we get

\[ S_k^{(1)} = \left\{ \left[ - (96\omega_1/\pi) a^4 \ln(\epsilon|a|) + C_1 a^4 - \alpha_1 D/4\pi^2 \right. \right. \]

\[- 6\alpha_1^3 r_3 + 6\alpha_1 a_0/\pi \} \phi_k - 6\alpha_2^2 \}

\[ \times (2\pi)^3 \delta(\mathbf{q}) \} + Y(\mathbf{q}, \mathbf{k}) J(\mathbf{q}), \quad (105) \]

where

\[ C_1 \equiv C_1 + 6\omega_1 (7/\sqrt{3} - 8/\pi) \]

\[ = 810.053 286 803 649 420, \quad (106) \]

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

**Step 10.** Substituting the latest results for \( S_0^{(1)} \) and \( R_{q_1,q_2,q_3} \) into Eq. (66c), extracting all the terms that contain the factor \( (2\pi)^3 \delta(\mathbf{q}_1) \delta(\mathbf{q}_2) \) from this equation, noting that \( T_{q_1,q_2,q_3} - (2\pi)^3 \delta(\mathbf{q}_1) \delta(\mathbf{q}_2) \) vanishes at \( q_1 = q_2 = 0 \), and using Eqs. (12) and (39) to simplify the result, we get

\[ E = 12\pi a^3 \left( 1 - \alpha_1 a\pi/\pi + (\alpha_1^2 + \alpha_2) a^2 e^2 /\pi^2 \right) \]

\[ + \left[ 16w a^3 \ln(\epsilon|a|) + C_0 a^3 + 3\pi^2 r_3 \right] \epsilon^3 \]

\[ + \left[ - (96\omega_1/\pi) a^4 \ln(\epsilon|a|) + C_1 a^4 - 6\alpha_3 /\pi \right] \epsilon^4 \}

\[ + (\epsilon^6 - 6\alpha_1 a^7 /\pi) D + O(\epsilon^8). \quad (107) \]

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 \( T_{q_1,q_2,q_3} \), in this paper.

**B. Results for Wu’s parameter \( \varepsilon_3 \)**

Wu computed the three-boson energy in the large periodic cubic volume to order \( L^{-6} \), and he left an unknown parameter \( \varepsilon_3 \) for the three-boson interaction strength at low energy [4]. \( \varepsilon_3 \) is needed to determine the full order-\( \rho^2 \) correction to the many-body energy [4].

Comparing our Eq. (100) with Wu’s result, Eq. (5.29) of Ref. [4] (note that the unit of mass in [4] is \( 2a^3 \)), we find that Huang and Yang’s constant [20] \( C = -\alpha_1/\pi = 2.837 \cdots \), [21] different from the number 2.37 which was first provided in Ref. [20] and then adopted by [4]; the symbols \( \varepsilon_3 \) in Ref. [4] equal \( \alpha_3 /\pi^2 \); the symbol \( \varepsilon_3 \) in Ref. [4] is now expressed in terms of \( D \) of the present paper:

\[ \varepsilon_3 = D/12\pi a^4 + 3\pi r_3 /a \]

\[ - 4\alpha_1 a^3 /\pi^3 + 16w \ln(2\pi) - (14\pi /\sqrt{3} - 16)w \]

\[ = D/12\pi a^4 + 3\pi r_3 /a + 73.699 808 371 935 4035. \quad (108) \]

For hard-sphere bosons, \( D \) is given by Eq. (4) and \( r_3 = 2a/3 \), so

\[ \varepsilon_3 = 126.709 37 \pm 0.000 06 \quad \text{(for hard spheres)}. \quad (109) \]

**C. Results for the ground state wave function**

There are 6 expansion formulas for \( A_{n_1,n_2,n_3} \), each of which is valid in a sub-region of the discrete momentum configuration space:

\[ A_{000} \equiv L^0, \quad (110a) \]
\[ A_{0,n,-n} = -aL^5/\pi n^2 + (\alpha_1/n^2 + 1/n^4)a^2L^4/\pi^2 + \left\{ -[\alpha_1^2 + \alpha_2 + 4\alpha_3]/(n^2 + 2\alpha_1/n^4 + 15/n^6)\right\} a^3L^3/\pi^3 + u_0L^3 + \left\{ -4\bar{\rho}_{AA}(n)/n^2 + 48\pi^2wn^{-2}\ln(L/|a|) - \pi^3C_0/n^2 - (9\alpha_1^2 + 6\alpha_2)/n^4 - 12\rho_{AA}(n)/n^4 + 3\alpha_1/n^6 + 48/n^8\right\} a^4L^4/\pi^4 \\
- (\alpha_1 + n^{-2})au_0/\pi - D/4\pi^2n^2 - 3a^3r_s/n^2 \right\} L^2 + O(L^1), \quad (110b) \]

\[ A_{n,n_2n_3} = \sum_{i=1}^{3} \left\{ 2a^2L^4/\pi^2n_i^2 - 2[\rho_{AA}(n_i) + \alpha_1/n_i^2 - 3/n_i^4]a^3L^3/\pi^3 - DL^2/12\pi^2 + 2[8\pi^2w\ln(L/|a|) - \bar{\rho}_{AA}(n_i)]a^4L^4/\pi^4 \right\} \\
\times G_{n_1n_2n_3} + \left\{ 6a^3L^3/\pi^3n_i^3 - 6[\rho_{AA}(n_i) + 2\alpha_1/n_i^2 - 3/n_i^4]a^4L^4/\pi^4 \right\} G_{n_1n_2n_3} + 18a^4L^4G_{n_1n_2n_3}^3/\pi^3n_i^2 - 2au_0L^2/\pi n_i^2 \\
+ O(L^1), \quad (11c) \]

\[ A_{0,N,-N} = \left\{ L^3 - \alpha_1aL^2/\pi + (\alpha_1^2 + \alpha_2)a^2L/\pi^2 - 16L^2\pi^2\ln(|a|) + C_0a^3 + 3\pi^2r_s - 3u_0 + \left\{ (96\pi\alpha_1/\pi) a^4L^4/\pi^4 \right\} \phi_k \right\} (1 - 3\alpha_1a/\pi L) \right\} \left\{ (6\pi a - 6\alpha_1a^2/\pi) f_k + O(L^{-2}), \quad (11d) \right\} \]

