

Calculations of long-range three-body interactions for $\text{He}(n_0^\lambda S)\text{-He}(n_0^\lambda S)\text{-He}(n_0^\lambda L)$

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We theoretically investigate long-range interactions between an excited L -state He atom and two identical S -state He atoms for the cases of the three atoms all in spin-singlet states or all in spin-triplet states, denoted by $\text{He}(n_0^\lambda S)\text{-He}(n_0^\lambda S)\text{-He}(n_0^\lambda L)$, with n_0 and n_0' principal quantum numbers, $\lambda = 1$ or 3 the spin multiplicity, and L the orbital angular momentum of a He atom. Using degenerate perturbation theory for the energies up to second-order, we evaluate the coefficients C_3 of the first-order dipolar interactions and the coefficients C_6 and C_8 of the second-order additive and nonadditive interactions. Both the dipolar and dispersion interaction coefficients, for these three-body degenerate systems, show dependences on the geometrical configurations of the three atoms. The nonadditive interactions start to appear in second-order. To demonstrate the results and for applications, the obtained coefficients C_n are evaluated with highly accurate variationally generated nonrelativistic wave functions in Hylleraas coordinates for $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1S)$, $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1P)$, $\text{He}(2^1S)\text{-He}(2^1S)\text{-He}(2^1P)$, and $\text{He}(2^3S)\text{-He}(2^3S)\text{-He}(2^3P)$. The calculations are given for three like nuclei for the cases of hypothetical infinite mass He nuclei, and of real finite mass ^4He or ^3He nuclei. The special cases of the three atoms in equilateral triangle configurations are explored in detail, and for the cases in which one of the atoms is in a P state, we also present results for the atoms in an isosceles right triangle configuration or in an equally spaced collinear configuration. The results can be applied to construct potential energy surfaces for three helium atom systems.

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I. INTRODUCTION

We recently demonstrated for the case of three Li atoms with two atoms in their ground states and one atom in the first excited P state that their long-range (i.e., atoms sufficiently separated that electron exchange is negligible) interactions exhibit a first-order interaction potential that is dependent on the geometrical configuration of the atoms, and that in second order additive and nonadditive dispersion interactions appear in Ref. [1]. These long-range interactions are in sharp contrast to the case of three ground-state atoms, where geometric-configuration nonadditive dispersion interactions (sometimes called Axilrod-Teller-Muto terms) appear in third order; cf. Ref. [2]. Our results provide accurate long-range potential energies of electronically excited Li trimers, and the results may be useful in the analysis of processes such as optical blockade effects [3] and cooperative spontaneous emission [4], where long-range dipole-dipole interactions among several atoms appear.

In the present paper, we extend the theory of Ref. [1] to the case of three He atoms. We investigate the long-range interactions between an excited L -state He atom and two identical S -state He atoms, for the cases of the three atoms all in spin-singlet states or all in spin-triplet states, denoted by $\text{He}(n_0^\lambda S)\text{-He}(n_0^\lambda S)\text{-He}(n_0^\lambda L)$, with n_0 and n_0' principal quantum

numbers, $\lambda = 1$ or 3 the spin multiplicity, and L the orbital angular momentum of a He atom.

Interactions between three ground-state He atoms were studied extensively, and elaborate calculations of three-body interactions, including dispersion interactions contributions, are available (see, for example, Ref. [5] and references therein). The three-ground state He-atom calculations are valuable for modeling liquid ^4He and solid He [6], for recombination and scattering studies [7], investigations of Efimov states [7,8], and thermophysics [5].

Rare-gas metastable helium atoms have been widely used in many studies [9], such as photoassociation spectroscopy [10], metastable loss in magneto-optical traps [11], Penning ionization [12–15], and associative ionization [11]. Indeed, the three-body loss rate in a $^4\text{He}(2^3S)$ Bose-Einstein condensate was measured providing evidence from the trimer system $^4\text{He}_3(2^3S)$ for a universal three-body parameter [16]. For the case of two metastable He atoms, with one atom in an excited P -state level, the first-order resonant dipole-dipole interaction produces an interatomic potential varying as C_3/R^3 , where the corresponding coefficients C_3 for weakly bound dimers of helium atoms were given in many papers (see Refs. [17,18] and references therein). However, due to the degeneracy, these coefficients may not be used in the study of helium clusters or the study of atom-molecule and molecule-molecule collision that involve a P -state atom. This is because when a helium excited dimer turns into an excited trimer or a cluster involving excited atoms, the interactions between atoms are changed due

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to quantum many-body effects. So to proceed with calculations of molecular He_n^* excimer potential energy surfaces, investigations of the long-range multibody interactions are warranted. For example, early work by Phelps [19] studying the destruction of $\text{He}(2^3S)$ atoms using absorption measurements in a discharge found evidence for the formation of metastable helium dimers through the reaction $\text{He}(2^3S) + \text{He}(1^1S) + \text{He}(1^1S)$ and evidence that the three-body interaction between a bound $\text{He}_2(2^3\Sigma)$ molecule and a $\text{He}(1^1S)$ atom may be “repulsive or, at most, weakly attractive.” However, trimer excited potential energy calculations were not available at the time, and, to date, may still be unavailable, making interpretations based on collisional dynamics uncertain. Later studies, however, confirm the importance and complexity (see Ref. [20] and references therein) of the kinetics between the $\text{He}(2^3S)$ atoms and the vibrationally excited $\text{He}_2(a^3\Sigma_u)$ molecules. Further work, such as we present here, concerning the long-range interactions of combinations of three He atoms when at least one is metastable, is desirable, and it may lead to an understanding of various recombination and scattering processes.