\[ A_{n,-n/2+N,-n/2-N} = \left\{ -2aL^2/\pi n^2 + (2\rho_{AA}(n) + 2\alpha_1/n^2 - 6/n^4) a^2L/\pi^2 - 16w^2\ln(L/|a|) + 2a^3\bar{\rho}_{AA}(n)/\pi^3 \right\} \phi_k \\
+ 10\pi \alpha_0 \phi^{(d)}_{nk} \right\} (1 - 3\alpha_1a/\pi L) \right\} \left\{ (6\pi a - 6\alpha_1a^2/\pi) f_k + O(L^{-1}), \quad (11e) \right\} \]

\[ A_{N_1, N_2 N_3} = \left\{ 1 - 3\alpha_1a/\pi L + 3(2\beta_{1A} + \alpha_2^2 - 3\alpha_2)a^2/\pi^2 L^2 \right\} \left\{ (6\pi a - 6\alpha_1a^2/\pi) f_k + O(L^{-1}), \quad (11f) \right\} \]

where \( \mathbf{n} \)'s are \textit{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), \( k \equiv 2\pi N/L, k_1 \equiv 2\pi N_1/L \), and \( G_{n_1n_2n_3} = 2/(n_1^2 + n_2^2 + n_3^2) \). The formulas for \( A_{0,0,0} \), \( A_{0,n,-n} \), and \( A_{n,n_2n_3} \) are extracted from the above results for \( N_1=0, Q_1 \); those for \( A_{0,N,-N} \) and \( A_{n,-n/2+N,-n/2-N} \) are extracted from \( S_k \); the formula for \( A_{N_1, N_2 N_3} \) results from the expansion of \( R_{k_1k_2k_3} \). The numerical constants in the above formulas are computed in Appendix C.

\section*{D. Momentum distribution}

The expectation value of the number of bosons with momentum \( 2\pi n/L \) is \( N_n = c \sum_{n,n'} |A_{n,n',-n-n'}|^2 \) for some constant \( c \) such that \( c \sum_{n,n}' |A_{n,n',-n-n'}|^2 = 3 \).

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

\[ N_0 = c|A_{000}|^2 + c \sum_{0<n\leq N_c} |A_{0,n,-n}|^2 + c \sum_{N>N_c} |A_{0,N,-N}|^2, \quad (11a) \]

\[ N_n = 2c|A_{0,n,-n}|^2 + c \sum_{n' \neq n/2, n' \leq N_c} |A_{n,-n/2+n',-n/2-n'}|^2 \\
+ c \sum_{N>N_c} |A_{n,-n/2+N',-n/2-N'}|^2, \quad (11b) \]

\[ N_N = 2c|A_{0,0,-N}|^2 + 2c \sum_{n' \neq 0, n' \leq N_c} |A_{n',-n'-N}|^2 \]

\[ + c \sum_{N>N_c} |A_{N',-N}|^2, \quad (11c) \]

where \( N_c \) satisfies \( 1 < N_c < L/\max(r_e, |a|) \); in Eq. (11b), \( n' \pm n/2 \) and \( N' \pm n/2 \) have integral Cartesian components. Substituting Eqs. (110) and using Eq. (14), we get

\[ N_0/c = L^{12} + \alpha_2a^2L^{10}/\pi^2 - 2(\alpha_1\alpha_2 + \alpha_3)a^3L^9/\pi^3 \\
- 3\alpha_1aL^{10} - 2\alpha_2r_sL^9 + O(L^8), \]

\[ N_n/c = 2a^2L^{10}/\pi^2n^4 - 4(\alpha_1/n^4 + 1/n^6)a^3L^9/\pi^3 \\
+ O(L^8), \]

\[ N_N/c = 2L^6(1 - 2\alpha_1/\pi L) |\phi_{2\pi N/L}|^2 + O(L^4), \]

Solving \( \sum_{n,n'} N_n = 3 \) [using Eq. (14) again], we get

\[ c = 3L^{12} \left\{ 1 - 3\alpha_2a^2/\pi^2 L^2 + 6(\alpha_1\alpha_2 + \alpha_3)a^3/\pi^3 L^3 \\
+ 6\alpha_1aL^{10}/L^3 + 6\pi^2r_sL^3 + O(L^{-4}) \right\}, \]
\[
\mathcal{N}_0/3 - 1 = -2\alpha_2 a^2/\pi^2 L^2 + 4(\alpha_1\alpha_2 + \alpha_3) a^3/\pi^3 L^3 + (4\Re u_0 + 4\pi a^2 r_s)/L^3 + O(L^{-4})
\]
\[
= -3.350147643 a^2/L^2 + (4\Re u_0 + 4\pi a^2 r_s - 17.92683116 a^3)/L^3 + O(L^{-4}),
\]  
(113a)

\[
\mathcal{N}_n = 6a^2/\pi^2 L^2 n^4 - (12a^3/\pi^3 L^3)(\alpha_1/n^4 + 1/n^6) + O(L^{-4})
\]
\[
= (0.607927102/n^4)(a/L)^2 + (3.449740068/n^4 - 0.387018413/n^6)(a/L)^3 + O(L^{-4}),
\]  
(113b)

\[
\mathcal{N}_\mathcal{N} = 6L^{-6}(1 - 2\alpha_1 a/\pi L)|\phi_{2\pi \mathcal{N}/L}|^2 + O(L^{-8}) = 6L^{-6}(1 + 5.674594959 a/L)|\phi_{2\pi \mathcal{N}/L}|^2 + O(L^{-8}).
\]  
(113c)

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

Equation (113a) shows that the depletion of the population of the zero momentum state depends on the parameter \(u_0\) at the next-to-leading order in the volume expansion.

Given \(\phi(r)\), one can compute \(u_0\) and \(r_s\) from the formulas

\[
u_0 = \int \left[ \phi(r) - (1 - a/r) \right] d^3r, \quad (114a)
\]
\[
-2\pi a^2 r_s = \int \left[ |\phi(r)|^2 - (1 - a/r)^2 \right] d^3r. \quad (114b)
\]

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

After repeated failure to find a general relation between \(R_{u_0}\) and any finite number of parameters in Eq. (9), the author conjectures that such a relation does not exist at all [22]. Because the EFT [9] is formulated in terms of parameters in Eq. (9) along with 3-body, 4-body, ... parameters, the two-body parameter \(u_0\) is absent in the EFT.

E. 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 to \(\mathcal{N}\) bosons (\(\mathcal{N} = 1, 2, 3, \ldots\)).

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 Beane, Detmold, and Savage’s result for \(E\) [23] which was derived with zero-range pseudopotentials [23], if the three-boson contact interaction parameter \(\eta_3(\mu)\) in Ref. [23] satisfies

\[
\eta_3(|\alpha|^{-1}) - 48a^4(4Q + 2\Re)/\pi^2
\]
\[
= D + 12\pi^2 a^3 r_s - 48a^4 \alpha_{1A1}/\pi^2
\]
\[
+ 24\pi a^4 \left[ 8 \ln(2\pi) - (7\pi/\sqrt{3} - 8) \right]
\]
\[
= D + 12\pi^2 a^3 r_s + 2778.417318626 973 645a^4,
\]  
(115)

where \(4Q + 2\Re\) is a number defined in Ref. [23]. It is the combination \(\eta_3(\mu) - 48a^4(4Q + 2\Re)/\pi^2\) that appears in their formula [23] for \(E\). In summary,

\[
E = P(1/L; a, N) - \frac{192\pi^2 a^4}{L^6} \left( \frac{N}{3} \right) \frac{\ln L}{|\alpha|}
\]
\[
+ \left( \frac{N}{2} \right) D + \frac{12\pi^2 a^3 r_s}{L^6} + \left( \frac{N}{2} \right) \frac{8\pi^2 a^3 r_s}{L^6} + O(L^{-7}),
\]  
(116)

where \(P\) is a well-determined [23] power series in \(1/L\) with \(a\) and \(N\) as the only parameters, and \(\left( \alpha_i \right) = \frac{a_i}{\nu_i(\alpha_{ij};)}\).

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

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

\[
\mathcal{N}_n = \mathcal{N}(N - 1)n^{-4}(a/\pi L)^2
\]
\[
- 2\mathcal{N}(N - 1)\left[ \alpha_1/n^4 + (2N - 5)/n^6 \right] (a/\pi L)^3
\]
\[
+ O(L^{-4}),
\]  
(117b)

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

Equations (117), unlike \(E\), can not be derived from the zero-range pseudopotentials or the effective field theory. [Even in Eq. (117b), the \(L^{-4}\) correction will contain the short-range parameter \(u_0\).]
2. Implications for dilute Bose-Einstein condensates in the thermodynamic limit

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

- \( L \gg N/a \), so that \( L \) is small compared to the BEC healing length \( \xi \sim (\rho a)^{-1/2} \);
- \( N^{1/3} a \ll L \ll N/a \), 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 \( \sum_{i=0}^{\infty} c_i (a/N/L)^i \). Nevertheless, one can infer many properties of the BEC in the second regime.

Now we tentatively take the thermodynamic limit \( (\rho \text{ fixed, } N \text{ and } L \text{ large}) \) of the \( 1/L \) expansions of \( E_0 = E/N \) and \( x \) [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 \( \sim -32\pi w a^4 \rho^2 \ln (L/a) \) 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 \( \rho^2 (D/6 + 2\pi^2 a^3 r_s) \). Comparing these findings with Eq. (1), we infer that

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

where \( C^E \) is a universal constant that remains the same for all Bose gases. Because \( E_0 \) was computed by Braaten and Nieto \([7]\), a comparison will be made between Eq. (118) and Ref. [7] (in Sec. V D).

The contributions to \( x \) that depend on \( a \) only are divergent in the thermodynamic limit. After a resummation that includes higher order terms in \( N/a/L \) (analogous to Eq. (55) of Ref. [3]), they must reproduce Bogoliubov’s well-known formula \( x = -\frac{8}{3\sqrt{\pi}} \sqrt{\rho a^3} + \ldots \). The leading nonuniversal term becomes \( \rho (2\Re u_0 + 2\pi a^2 r_s) \); 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 for the condensate depletion \([9]\) (which should be valid through order \( \rho^1 \) at \( u_0 = a^2 r_s = 0 \), at the very least), we infer that

\[
x = -\frac{8}{3\sqrt{\pi}} \sqrt{\rho a^3} + \rho (2\Re u_0 + 2\pi a^2 r_s) + C^x \rho a^3
\]

plus higher order terms in \( \rho \), where \( C^x \) is another universal numerical constant. Thus the nonuniversal effect in the quantum depletion of the condensate is larger than the EFT prediction \([9]\) 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 \( k \sim 1/r_s \gg (\rho a)^{1/2} \) is approximately \( \rho^2 |\delta_k|^2 \), rather than a structureless function \( \sim 16\pi^2 a^2 \rho^2 /k^4 \) as implied by the EFT.

The condensate fraction \( (\text{namely } N_0/N, \text{or } 1 + x) \) of a dilute Bose gas of hard spheres \( (\text{for which } 2u_0 + 2\pi a^2 r_s = \frac{8\pi}{3}a^3) \) is thus slightly greater than that of a Bose gas with \( r_s \ll a \) \( (\text{for which } |2u_0 + 2\pi a^2 r_s| \ll a^3) \) 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 SCATTERING AMPLITUDES OF THREE IDENTICAL BOSONS

In this section we compute the T-matrix elements of three identical bosons at low energy. We will compare our results with a similar calculation in Ref. [7], to establish the relation between the parameter \( D \) in the present paper and the three-body contact interaction parameter \( g_3(\kappa) \) in [7].

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.

A. 2-boson scattering amplitude

The two-boson T-matrix can be expressed in terms of the scattering phase shifts \([24]\) \((\hbar = m_\text{boson} = 1)\):

\[
T(b, \hat{b} \cdot \hat{q}) = (4\pi/|q|) \sum_{l=0,2,4,\ldots} \left[ e^{2\delta_l(q)} - 1 \right] (2l + 1) P_l(\hat{b} \cdot \hat{q}),
\]

where \( \pm b \) and \( \pm \hat{q} \) 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

\[
T(b, \hat{b} \cdot \hat{q}) = -8\pi a + i8\pi a^2 q + 8\pi a^2 (a - r_s/2) q^2
- i8\pi a^3 (a - r_s) q^3 + O(q^4).
\]

The first two terms in this expansion agree with Ref. [7], and all higher order corrections disagree, since the effective range \( r_s \) is not included in [7].

Equation (121) agrees with Ref. [9] where \( r_s \) is taken into account.