In this work, we present our research on long-range interactions for three like helium atoms involving at least one atom in an excited state. Using variationally optimized nonrelativistic atomic helium wave functions in Hylleraas coordinates, we present our theoretical calculations of long-range interaction coefficients for $\text{He}(n_0^\lambda S)\text{-He}(n_0^\lambda S)\text{-He}(n_0^\lambda L)$ considering the energetically lowest five states: $\text{He}(1^1S)$, $\text{He}(2^3S)$, $\text{He}(2^1S)$, $\text{He}(2^3P)$, and $\text{He}(2^1P)$. We present the additive “dipolar” interaction coefficients C_3 and additive dispersion interaction coefficients C_6 , C_8 that enter, respectively, in first- and second-order perturbation theory. We also evaluate the second-order nonadditive dispersion interactions coefficients C_6 , C_8 that contain a dependence on the geometrical configuration of the three atoms. In addition, the coefficients are given explicitly and as numerical values for the three basic geometrical

configurations of the nuclei in an equilateral triangle, in an isosceles right triangle, or equally spaced collinearly. Finally, long-range potentials in the sum of first- and second-order energies for these three geometrical configurations are given (see Fig. 1).

Due to the quantum three-body effect, both the dipolar and dispersion interaction coefficients, for the degenerate $\text{He}(n_0^\lambda S)\text{-He}(n_0^\lambda S)\text{-He}(n_0^\lambda L)$ system, show a dependence on the geometrical configurations of the three atoms. In the present work, the coefficients obtained are given for three very common configurations. We also discuss the connection of this degenerate three-body system with the nondegenerate three-body system and the three-body atom-molecule system, which could be used in the study of three-body recombination or ultracold atom-molecule collisions.

II. THEORETICAL FORMULATION

In this paper, atomic units are used throughout. The three atoms are labeled by I , J , and K , with, respectively, internal coordinates σ , ρ , and ζ . When the labels I , J , or K appear, it is understood that cyclic permutation can be used.

In the present work, we take the electrostatic interactions V_{123} between pairs of atoms for the $\text{He}(n_0^\lambda S)\text{-He}(n_0^\lambda S)\text{-He}(n_0^\lambda L)$ system as a perturbation,

$$H' = V_{123} = V_{12} + V_{23} + V_{31}, \quad (1)$$

with V_{12} , V_{23} , and V_{31} the two-body mutual electrostatic interactions between atoms 1, 2, and 3. According to degenerate perturbation theory, the zeroth-order wave function of the unperturbed system can be written as

$$|\Psi^{(0)}\rangle = a|\phi_1\rangle + b|\phi_2\rangle + c|\phi_3\rangle, \quad (2)$$

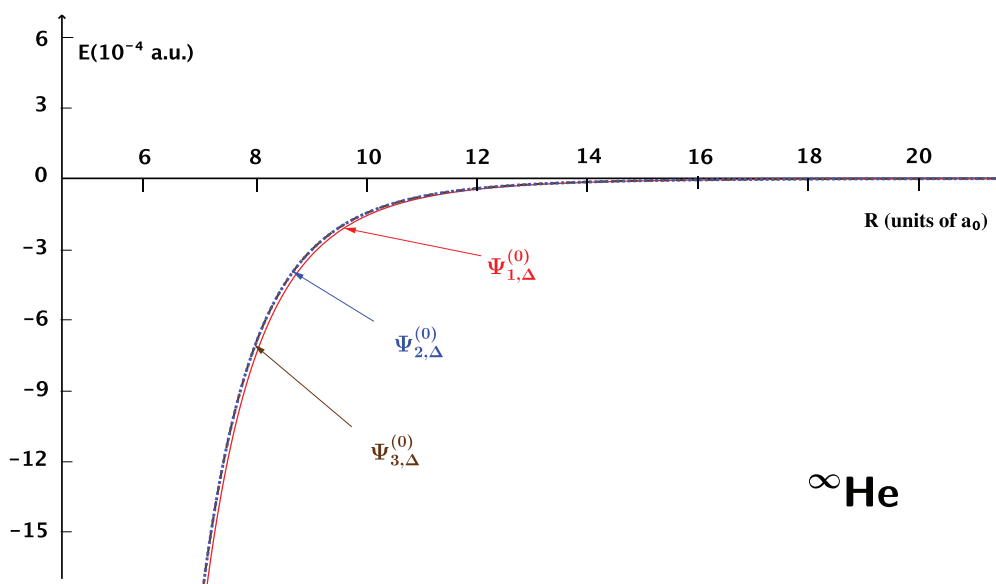


FIG. 1. Long-range potentials for the $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1S)$ system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. For each curve labeled by a wave function, the plotted curve is the sum of $\Delta E^{(1)}$ and $\Delta E^{(2)}$, where $\Delta E^{(1)} = 0$.

where ϕ_1 , ϕ_2 , and ϕ_3 are three orthogonal eigenvectors corresponding to the same energy eigenvalue $E_{n_0 n_0 n_0'}^{(0)} = 2E_{n_0 S}^{(0)} + E_{n_0' L}^{(0)}$,

$$|\phi_1\rangle = |\varphi_{n_0'}(LM; \sigma)\varphi_{n_0}(0; \rho)\varphi_{n_0}(0; \zeta)\rangle, \quad (3)$$

$$|\phi_2\rangle = |\varphi_{n_0}(0; \sigma)\varphi_{n_0'}(LM; \rho)\varphi_{n_0}(0; \zeta)\rangle, \quad (4)$$

$$|\phi_3\rangle = |\varphi_{n_0}(0; \sigma)\varphi_{n_0}(0; \rho)\varphi_{n_0'}(LM; \zeta)\rangle. \quad (5)$$

The expansion coefficients a , b , and c are determined by diagonalizing the perturbation in the basis set $\{\phi_1, \phi_2, \phi_3\}$, which depends on the geometrical configuration formed by the three atoms. In the following, we show that all the dispersion interaction coefficients contain some or all of these three

expansion coefficients a , b , and c leading to dependences on the configuration of the three atoms.