B. 3-boson scattering amplitude

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

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

where \(-i\eta\) specifies an outgoing wave \((\eta \to 0^+)\).
Similarly, from the stationary wave function $\Psi_{q_1,q_2,q_3}$ describing the scattering of three bosons with incoming momenta $b_1$, $b_2$, and $b_3$, and energy
\[ E = (b_1^2 + b_2^2 + b_3^2)/2, \] (122)
one can extract the three-boson T-matrix elements:
\[
\begin{align*}
\Psi_{q_1,q_2,q_3} &= \frac{(2\pi)^6}{6} \sum_P \delta(q_1 - b_{P1})\delta(q_2 - b_{P2}) \\
&+ \frac{1}{6} G_{q_1,q_2,q_3}^E \left[T(b_1,b_2,b_3;q_1,q_2,q_3) + \sum_{i,j=1}^3 T(h_i,\hat{h}_i,\hat{p}_j)(2\pi)^3\delta(q_j - b_i)\right] \\
&+ \text{[terms that are regular at $(q_1^2 + q_2^2 + q_3^2)/2 = E$]}.
\end{align*}
\] (123)
Here $P$ refers to all 6 permutations of “$123$”, $\sum_{i=1}^3 b_i \equiv \sum_{i=1}^3 q_i \equiv 0$, $p_i$ is defined in Eq. (19), and
\[
G_{q_1,q_2,q_3}^E = \left((q_1^2 + q_2^2 + q_3^2)/2 - E - i\eta\right)^{-1},
\] (124)
$h_1 = (b_2 - b_3)/2$, and similarly for $h_2$, $h_3$. (125)

Let $b_i \approx q_i \approx q$ 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: 1) the box size $L = \infty$ here, so $I(q) = 1$, 2) $E \sim q^2$ here, instead of $1/L^3$ in Sec. IV, and 3) the leading contribution to $\Psi_{q_1,q_2,q_3}$ is
\[
T_{q_1,q_2,q_3}^{(i-6)} = \frac{(2\pi)^6}{6} \sum_P \delta(q_1 - b_{P1})\delta(q_2 - b_{P2}).
\] (126)

Naturally, $\Psi_{q_1,q_2,q_3} \to \phi_{q_1,q_2,q_3}^{(3)}$ 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 $T$ and $S$ as in Sec. II, in the asymptotic expansions
\[
\begin{align*}
\Psi_{q_1,q_2,q_3} &= \sum_{s=-6}^{\infty} T_{q_1,q_2,q_3}^{(s)}; \\
\Psi_{k}^{q} &= \Psi_{q,-q/2+k,-q/2-k} = \sum_{s=-3}^{\infty} S_{k}^{(s)q},
\end{align*}
\] (127)
(128)
where $T_{q_1,q_2,q_3}^{(s)}$ and $S_{k}^{(s)q}$ scale like $q^s$ (not excluding $q^a \ln^n q$). When $E, b_i \to 0$ but $q_i$’s and $k$ 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 $k_i \sim 1/r_e \gg \sqrt{E}$
\[
\Psi_{k_1,k_2,k_3} = \phi_{k_1,k_2,k_3}^{(3)} + O(\sqrt{E}).
\] (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):
\[
\begin{align*}
S_{k}^{(-3)q} &= \frac{1}{3} \sum_{i=1}^{3} (2\pi)^3\delta(q - b_i)\phi_k, \\
T_{q_1,q_2,q_3}^{(-5)} &= -\frac{4\pi a}{3} G_{q_1,q_2,q_3}^E \sum_{i,j=1}^{3} (2\pi)^3\delta(q_j - b_i), \\
S_{k}^{(-2)q} &= -\frac{1}{3} \sum_{i=1}^{3} \left[8\pi a G_{q_i}^E + i\hbar_i (2\pi)^3\delta(q - b_i)\right]\phi_k, \tag{130a} \\
T_{q_1,q_2,q_3}^{(-4)} &= \frac{16\pi a^2}{3} G_{q_1,q_2,q_3}^E \sum_{i,j=1}^{3} \left[2G_{q_i,b_i}^E + \frac{i\hbar_i}{4\pi} (2\pi)^3\delta(q_j - b_i)\right], \tag{130b} \\
S_{k}^{(-1)q} &= \frac{1}{3} \sum_{i=1}^{3} \left[8\pi a^2 (i\hbar_i - \sqrt{3q_i^2/4 - E - i\eta}) G_{q_i,b_i}^E + 64\pi^2 a^2 c_1^E(q_i,b_i)\right]\phi_k + \hbar_i^2 (2\pi)^3\delta(q_i - b_i) \left[f_k - a(a - r_s/2)\phi_k - 5\phi(d)_{h,k}\right], \tag{130c} \\
T_{q_1,q_2,q_3}^{(-3)} &= \frac{1}{3} G_{q_1,q_2,q_3}^E \sum_{i,j=1}^{3} \left[32\pi^2 a^3 (\sqrt{3q_j^2/4 - E - i\eta} - i\hbar_i) G_{q_j,b_j}^E - 256\pi^3 a^3 c_1^E(q_j,b_j) + 4\pi a^2 (a - r_s/2)\hbar_i^2 (2\pi)^3\delta(q_j - b_i)\right] \\
&+ \frac{u_0}{3} \sum_{i,j=1}^{3} (2\pi)^3\delta(q_j - b_i), \tag{130d}
\end{align*}
\]
where \( i \neq i', q'_i \equiv q + 2b_i \) (not the outgoing momenta), \( \sqrt{\varepsilon} \) is defined with a branch cut along the negative \( z \)-axis, and

\[
G^{E}_{qb} \equiv (q^2 + q \cdot b + b^2 - E - i\eta)^{-1},
\]

\[
c^E_i(q, b) \equiv \int \frac{d^3k}{(2\pi)^3} G^{E}_{qkb} G^{E}_{kq},
\]

\[
c^E_2(q, b, \kappa) \equiv \lim_{K \to \infty} -\frac{w}{16\pi^3} \ln \frac{K}{\kappa} + \int_{K<K} \frac{d^3k}{(2\pi)^3} G^{E}_{qk} \times \left[ 2c^E_1(k, b) - \sqrt{\frac{3}{4}} \frac{E - i\eta}{4\pi} G^{E}_{kb} \right].
\]

The loop integrals \( c^E_1 \) and \( c^E_2 \) emerge from the \( Z - \delta \) expansions (Appendix B) of \( T^{(-3)}_{q_i - q_j - k_1} \) and \( T^{(-3)}_{q_i - q_j - k_1 - q_k - k_2} \) respectively.

Remarkably, \( c^E_2 \) (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 \( \Psi_{q_1q_2q_3} \) \( \equiv \sum_{s = -2}^{\infty} T^{(s)}_{q_1q_2q_3} \) with Eq. (123), we find the same result for the two-boson T-matrix as Eq. (121), and the first 3 terms in the low-energy expansion of the three-boson T-matrix:

\[
T(b_1b_2b_3; q_1q_2q_3) = \sum_{s=-2}^{\infty} T^{(s)}(b_1b_2b_3; q_1q_2q_3),
\]

Where \( T^{(s)}(b_1b_2b_3; q_1q_2q_3) \sim E^{s/2} \) (not excluding \( E^{5/2} \ln \eta \) \( E \)).

\[
T^{(-2)}(b_1b_2b_3; q_1q_2q_3) = 64\pi^2 a^2 \sum_{i,j=1}^{3} G^E_{q_i b_j},
\]

The momentum-independent term in this expression is proportional to \( D - 36\pi^2 a^2 r_s \), while the leading nonuniversal contribution to the BEC energy (as in Eq. (118)) is proportional to \( D + 12\pi^2 a^3 r_s \). We conclude that they can not be absorbed into a single 3-body contact interaction parameter \( g_3 \), unless the two-body effective range \( r_s = 0 \). This disagrees with Ref. [7].