For three well-separated helium atoms, the mutual interaction energy V_{IJ} can be expanded according to Refs. [2,21],

$$V_{IJ} = \sum_{l_I l_J} \sum_{m_I m_J} T_{l_I - m_I}(\sigma) T_{l_J m_J}(\rho) W_{l_I l_J}^{m_I - m_J}(IJ). \quad (6)$$

In Eq. (6), the multipole transition operators are

$$T_{l_I - m_I}(\sigma) = \sum_{i=1}^3 Q_i \sigma_i^{l_I} Y_{l_I - m_I}(\hat{\sigma}_i), \quad (7)$$

$$T_{l_J m_J}(\rho) = \sum_{j=1}^3 q_j \rho_j^{l_J} Y_{l_J m_J}(\hat{\rho}_j), \quad (8)$$

where Q_i and q_j are the charges of the i th and j th particles of the atoms I and J , respectively. The geometry factor is

$$W_{l_I l_J}^{m_I - m_J}(IJ) = \frac{4\pi(-1)^{l_I}}{R_{IJ}^{l_I + l_J + 1}} \frac{(l_I + l_J - m_I + m_J)!(l_I, l_J)^{-1/2}}{[(l_I + m_I)!(l_I - m_I)!(l_J + m_J)!(l_J - m_J)!]^{1/2}} P_{l_I + l_J}^{m_I - m_J}(\cos \theta_{IJ}) \exp[i(m_I - m_J)\Phi_{IJ}], \quad (9)$$

where $\mathbf{R}_{IJ} = \mathbf{R}_J - \mathbf{R}_I$ is the relative position vector from atom I to atom J , the notation $(l_I, l_J, \dots) = (2l_I + 1)(2l_J + 1) \dots$, and $P_{l_I + l_J}^{m_I - m_J}(\cos \theta_{IJ})$ is the associated Legendre function with θ_{IJ} representing the angle between \mathbf{R}_{IJ} and the z axis. If we now choose the z axis to be normal to the plane of the three atoms, giving $\theta_{12} = \theta_{23} = \theta_{31} = \pi/2$, the associated Legendre functions can be simplified as

$$P_l^m(0) = \frac{1}{2^{l+1}} [1 + (-1)^{l+m}] (-1)^{\frac{l+m}{2}} (l+m)! \times \left[\left(\frac{l+m}{2} \right)! \right]^{-1} \left[\left(\frac{l-m}{2} \right)! \right]^{-1}. \quad (10)$$

Φ_{IJ} denotes the angle between \mathbf{R}_{IJ} and the x axis. It shows the dependence of the mutual dipole-dipole interaction between two atoms on the orientation of the interacting dipoles relative to the line connecting them [22]. Similar expressions result for V_{JK} and V_{KI} . For simplicity, in this work, we transfer all these Φ_{IJ} into interior angles (α, β, γ) of the triangle formed by the three helium atoms with the same method as used in Ref. [1].

A. The formulas for He(1¹S)-He(1¹S)-He(2¹S)

1. The first-order energy

According to the perturbation theory, the first-order energy correction for the He(1¹S)-He(1¹S)-He(2¹S) system is

$$\Delta E^{(1)} = \langle \Psi^{(0)} | V_{123} | \Psi^{(0)} \rangle = \sum_{l_I, l_J} \left(\frac{C_n^{(12)}}{R_{12}^n} + \frac{C_n^{(23)}}{R_{23}^n} + \frac{C_n^{(31)}}{R_{31}^n} \right), \quad (11)$$

and the corresponding interaction coefficients are

$$C_n^{(IJ)} = |A_I|^2 \mathbb{B}_0^{(IJ)} + (A_I^* A_J + A_J^* A_I) \mathbb{B}_1^{(IJ)}, \quad (12)$$

where

$$A_1 = a, A_2 = b, A_3 = c, \quad (13)$$

$$\mathbb{B}_0^{(IJ)} = \sum_{m_I m_J} W_{l_I l_J}^{m_I - m_J}(IJ) R_{IJ}^{l_I + l_J + 1} \begin{pmatrix} 0 & l_I & 0 \\ 0 & -m_I & 0 \end{pmatrix} \begin{pmatrix} 0 & l_J & 0 \\ 0 & m_J & 0 \end{pmatrix} \times \langle \varphi_{n_0}(0; \sigma) \| T_{l_I}(\sigma) \| \varphi_{n_0}(0; \sigma) \rangle \times \langle \varphi_{n_0}(0; \rho) \| T_{l_J}(\rho) \| \varphi_{n_0}(0; \rho) \rangle, \quad (14)$$

and

$$\mathbb{B}_1^{(IJ)} = \sum_{m_I m_J} W_{l_I l_J}^{m_I - m_J}(IJ) R_{IJ}^{l_I + l_J + 1} \begin{pmatrix} 0 & l_I & 0 \\ 0 & -m_I & 0 \end{pmatrix} \begin{pmatrix} 0 & l_J & 0 \\ 0 & m_J & 0 \end{pmatrix} \times \langle \varphi_{n_0}(0; \sigma) \| T_{l_I}(\sigma) \| \varphi_{n_0'}(0; \sigma) \rangle \times \langle \varphi_{n_0'}(0; \rho) \| T_{l_J}(\rho) \| \varphi_{n_0}(0; \rho) \rangle. \quad (15)$$

From the 3 - j symbols above, one has $l_I=0, m_I=0, l_J=0$, and $m_J = 0$. Thus

$$\sum_{i=1}^3 Q_i \sigma_i^{l_I} Y_{l_I, m_I}(\hat{\sigma}_i) = \frac{1}{\sqrt{4\pi}} \sum_{i=1}^3 Q_i = 0, \quad (16)$$

$$\sum_{j=1}^3 q_j \rho_j^{l_J} Y_{l_J, m_J}(\hat{\rho}_j) = \frac{1}{\sqrt{4\pi}} \sum_{j=1}^3 q_j = 0. \quad (17)$$