C. Comparison with Ref. [7]

If \( r_s = 0 \), Eqs. (135) then agree with Ref. [7]. To see this, we use the power series for the 2-boson T-matrix to expand
the last term in Eq. (77) of [7] (note that \( q_{12} \) in [7] is twice \( h_3 \) here), and get all the 4 terms in Eqs. (135) of the present paper which contain \( G_{q_{1},b_{j}}^{E} \). The quantity \( T_{2}^{\text{PI}} \) of [7] corresponds to the first term on the right hand side of Eq. (135b) above; the finite contribution to \( T_{1}^{\text{PI}} \) in Eq. (80) of [7] corresponds to the last term of Eq. (135c) above. The sum of the divergent terms in \( T_{2}^{\text{PI}} \) and the 3-body term \(-[g_{3}(\kappa) + \delta g_{3}(\kappa)]\) [7] can be expressed in terms of \( c^{E}_{2} \) defined above:

\[
\frac{(8\pi a)^{4}}{2} \left[ \text{CMS} + \sum_{i,j=1}^{3} c^{E}_{2}(k_{i}, k_{j}', \kappa) \right] - g_{3}(\kappa),
\]

where

\[
\text{CMS} = \frac{18w\left[ \ln(2\pi) + 1 - \gamma + \sqrt{3}(2\delta' + 9\ln3 - 18) \right]}{64\pi^{3}}
= 0.055 \, 571 \, 793 \, 27.
\]

Here \( \delta' = \sum_{n=0}^{\infty} \left[ (1/3 + n)^{-2} - (2/3 + n)^{-2} \right] \). The momentum-dependent terms in Eqs. (135) thus completely agree with Ref. [7] at \( r_{s} = 0 \). Further matching the constant terms, we find the relation between the 3-body parameter \( g_{3}(\kappa) \) in Ref. [7] and the scattering hypervolume \( D \) defined in the present paper at \( r_{s} = 0 \):

\[
g_{3}(|a|^{-1}) = \frac{6(D - 24w(7\pi/\sqrt{3} - 8)a^{4}) + (8\pi a)^{4}}{2} \text{CMS}
= 6(D + 977.736 \, 695 \, 4 \, a \, a^{4}).
\]

At \( r_{s} \neq 0 \), the discrepancy between Ref. [7] and our result, Eqs. (135), disappears if \( r_{s} \) is included in the effective field theory. The 2-boson interaction vertex becomes [9]

\[
i(-8\pi a - 2\pi a^{2} r_{s} k^{2} - 2\pi a^{2} r_{s} k'^{2}),
\]

where \( k_{c}/2 \leq k \) and \( k_{c}'/2 \leq k' \) 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 3-boson T-matrix, Fig. 5(a) of Ref. [7], is modified as

\[
\sum_{i,j=1}^{3} \, G_{q_{1},b_{j}}^{E} \left[ 8\pi a + 2\pi a^{2} r_{s} p_{j}^{2} + 2\pi a^{2} r_{s} (b_{i} + q_{j}/2)^{2} \right] \\
\times \left[ 8\pi a + 2\pi a^{2} r_{s} h_{i}^{2} + 2\pi a^{2} r_{s} (q_{i} + b_{i}/2)^{2} \right] \\
\left[ (2\pi a)^{2} \sum_{i,j=1}^{3} G_{q_{1},b_{j}}^{E} + 32\pi a^{2} r_{s} \sum_{i,j=1}^{3} \left( p_{j}^{2} + h_{i}^{2} \right) G_{q_{1},b_{j}}^{E} \right] \
+ 288\pi a^{3} r_{s} + O(E^{1}).
\]

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

\[
g_{3}(|a|^{-1}) = \frac{6h_{a}^{2}}{m_{\text{boson}}} \left( D + 12\pi^{2} a^{3} r_{s} + 977.736 \, 695 \, 4 \, a^{4} \right),
\]

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 \( r_{s}^{2} \) by Braaten and Nieto [7]. The result, Eq. (96) of Ref. [7], 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 \( r_{s}^{3} \) in the thermodynamic limit, if it is expressed in terms of \( g_{3}(\kappa) \) [9].

Using Eq. (136), we can now express Braaten and Nieto’s result for the BEC energy [7] in terms of the scattering hypervolume \( D \) defined in Eq. (3). The outcome is precisely the same as Eq. (118), and \( C^{E} \) in Eq. (118) is found to be

\[
C^{E} = 977.7366695/12\pi + 8w\left[ \ln(16\pi) + 0.80 \pm 0.005 \right]
= 118.65 \pm 0.10.
\]

(137)

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

\[
C^{E} = 118.498 \, 920 \, 346 \, 444 \quad \text{(exactly rounded)},
\]

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

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

\[
E_{3}' = 167.319 \, 69 \pm 0.000 \, 06.
\]

(139)

This completes our calculation of the ground state energy per particle of a dilute Bose gas of hard spheres, through order \( r_{s}^{2} \).

For a dilute Bose gas with \( a \gg r_{c} \) (\( r_{c} \) is the range of interparticle forces), Braaten, Hammer, and Mehen found that \( E_{3}' \) is near 141 [8] and has a small imaginary part associated with 3-body recombination [8]. 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 \( \approx 39\rho a^{3} \), and a specific heat that is smaller by a fraction \( \approx 39\rho a^{3} \). Here the specific heats are compared at the same temperature \( T \ll \rho_{c}^{1/3}aT_{c} \), where they are dominated by phonons with wavelengths \( \gg 1/\sqrt{\rho_{c}} \). (\( T_{c} \) is the critical temperature.)

These differences, \( s \), in 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.)

For \( T/T_{c} \sim O(1) \) and \( \rho a^{3}, \rho_{c} a^{3} \ll 1 \), the thermal de Broglie wavelength greatly exceeds \( r_{c} \), and the interaction is well described by the constants \( a, r_{c}, \) and \( D \), etc.