Thus $\mathbb{B}_0^{(IJ)} = \mathbb{B}_1^{(IJ)} = 0$ and

$$\Delta E^{(1)} = 0. \quad (18)$$

2. The second-order energy

The second-order energy correction for the He(1 1S)-He(1 1S)-He(2 1S) system can be written as

$$\Delta E^{(2)} = - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \frac{|\langle \Psi^{(0)} | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\zeta}) \rangle|^2}{E_{n_s L_s; n_t L_t; n_u L_u} - E_{n_0 S; n_0 S; n_0 S}^{(0)}} = - \sum_{n \geq 3} \left(\frac{C_{2n}^{(12)}}{R_{12}^{2n}} + \frac{C_{2n}^{(23)}}{R_{23}^{2n}} + \frac{C_{2n}^{(31)}}{R_{31}^{2n}} \right), \quad (19)$$

where $\chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\zeta})$ is an intermediate state of the system with the energy eigenvalue $E_{n_s L_s; n_t L_t; n_u L_u} = E_{n_s L_s} + E_{n_t L_t} + E_{n_u L_u}$. It is noted that the above summations should exclude terms with $E_{n_s L_s; n_t L_t; n_u L_u} = E_{n_0 S; n_0 S; n_0 S}^{(0)}$. $C_{2n}^{(12)}$, $C_{2n}^{(23)}$, and $C_{2n}^{(31)}$ are the additive dispersion coefficients. In this work, we are only concerned with $n = 3$ and 4 in Eq. (19). The corresponding dispersion coefficients are

$$C_6^{(IJ)} = (|A_I|^2 + |A_J|^2) \mathbb{T}_1 + |A_K|^2 \mathbb{T}_2 + (A_I^* A_J + A_J^* A_I) \mathbb{T}_3, \quad (20)$$

$$C_8^{(IJ)} = (|A_I|^2 + |A_J|^2) \mathbb{R}_1 + |A_K|^2 \mathbb{R}_2 + (A_I^* A_J + A_J^* A_I) \mathbb{R}_3, \quad (21)$$

$$A_1 = a, \quad A_2 = b, \quad A_3 = c, \quad (22)$$

where a , b , and c are defined in Eq. (2). The other terms in Eqs. (20) and (21) are given by

$$\mathbb{T}_1 = \sum_{n_s n_t} K_1(n_s, n_t, 1, 1), \quad (23)$$

$$\mathbb{T}_2 = \sum_{n_s n_t} K_2(n_s, n_t, 1, 1), \quad (24)$$

$$\mathbb{T}_3 = \sum_{n_s n_t} K_3(n_s, n_t, 1, 1), \quad (25)$$

$$\mathbb{R}_1 = \sum_{n_s n_t} [K_1(n_s, n_t, 1, 2) + K_1(n_s, n_t, 2, 1)], \quad (26)$$

$$\mathbb{R}_2 = \sum_{n_s n_t} [K_2(n_s, n_t, 1, 2) + K_2(n_s, n_t, 2, 1)], \quad (27)$$

and

$$\mathbb{R}_3 = \sum_{n_s n_t} [K_3(n_s, n_t, 1, 2) + K_3(n_s, n_t, 2, 1)]. \quad (28)$$

The K_i functions are defined by Eqs. (A13)–(A15) in Appendix A.

B. The formulas for He($n_0^\lambda S$)-He($n_0^\lambda S$)-He($n_0^\lambda P$)

1. The first-order energy

According to the perturbation theory, the first-order energy correction for the He($n_0^\lambda S$)-He($n_0^\lambda S$)-He($n_0^\lambda P$) system is

$$\Delta E^{(1)} = \langle \Psi^{(0)} | V_{123} | \Psi^{(0)} \rangle = - \frac{C_3^{(12)}(1, M)}{R_{12}^3} - \frac{C_3^{(23)}(1, M)}{R_{23}^3} - \frac{C_3^{(31)}(1, M)}{R_{31}^3}, \quad (29)$$

where

$$C_3^{(IJ)}(1, M) = (A_I^* A_J + A_J^* A_I) \mathbb{D}_0(M), \quad (30)$$

$$A_1 = a, \quad A_2 = b, \quad A_3 = c, \quad (31)$$

and

$$\mathbb{D}_0(M) = \frac{4\pi(-1)^{1+M}}{9(1-M)!(1+M)!} \left| \langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_1(\boldsymbol{\sigma}) \| \varphi_{n_0'}(1; \boldsymbol{\sigma}) \rangle \right|^2, \quad (32)$$

where a , b , and c are defined in Eq. (2). It should be mentioned that there exist only additive long-range interaction terms at this order of perturbation.

2. The second-order energy

The second-order energy correction for the He($n_0^\lambda S$)-He($n_0^\lambda S$)-He($n_0^\lambda P$) system can be written as

$$\Delta E^{(2)} = - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \frac{|\langle \Psi^{(0)} | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\zeta}) \rangle|^2}{E_{n_s L_s; n_t L_t; n_u L_u} - E_{n_0 S; n_0 S; n_0 L}^{(0)}} = - \sum_{n \geq 3} \left(\frac{C_{2n}^{(12)}(1, M)}{R_{12}^{2n}} + \frac{C_{2n}^{(23)}(1, M)}{R_{23}^{2n}} + \frac{C_{2n}^{(31)}(1, M)}{R_{31}^{2n}} + \frac{C_{2n}^{(12,23)}(1, M)}{R_{12}^n R_{23}^n} + \frac{C_{2n}^{(23,31)}(1, M)}{R_{23}^n R_{31}^n} + \frac{C_{2n}^{(31,12)}(1, M)}{R_{31}^n R_{12}^n} \right), \quad (33)$$

where $\chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\zeta})$ is an intermediate state of the system with the energy eigenvalue $E_{n_s L_s; n_t L_t; n_u L_u} = E_{n_s L_s} + E_{n_t L_t} + E_{n_u L_u}$. It is noted that the above summations should exclude terms with $E_{n_s L_s; n_t L_t; n_u L_u} =$