The nonuniversal corrections to \( T_{c} \), as an extension of the calculations reviewed in Ref. [27], are of particular interest. Is the leading order nonuniversal correction determined by \( r_{s} \), or \( D \), or both? The present author speculates it is perhaps by \( r_{s} \) alone, and is of the form \( c'\rho a^{3} r_{s} T_{c}^{2} \), where \( T_{c}^{2} \) is the critical temperature of the noninteracting Bose gas, and \( c' \) is a universal numerical constant.
VI. SUMMARY

We have shown that the 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 an explicit calculation of the three-body force is given for hard spheres only, one can apply the general formulas, Eqs. (45), to many other interaction potentials, to predict the effective three-body forces. The unknown wave function has 3 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 with finite-range interactions. For weakly bound dimers of fermionic atoms, the two-dimer scattering length $a_d \approx 0.6a_f$ [28], where $a_f$ is the atomic scattering length, but the parameters $r_s$ and $D$ for these dimers are still unknown, which must be computed to determine the equation of state of many such dimers [28–30] more accurately [31].

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 $\phi^3$. The result, Eq. (5), may be combined with a Monte-Carlo simulation (for nonrelativistic particles such as atoms) or Lattice QCD simulation (for low energy pions) to determine the three-body force.

Equation (5) suggests that, to determine $D$ accurately, $L$ should greatly exceed $17a$ in these simulations, or the higher order corrections can overwhelm the lower order terms.

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

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.

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 [7] at $r_s \neq 0$. By including $r_s$ corrections in the EFT, however, one can eliminate the discrepancy completely. The resultant relation between $g(k)$ and $D$, combined with the many-body energy formula of Ref. [7], and the three-body force computed in the present paper [Eq. (4)], solves a longstanding problem of theoretical interest, namely the complete second-order correction to the ground state energy of a dilute Bose gas of hard spheres. The result shows small differences between this system and a dilute Bose gas with large scattering length considered by Ref. [8].

We have studied the energies and momentum distributions of $N$ bosons in a large volume, from which we deduce the energies and condensate fractions of dilute BECs with sizes greatly exceeding the healing length. The result for the energy, Eq. (118), agrees with the effective field theory, but the condensate depletion, Eq. (119), disagrees. It is found that at low density, even the population of the zero-momentum state, or the off-diagonal long-range order [32], is affected by short-range physics missed by the EFT.

Although the three-body force is usually a small correction to physical observables in a dilute BEC, dramatic effects may be obtained near a three-body resonance [8, 33]. Alternatively, one may reduce the two-body force by tuning the scattering length to a zero crossing [34]. At $a = 0$ the BEC ground state energy density $\approx h^2Dp^3/6m$.

The author would like to draw the readers’ attention to a few mathematical techniques. The $Z$-functions and $Z-\delta$ expansions (Appendices 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 $Z_\eta(k)/k^{2n+1}$ ($n = 1, 2, 3, \ldots$, and $b > 0$ is a constant):

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

$$\int_{|k|<b} d^3k \frac{Z}{k^{2n}} (k) = 0 \quad (s \leq 2n - 4), \quad (A2)$$

$$\int_{|k|<b} d^3k \frac{Z_\eta(k)}{k^{2n+1}} (k) = 0 \quad (k_0 > 0 \text{ and } n \geq 2), \quad (A3)$$

$$\int_{|k|<b} d^3k \frac{Z_\eta(k)}{k^{2n+1}} (k) = 0 \quad (s \leq 2n - 3), \quad (A4)$$

$$\int_{|k|<b} d^3k \frac{Z_\eta(k)}{k^{2n+1}} (k) = 0 \quad (A5)$$

where $p^{(s)}(k)$ is any homogeneous polynomial of $k$ with degree $s (\neq 0, 1, 2, \ldots)$. $Z/k^2$ 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 \((n = 1, 2, 3, \ldots)\):

\[
\int \frac{d^3k}{(2\pi)^3} \frac{Z}{k^{2n+1}} e^{ik \cdot r} = (-1)^{n+1} \frac{r^{2n-3}}{4\pi(2n-2)!},
\]

(A6)

\[
\lim_{\eta \to 0^+} \int d^3r \frac{(-1)^{n+1}r^{2n-3}}{4\pi(2n-2)!} e^{-ik \cdot r - \eta r} = \frac{Z}{k^{2n+1}},
\]

(A7)

\[
\int \frac{d^3k}{(2\pi)^3} \frac{Z_b(k)}{k^{2n+1}} e^{ik \cdot r} = F_b^{(n)}(r),
\]

(A8)

\[
\lim_{\eta \to 0^+} \int d^3r F_b^{(n)}(r) e^{-ik \cdot r - \eta r} = \frac{Z_b(k)}{k^{2n+1}},
\]

(A9)

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

where \(\gamma = 0.5772 \ldots\) is Euler’s constant.

\[\frac{Z_b(k)}{k^{2n+1}} = \frac{4\pi \ln(b'/b)}{(2n-1)!} \nabla_k^{2n-2} \delta(k),\]

(A10)

\[\frac{Z_b(ck)}{c(ck)^{2n+1}} = \frac{1}{c^{2n+1}} \frac{Z_b(k)}{k^{2n+1}} \text{ (constant } c > 0)\]

(A11)

APPENDIX B: Z-\(\delta\) EXPANSIONS

Example 1. Consider the expansion of \((k^2 + 3q^2/4)^{-1}\) at small \(q\). Naively, it is \(1/k^2 - 3q^2/(4k^4) + O(q^4)\). But this series fails around \(k = 0\). In particular, \(R_0(k, q) = (k^2 + 3q^2/4)^{-1} - 1/k^2\) has a finite integral over all \(k\):

\[
\int \frac{d^3k}{(2\pi)^3} R_0(k, q) = -\frac{\sqrt{3}}{8\pi} q^2, \text{ but the integral of } -3q^2/(4k^4) \text{ over all } k \text{ is infinite.}
\]

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

\[R_1(k, q) = \frac{-3q^2}{4} Z k^4\]

where \(Z/k^4\) is defined in Appendix A. Further subtracting \(-3q^2 Z/(4k^4)\) from \(R_1(k, q)\), we get a remainder \(\approx (\sqrt{3}/64\pi) q^3 \nabla_k^3 \delta(k)\). 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: first Fourier transform it for fixed \(q\), to obtain \(\exp(-\sqrt{3}qr/2)/(4\pi r)\), then expand it in powers of \(q^6\):

\[
1 - \frac{\sqrt{3} q^2}{8\pi} + \frac{3q^4}{32\pi} \left( \frac{\sqrt{3} q^2}{64\pi} r^2 - \frac{3q^4}{512\pi} r^4 \right) + O(q^6),
\]

and finally transform the series back to the \(k\)-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 \(k\) in this paper can not be found analytically.

Example 2 [needed in deriving Eq. (35)]. At small \(q\):

\[(k + q/2)^{-1} + (k - q/2)^{-1}/(k^2 + 3q^2/4)\]

\[= 2Z_0(k)/k^3 + \left[ 8\pi - 4\pi^2/\sqrt{3} - 8\pi \ln(q/n) \right] \delta(k) + O(q^6),\]

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

**Generics.** Consider a function \(F(k, o)\) (where \(o\) are a set of variables), with a finite integral over any finite region of the \(k\)-space for \(o \neq 0\), and a unique singularity at \(k = 0\) for \(o \to 0\). The \(Z-\delta\) expansion is of the form \(F(k, o) = F_Z(k, o) + F_0(k, o)\), where \(F_Z\) is a series including ordinary and/or \(Z\) functions of \(k\) and may be directly inferred from the Taylor expansion of \(F(k, o)\) at small \(o\), and

\[
F_b(k, o) = \sum_{m_j} c_{m_j} o^{\delta^m} (\nabla_k^m \delta(k))^{(2\pi)^3}(2\pi)^3 (2\pi)^3 (2\pi)^3 \delta(k),
\]

(B1a)

\[
c_{m_j} o^{\delta^m} (\nabla_k^m \delta(k))^{(2\pi)^3}(2\pi)^3 (2\pi)^3 \delta(k)\]

(B1b)

Here \(Q^{(j)}\) are all the independent homogeneous harmonic polynomials, satisfying \(\int Q^{(j)}(k)\delta(k)d^3k = 0\) for \(j \neq j'\). The degree of \(Q^{(j)}\) is \(l_j\).

If \(F(k, o)\) is rotationally invariant around an axis \(q\), only \(Q^{(j)}\) are needed above, and the coefficient before the integral sign in Eq. (B1b) becomes \(\gamma_j (2\pi)^3 (2\pi)^3 (2\pi)^3 \delta(k)\).

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

\[
Q^{(j)}(v) = v_x^j + v_y^j + v_z^j - 3(v_x^j v_y^j + v_x^j v_z^j + v_y^j v_z^j),
\]

(B2a)

\[
Q^{(j)}(v) = v_x^j + v_y^j + v_z^j - (15/2)(v_x^j v_y^j + v_x^j v_z^j + v_y^j v_z^j) + v_x^j v_y^j + v_y^j v_z^j + 9v_x^j v_z^j,
\]

(B2b)

\[
Q^{(j)}(v) = v_x^j + v_y^j + v_z^j - 14(v_x^j v_y^j + v_x^j v_z^j + v_y^j v_z^j) + v_x^j v_y^j + v_y^j v_z^j + 35(v_x^j v_y^j + v_y^j v_z^j + v_z^j v_x^j).
\]

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-\(n\) asymptotics of the summands).

To evaluate a lattice sum \(\sum_n X(n)\) (sum over \(3\)-vectors of integers), where \(X(n)\), as a continuous function, has both singularity in the real-\(n\) space and a power-law tail at large \(n\), we sometimes break \(X(n)\) in two pieces: \(X(n) = X_1(n) + X_2(n)\), such that \(X_1(n)\) has singularity but no power-law tail (i.e., decays much more rapidly at large \(n\)), while \(X_2(n)\) has power-law tail but is sufficiently smooth. \(\sum_n X_1(n)\) is done directly, while \(\sum_{n=1}^{\infty} X_2(n)\) is approximated by \(\int d^3n X_2(n)\) to a very high precision. We call this method tail-singularity separation (TSS).

For instance, to compute \(O_s\) \((s = 1, 2, 3, \ldots)\), we write \(n^{-2s} = \sum_{i=0}^{s-1} (m^2)^i \exp(-m^2) + X_2(n)\), where \(\eta > 0\) is small. \(X_2(n)\) is very smooth, so \(\sum_{n=1}^{\infty} X_2(n)\) is approxi-
mated by an integral. Straightforward algebra yields
\[ \alpha_s = c_s \pi^{3/2} \eta s^{-3/2} - \frac{\eta^2}{s!} + \sum_{n=0}^{\infty} \frac{(\eta n)^2}{n!} e^{-\eta n^2} \]
\[ + O(e^{-\eta^2/n}), \]  
(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 \( \sim O((e^{-\eta^2/n}) \) results from
the approximation \( \sum_{n=0}^{\infty} X_2(n) \approx \int d^3 n X_2(n) \) [35].
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 acceleration
method. For example, \( \sum_{n \neq 0} n^{-3} / \) is not sufficiently acceler-
ated by an integral. Straightforward algebra yields
\( \sum_{n \neq 0} n^{-3} \approx \int d^3 n X_2(n) \) [35].
Equation (C1) applies to both \( s = 1 \) and \( s = 2, 3, \ldots \).

Using the Poisson summation formula and the TSS method, we get
\[ \alpha_{5,5}^{(g)} = -(2^{6} \pi^5 / 9!) \sum_{n \neq 0} Q^{(g)}(n) \bar{I}(\eta n) + O(e^{-\eta^2/n}), \]  
(C5a)
\[ \alpha_{7,5}^{(i)} = (2^{8} \pi^7 / 13!) \sum_{n \neq 0} Q^{(i)}(n) \bar{I}(\eta n) + O(e^{-\eta^2/n}), \]  
(C5b)
\[ \alpha_{9,5}^{(s)} = -(2^{10} \pi^9 / 17!) \sum_{n \neq 0} Q^{(s)}(n) \bar{I}(\eta n) + O(e^{-\eta^2/n}), \]  
(C5c)
where \( \bar{I}(x) \equiv \ln [\tanh (\frac{x}{2} \sinh x)] \).

Using the Poisson summation formula, we get
\[ W_A(n) = -\sqrt{3} \pi^2 n + \pi \sum_{m \neq 0} e^{-\sqrt{3} \pi mn - i \pi m n / m}, \]  
(C6a)
\[ W_B(n) = (2 \pi^2 / \sqrt{3}) \sum_{m \neq 0} e^{-\sqrt{3} \pi mn - i \pi m n} \]  
(C6b)
For $\alpha_{1A1}$, $\alpha_{2A1}$, and $\alpha_{1B1}$, we thus have

$$\alpha_{sA1} = \pi^2 w_{0.5+s} + 2\alpha_{1}\alpha_{1+s} + 4\alpha_{2+s}/3 + 4\alpha_{1}^{(g)}(g)/15 + 4\alpha_{1}^{(i)}\alpha_{7+s}/231 + 4\alpha_{1}^{(i)}\alpha_{9+s}/195 + \sum_{n\neq 0} n^{-2}\left[\rho_{A1}(n) - \rho_{A1}^{(11)}(n)\right],$$  \hspace{1cm} (C8a)