$E_{n_0 S; n_0 S; n_0 L}^{(0)}$. $C_{2n}^{(12)}(1, M)$, $C_{2n}^{(23)}(1, M)$, and $C_{2n}^{(31)}(1, M)$ are the additive dispersion coefficients, and $C_{2n}^{(12,23)}(1, M)$, $C_{2n}^{(23,31)}(1, M)$, and $C_{2n}^{(31,12)}(1, M)$ are the nonadditive dispersion

TABLE I. Values of \mathbb{T}_1 , \mathbb{T}_2 , \mathbb{T}_3 , \mathbb{R}_1 , \mathbb{R}_2 , and \mathbb{R}_3 for the He(1^1S)-He(1^1S)-He(2^1S) system, in atomic units. All these quantities are independent of the geometrical configuration formed by the three atoms. The numbers in parentheses represent the computational uncertainties.

Atom	\mathbb{T}_1	\mathbb{T}_2	\mathbb{T}_3	\mathbb{R}_1	\mathbb{R}_2	\mathbb{R}_3
$^\infty\text{He}$	41.8413161(1)	1.4609778377(1)	2.90911603(1)	3310.4418(1)	14.11785735(1)	96.090681(2)
^4He	41.8723173(1)	1.4621228531(1)	2.91128666(1)	3312.0535(1)	14.12578804(1)	96.141508(2)
^3He	41.8824647(1)	1.4624976699(1)	2.91199719(1)	3312.5809(1)	14.12838381(1)	96.158143(2)

coefficients. In this work, we are only concerned with $n = 3$ and 4 in Eq. (33). The corresponding dispersion coefficients are

$$C_6^{(IJ)}(1, M) = (|A_I|^2 + |A_J|^2)\mathbb{D}_1(M) + |A_K|^2\mathbb{D}_2, \quad (34)$$

$$C_8^{(IJ)}(1, M) = (|A_I|^2 + |A_J|^2)\mathbb{Q}_1(M) + |A_K|^2\mathbb{Q}_2 + (A_I^*A_J + A_J^*A_I)\mathbb{Q}_3(M), \quad (35)$$

$$C_6^{(IJ,JK)}(1, M) = \mathbb{Q}_4(A_K, A_I, 1, M, \eta_J), \quad (36)$$

$$C_8^{(IJ,JK)}(1, M) = \mathbb{Q}_4(A_K, A_I, 2, M, \eta_J), \quad (37)$$

with

$$A_1 = a, A_2 = b, A_3 = c, \eta_1 = \alpha, \eta_2 = \beta, \eta_3 = \gamma, \quad (38)$$

where a , b , and c are defined in Eq. (2) and α , β , and γ are the interior angles, and the other terms in Eqs. (34)–(37) are given by

$$\mathbb{D}_1(M) = \sum_{n_s n_t L_s} F_1(n_s, n_t, L_s, 1; 1, 1; 1, M), \quad (39)$$

$$\mathbb{D}_2 = \sum_{n_s n_t} F_2(n_s, n_t, 1, 1), \quad (40)$$

$$\begin{aligned} \mathbb{Q}_1(M) = \sum_{n_s n_t L_s} [& F_1(n_s, n_t, L_s, 1; 1, 3; 1, M) \\ & + F_1(n_s, n_t, L_s, 1; 2, 2; 1, M) \\ & + F_1(n_s, n_t, L_s, 1; 3, 1; 1, M) \\ & + F_1(n_s, n_t, L_s, 2; 1, 1; 1, M)], \end{aligned} \quad (41)$$

$$\mathbb{Q}_2 = \sum_{n_s n_t} [F_2(n_s, n_t, 1, 2) + F_2(n_s, n_t, 2, 1)], \quad (42)$$

$$\begin{aligned} \mathbb{Q}_3(M) = \sum_{n_s n_t} [& F_3(n_s, n_t, 1, 1; 1, 2; 2; 1, M) \\ & + F_3(n_s, n_t, 1, 2; 2, 1; 1, M) \\ & + F_3(n_s, n_t, 2, 1; 1, 2; 1, M) \\ & + F_3(n_s, n_t, 2, 2; 1, 1; 1, M)], \end{aligned} \quad (43)$$

TABLE II. Values of $\mathbb{D}_0(M=0)$, $\mathbb{D}_0(M=\pm 1)$, $\mathbb{D}_1(M=0)$, $\mathbb{D}_1(M=\pm 1)$, \mathbb{D}_2 , $\mathbb{Q}_1(M=0)$, $\mathbb{Q}_1(M=\pm 1)$, \mathbb{Q}_2 , $\mathbb{Q}_3(M=0)$, and $\mathbb{Q}_3(M=\pm 1)$ for the He(n_0^1S)-He(n_0^1S)-He(n_0^1P) system, in atomic units. All these quantities are independent of the geometrical configuration formed by the three atoms. The numbers in parentheses represent the computational uncertainties.