$$\alpha_{1B1} = 2\sqrt{3}\pi^2\omega_{2.5} + 2\alpha_{1}\omega_{3} + 2\alpha_{4} + 4\alpha_{1}^{(g)}\alpha_{7}/3 + 4\alpha_{1}^{(i)}\alpha_{9}/65 + \sum_{n\neq 0} n^{-2}\left[\rho_{B1}(n) - \rho_{B1}^{(13)}(n)\right],$$  \hspace{1cm} (C8b)

and the sums over $n$ 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

$$\tilde{\alpha}_{1A1} = -\alpha_{1A1} - \pi^3 w(7\pi/\sqrt{3} - 8)\alpha_{1} + 8\pi^3 w_{0.1} \ln(2\pi) - \alpha_{1} \alpha_{A1} + 3\alpha_{A2} + 3\alpha_{B1} - (\alpha_2 + 6\alpha_{1}\alpha_{3} - 9\alpha_{4}),$$

$$\alpha_{1A1} = \lim_{N\to\infty} \sum_{n\neq 0; n < N} n^{-2}\rho_{A1}(n) - 8\pi^3 w_{0.1} \ln N$$

$$+ 4\pi^4 w N (8 \ln N - 16 + 7\pi/\sqrt{3}).$$  \hspace{1cm} (C10)

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

$$\alpha_{1A1} = \lim_{N\to\infty} \sum_{n\neq 0; n < N} \rho_{A1}^2(n) - 4\pi^5 w^2 N - 16\pi^3 w_{0.1} \ln N.$$  \hspace{1cm} (C11)

At large $n$ we derive from Eq. (C7a)

$$\rho_{A1}^2(n) = K^{(12)}(n) + O(n^{-13}),$$  \hspace{1cm} (C12)

where the sum over $n$ converges very rapidly; truncating it at $|n_x|, |n_y|, |n_z| \leq 15$ we obtain the result for $\alpha_{1A1}$ with 18-digit precision.

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

1-fold lattice sums (rounded to fit the 2-column format):

| $\alpha_1$ | -8.913 632 917 585 151 272 687 120 136 |
| $\alpha_{1.5}$ | 3.821 923 503 940 635 799 730 123 034 |
| $\alpha_2$ | 16.532 315 599 761 669 643 892 704 593 |
| $\alpha_{2.5}$ | 10.377 524 830 847 083 864 728 948 355 |
For any two-body potential $V$, the following equations hold:

\[ \alpha_3 = 8.401 \times 10^2 827 539 993 146 138 987, \]  
\[ \alpha_4 = 6.945 807 922 266 369 624 170 778 023, \]  
\[ \alpha_6 = 6.292 149 045 047 128 551 930 416 392, \]  
\[ \alpha_7 = 1.127 575 148 686 792 075 014 583 731, \]  
\[ \alpha_8^{(o)} = 5.672 650 625 242 259 129 524 572 370, \]  
\[ \alpha_8^{(p)} = 5.772 772 158 341 296 181 095 291 055, \]  
\[ \alpha_8^{(q)} = 5.594 443 615 615 246 912 541 646 623, \]  
\[ \alpha_8^{(i)} = -2.434 385 049 385 522 287 574 679 853, \]  
\[ \alpha_7^{(i)} = 5.242 702 841 443 828 214 862 689 624, \]  
\[ \alpha_8^{(i)} = 5.391 072 910 162 494 739 294 958, \]  
\[ \alpha_9^{(i)} = 5.175 464 651 152 249 495 454 861 607, \]  
\[ \alpha_9^{(i)} = 16.571 410 717 431 131 178 469 668 510, \]  
\[ \alpha_9^{(i)} = 6.156 579 477 795 506 959 879 789 010, \]  
\[ \alpha_{10}^{(i)} = 6.109 685 927 989 065 132 252 619 095, \]  
\[ \alpha_{11}^{(i)} = 6.054 088 533 916 337 242 283 438 742. \]

2-fold lattice sums:

\[ \alpha_{1A1} = -190.172 897 984 865 754 8, \]  
\[ \alpha_{1A2} = 221.523 005 675 695 107 22, \]  
\[ \alpha_{1A1} = -659.229 842 103 439 89. \]

3-fold lattice sums:

\[ \alpha_{1A1}^{(a)} = -2996.889 395 378 764 86, \]  
\[ \alpha_{1A1}^{(b)} = -6591.229 842 103 439 89. \]

Finally, from Eq. (C6a) we get

\[ \beta_{1A} = -\sqrt{3} \pi^2 \alpha_{0.5} + \pi \sum_{n,m=0}^{\infty} e^{-\sqrt{3} \pi (m-n)^2/2} / n. \]

\[ = 48.614 754 175 227 821 038 934 419 912. \]

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

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[11] The $|a|$ in $<n|a|k|$ ensures that Eq. (3) is also valid for $\alpha < 0$.
[12] The first term in this expansion was first found by P. Price, thesis, Cambridge University, Cambridge, 1951 (unpublished); the second and third terms found by Huang and Yang for $N$ particles [20], although numerical coefficients were inexact; the term $\propto L^{-6} \ln L$ was discovered by Wu [4].
[13] For any two-body potential $V(r)$, $U_{k_1k_2k_3k_4} = \sum_{r=0}^{\infty} e^{ik_1r}V(r)e^{ik_2r}$, where $k_1 + k_2 \equiv k_3 + k_4$, and $\overline{V}_k = \frac{1}{2\pi} V(r)e^{ikr}$.
[14] These functions can be obtained from the wave function of the two-body $l$-wave scattering state at energy $E \rightarrow 0$: $\phi_{nk}(l,E) = \phi_{nk}^{(E)} + E\phi_{nk}^{(g)} + O(E^2)$, whose amplitude is defined by $\sum_{n,m=0}^{\infty} e^{-\sqrt{3} \pi (m-n)^2/2} / n$. 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 $Q_n^{(l)}$ is defined by Eq. (10).
[15] Note that $Q_n^{(l)}(\nabla k)(2\pi)^3 \delta(k)$ scales with $k$ like $k^{-3-\epsilon}$.
[16] It can be shown that $\alpha$ and $r_s$ are real.
[17] The vector sum of the three subscripts of $\phi^{(3)}$ is fixed as zero.
[18] Using the expansion formulas for $\phi_k$ and $\phi^{(3)}_{k-k,0} = \phi^{(3)}_{k,k,0}$ at small $k$, and noting that $\int_{k,k_0} U_{k,k_0} dk_0$ are smooth functions of $k_0$, one can readily verify that Eqs. (36a) and (36c) are compatible.
[19] Although $U_{k,k_0}$ 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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