Atom	$\mathbb{D}_0(M=0)$ $\mathbb{Q}_1(M=0)$	$\mathbb{D}_0(M=\pm 1)$ $\mathbb{Q}_1(M=\pm 1)$	$\mathbb{D}_1(M=0)$ \mathbb{Q}_2	$\mathbb{D}_1(M=\pm 1)$ $\mathbb{Q}_3(M=0)$	\mathbb{D}_2 $\mathbb{Q}_3(M=\pm 1)$
He(1^1S)-He(1^1S)-He(2^1P)					
$^\infty\text{He}$	-0.1770556027(1) 377.0136(1)	0.0885278013(1) 5123.8556(1)	32.6430764067(3) 14.1178573524(3)	45.758183356(1) 19.5357464(2)	1.4609778377(1) -78.9244427(5)
^4He	-0.1770765305(1) 376.9508(1)	0.0885382652(1) 5127.4835(1)	32.6709827359(1) 14.1257880415(1)	45.797120320(1) 19.5451867(2)	1.4621228531(1) -78.9606567(6)
^3He	-0.1770833800(1) 376.9301(1)	0.0885416900(1) 5128.6709(1)	32.6801176662(2) 14.1283838158(2)	45.809866024(1) 19.5482763(2)	1.4624976699(1) -78.9725084(6)
He(2^1S)-He(2^1S)-He(2^1P)					
$^\infty\text{He}$	-8.5048343026(1) 456379(2)	4.2524171513(1) 1547973(4)	4068.2(1) 817250.251(2)	4849.0(2) 36573.7501(1)	11241.0468(1) -962005.7512(1)
^4He	-8.5078707885(1) 456573(2)	4.2539353942(1) 1548946(5)	4071.8(1) 817626.242(2)	4853.3(2) 36641.8289(1)	11247.7393(1) -962545.9503(1)
^3He	-8.5088643582(1) 456635(3)	4.2544321791(1) 1549265(5)	4073.0(1) 817749.274(2)	4854.7(2) 36664.1093(1)	11249.9297(1) -962722.7314(1)
He(2^3S)-He(2^3S)-He(2^3P)					
$^\infty\text{He}$	-6.4077465538(1) 135961.610(2)	3.2038732769(1) 531453.96(2)	1862.5727(2) 210566.55(2)	2251.4034(2) 32944.5218(1)	3276.6801(3) -291050.4284(1)
^4He	-6.4090875602(1) 135980.281(2)	3.2045437801(1) 531566.81(2)	1863.4728(2) 210667.81(2)	2252.4905(1) 32941.0762(1)	3279.4590(3) -291128.5937(1)
^3He	-6.4095263009(2) 135986.388(2)	3.2047631504(1) 531603.71(1)	1863.7672(1) 210700.95(2)	2252.8465(2) 32939.9454(1)	3280.3686(2) -291154.1703(1)

TABLE III. The additive dispersion coefficients $C_6^{(IJ)}$ and $C_8^{(IJ)}$ of the He(1^1S)-He(1^1S)-He(2^1S) system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_6^{(12)}$	$C_6^{(23)}$	$C_6^{(31)}$	$C_8^{(12)}$	$C_8^{(23)}$	$C_8^{(31)}$
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	30.320614(1)	30.320614(1)	30.320614(1)	2275.727(1)	2275.727(1)	2275.727(1)
	$\Psi_{2,\Delta}^{(0)}$	21.651146(1)	21.651146(1)	38.932200(1)	1662.279(1)	1662.279(1)	3214.351(1)
	$\Psi_{3,\Delta}^{(0)}$	33.171849(1)	33.171849(1)	15.890795(1)	2696.994(1)	2696.994(1)	1144.922(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	30.343110(1)	30.343110(1)	30.343110(1)	2276.838(1)	2276.838(1)	2276.838(1)
	$\Psi_{2,\Delta}^{(0)}$	21.667220(1)	21.667220(1)	38.961030(1)	1663.089(1)	1663.089(1)	3215.912(1)
	$\Psi_{3,\Delta}^{(0)}$	33.196427(1)	33.196427(1)	15.902616(1)	2698.304(1)	2698.304(1)	1145.482(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	30.350473(1)	30.350473(1)	30.350473(1)	2277.202(1)	2277.202(1)	2277.202(1)
	$\Psi_{2,\Delta}^{(0)}$	21.672481(1)	21.672481(1)	38.970467(1)	1663.354(1)	1663.354(1)	3216.422(1)
	$\Psi_{3,\Delta}^{(0)}$	33.204472(1)	33.204472(1)	15.906485(1)	2698.733(1)	2698.733(1)	1145.665(1)

TABLE IV. The additive long-range coefficients $C_3^{(IJ)}(1, M)$ of the He(n_0^1S)-He(n_0^1S)-He(n_0^1P) system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_3^{(12)}(1, M=0)$	$C_3^{(23)}(1, M=0)$	$C_3^{(31)}(1, M=0)$	$C_3^{(12)}(1, M=\pm 1)$	$C_3^{(23)}(1, M=\pm 1)$	$C_3^{(31)}(1, M=\pm 1)$
He(1^1S)-He(1^1S)-He(2^1P)							
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	-0.1180370684(1)	-0.1180370684(1)	-0.1180370684(1)	0.0590185342(1)	0.0590185342(1)	0.0590185342(1)
	$\Psi_{2,\Delta}^{(0)}$	0	0	0.1770556027(1)	0	0	-0.0885278013(1)
	$\Psi_{3,\Delta}^{(0)}$	0.1180370684(1)	0.1180370684(1)	-0.0590185342(1)	-0.0590185342(1)	-0.0590185342(1)	0.0295092671(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	-0.1180510203(1)	-0.1180510203(1)	-0.1180510203(1)	0.0590255101(1)	0.0590255101(1)	0.0590255101(1)
	$\Psi_{2,\Delta}^{(0)}$	0	0	0.1770765305(1)	0	0	-0.0885382652(1)
	$\Psi_{3,\Delta}^{(0)}$	0.1180510203(1)	0.1180510203(1)	-0.0590255101(1)	-0.0590255101(1)	-0.0590255101(1)	0.0295127550(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	-0.1180555867(1)	-0.1180555867(1)	-0.1180555867(1)	0.0590277933(1)	0.0590277933(1)	0.0590277933(1)
	$\Psi_{2,\Delta}^{(0)}$	0	0	0.1770833800(1)	0	0	-0.0885416900(1)
	$\Psi_{3,\Delta}^{(0)}$	0.1180555867(1)	0.1180555867(1)	-0.0590277933(1)	-0.0590277933(1)	-0.0590277933(1)	0.0295138966(1)
He(2^1S)-He(2^1S)-He(2^1P)							
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	-5.6698895350(1)	-5.6698895350(1)	-5.6698895350(1)	2.8349447675(1)	2.8349447675(1)	2.8349447675(1)
	$\Psi_{2,\Delta}^{(0)}$	0	0	8.5048343026(1)	0	0	-4.2524171513(1)
	$\Psi_{3,\Delta}^{(0)}$	5.6698895350(1)	5.6698895350(1)	-2.8349447675(1)	-2.8349447675(1)	-2.8349447675(1)	1.4174723837(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	-5.6719138590(1)	-5.6719138590(1)	-5.6719138590(1)	2.8359569295(1)	2.8359569295(1)	2.8359569295(1)
	$\Psi_{2,\Delta}^{(0)}$	0	0	8.5078707885(1)	0	0	-4.2539353942(1)
	$\Psi_{3,\Delta}^{(0)}$	5.6719138590(1)	5.6719138590(1)	-2.8359569295(1)	-2.8359569295(1)	-2.8359569295(1)	1.4179784647(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	-5.6725762388(1)	-5.6725762388(1)	-5.6725762388(1)	2.8362881194(1)	2.8362881194(1)	2.8362881194(1)
	$\Psi_{2,\Delta}^{(0)}$	0	0	8.5088643582(1)	0	0	-4.2544321791(1)
	$\Psi_{3,\Delta}^{(0)}$	5.6725762388(1)	5.6725762388(1)	-2.8362881194(1)	-2.8362881194(1)	-2.8362881194(1)	1.4181440597(1)
He(2^3S)-He(2^3S)-He(2^3P)							
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	-4.2718310359(1)	-4.2718310359(1)	-4.2718310359(1)	2.1359155179(1)	2.1359155179(1)	2.1359155179(1)
	$\Psi_{2,\Delta}^{(0)}$	0	0	6.4077465538(1)	0	0	-3.2038732769(1)
	$\Psi_{3,\Delta}^{(0)}$	4.2718310359(1)	4.2718310359(1)	-2.1359155179(1)	-2.1359155179(1)	-2.1359155179(1)	1.0679577589(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	-4.2727250401(1)	-4.2727250401(1)	-4.2727250401(1)	2.1363625200(1)	2.1363625200(1)	2.1363625200(1)
	$\Psi_{2,\Delta}^{(0)}$	0	0	6.4090875602(1)	0	0	-3.2045437801(1)
	$\Psi_{3,\Delta}^{(0)}$	4.2727250401(1)	4.2727250401(1)	-2.1363625200(1)	-2.1363625200(1)	-2.1363625200(1)	1.0681812600(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	-4.2730175339(1)	-4.2730175339(1)	-4.2730175339(1)	2.1365087669(1)	2.1365087669(1)	2.1365087669(1)
	$\Psi_{2,\Delta}^{(0)}$	0	0	6.4095263009(1)	0	0	-3.2047631504(1)
	$\Psi_{3,\Delta}^{(0)}$	4.2730175339(1)	4.2730175339(1)	-2.1365087669(1)	-2.1365087669(1)	-2.1365087669(1)	1.0682543834(1)

TABLE V. The additive and nonadditive dispersion coefficients $C_6^{(IJ)}(1, M=0)$ and $C_6^{(IJ,JK)}(1, M=0)$ of the $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}P)$ system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_6^{(12)}(1, M=0)$	$C_6^{(23)}(1, M=0)$	$C_6^{(31)}(1, M=0)$	$C_6^{(12,23)}(1, M=0)$	$C_6^{(23,31)}(1, M=0)$	$C_6^{(31,12)}(1, M=0)$
He(1 ¹ S)-He(1 ¹ S)-He(2 ¹ P)							
∞He	$\Psi_{1,\Delta}^{(0)}$	22.2490435504(2)	22.2490435504(2)	22.2490435504(2)	0.3183512641(1)	0.3183512641(1)	0.3183512641(1)
	$\Psi_{2,\Delta}^{(0)}$	17.0520271221(1)	17.0520271221(1)	32.6430764067(3)	-0.4775268962(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	27.4460599786(3)	27.4460599786(3)	11.8550106940(1)	0.1591756320(1)	-0.3183512641(1)	-0.3183512641(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	22.2680294416(1)	22.2680294416(1)	22.2680294416(1)	0.3185403283(1)	0.3185403283(1)	0.3185403283(1)
	$\Psi_{2,\Delta}^{(0)}$	17.0665527945(1)	17.0665527945(1)	32.6709827359(1)	-0.4778104925(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	27.4695060888(1)	27.4695060888(1)	11.8650761474(1)	0.1592701641(1)	-0.3185403283(1)	-0.3185403283(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	22.2742443341(1)	22.2742443341(1)	22.2742443341(1)	0.3186022100(1)	0.3186022100(1)	0.3186022100(1)
	$\Psi_{2,\Delta}^{(0)}$	17.0713076681(1)	17.0713076681(1)	32.6801176662(2)	-0.4779033149(2)	0	0
	$\Psi_{3,\Delta}^{(0)}$	27.4771810002(2)	27.4771810002(2)	11.8683710021(1)	0.1593011050(1)	-0.3186022100(1)	-0.3186022100(1)
He(2 ¹ S)-He(2 ¹ S)-He(2 ¹ P)							
∞He	$\Psi_{1,\Delta}^{(0)}$	6459.14(5)	6459.14(5)	6459.14(5)	1277.7398(1)	1277.7398(1)	1277.7398(1)
	$\Psi_{2,\Delta}^{(0)}$	7654.62(4)	7654.62(4)	4068.2(1)	-1916.6097(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	5263.7(1)	5263.7(1)	8850.10(3)	638.8699(1)	-1277.7398(1)	-1277.7398(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	6463.79(6)	6463.79(6)	6463.79(6)	1278.5076(1)	1278.5076(1)	1278.5076(1)
	$\Psi_{2,\Delta}^{(0)}$	7659.77(4)	7659.77(4)	4071.8(1)	-1917.7614(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	5267.8(1)	5267.8(1)	8855.76(3)	639.2538(1)	-1278.5076(1)	-1278.5076(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	6465.31(6)	6465.31(6)	6465.31(6)	1278.7588(1)	1278.7588(1)	1278.7588(1)
	$\Psi_{2,\Delta}^{(0)}$	7661.47(5)	7661.47(5)	4073.0(1)	-1918.1383(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	5269.1(1)	5269.1(1)	8857.62(3)	639.3794(1)	-1278.7588(1)	-1278.7588(1)
He(2 ³ S)-He(2 ³ S)-He(2 ³ P)							
∞He	$\Psi_{1,\Delta}^{(0)}$	2333.9418(2)	2333.9418(2)	2333.9418(2)	376.6260(1)	376.6260(1)	376.6260(1)
	$\Psi_{2,\Delta}^{(0)}$	2569.6263(2)	2569.6263(2)	1862.5727(2)	-564.9390(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	2098.2571(1)	2098.2571(1)	2805.3109(2)	188.3130(1)	-376.6260(1)	-376.6260(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	2335.4680(1)	2335.4680(1)	2335.4680(1)	376.9477(1)	376.9477(1)	376.9477(1)
	$\Psi_{2,\Delta}^{(0)}$	2571.4658(2)	2571.4658(2)	1863.4728(2)	-565.4215(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	2099.4703(1)	2099.4703(1)	2807.4635(2)	188.4738(1)	-376.9477(1)	-376.9477(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	2335.9678(2)	2335.9678(2)	2335.9678(2)	377.0530(1)	377.0530(1)	377.0530(1)
	$\Psi_{2,\Delta}^{(0)}$	2572.0680(2)	2572.0680(2)	1863.7672(1)	-565.5795(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	2099.8674(1)	2099.8674(1)	2808.1682(2)	188.5265(1)	-377.0530(1)	-377.0530(1)

and

$$\mathbb{Q}_4(A_K, A_I, \lambda, M, \eta_J) = 2 \sum_{n_i, M_i} \text{Re}[A_K^* A_I e^{i(M_i - M)\eta_J}] F_4(n_i, \lambda, M_i; 1, M). \quad (44)$$

Recall, in the above, (I, J, K) forms a cyclic permutation of $(1, 2, 3)$. Many of the details of the perturbation theory were given in Ref. [1]. The expressions of the F_i appearing above are given by Eqs. (A10)–(A13) of Ref. [1].

III. RESULTS AND DISCUSSION

In the present work, the atomic wave functions of helium were constructed variationally using Hylleraas basis sets, and the intermediate states were generated by diagonalizing the helium Hamiltonian [23]. All relevant matrix elements of the multipole transition operators were thus calculated, including

the finite nuclear mass corrections [17]. With these, we calculate the first-order dipolar and second-order long-range dispersion coefficients for the $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}L)$ system.

According to Eqs. (19)–(44), we can see that the dependence of these interaction coefficients on the geometrical configurations of the three atoms is due to two reasons. First, all these coefficients contain the expansion coefficients a , b , and c . The cause of this dependence is the existence of the three degenerate states that are shown in Eqs. (3)–(5). Secondly, these nonadditive interaction coefficients contain the interior angles of the triangle α , β , and γ formed by these three helium atoms. So in this paper, the expansion coefficients a , b , and c and the interior angles α , β , and γ are called geometric parameters.

Now, let us reconsider the formulas of additive dispersion interaction coefficients that are shown in Eqs. (20), (21), (30), (34), and (35). Since these coefficients do not contain the

TABLE VI. The additive and nonadditive dispersion coefficients $C_6^{(IJ)}(1, M = \pm 1)$ and $C_6^{(IJ,JK)}(1, M = \pm 1)$ of the $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}P)$ system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_6^{(12)}(1, M = \pm 1)$	$C_6^{(23)}(1, M = \pm 1)$	$C_6^{(31)}(1, M = \pm 1)$	$C_6^{(12,23)}(1, M = \pm 1)$	$C_6^{(23,31)}(1, M = \pm 1)$	$C_6^{(31,12)}(1, M = \pm 1)$
He(1 1S)-He(1 1S)-He(2 1P)							
∞He	$\Psi_{1,\Delta}^{(0)}$	30.9924481829(1)	30.9924481829(1)	30.9924481829(1)	-0.2785573560(1)	-0.2785573560(1)	-0.2785573560(1)
	$\Psi_{2,\Delta}^{(0)}$	23.6095805966(1)	23.6095805966(1)	45.758183355(1)	0.4178360340(2)	0	0
	$\Psi_{3,\Delta}^{(0)}$	38.3753157692(1)	38.3753157692(1)	16.2267130103(1)	-0.13927867804(5)	0.2785573560(1)	0.2785573560(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	31.0187878317(2)	31.0187878317(2)	31.0187878317(2)	-0.2787227872(1)	-0.2787227872(1)	-0.2787227872(1)
	$\Psi_{2,\Delta}^{(0)}$	23.6296215870(2)	23.6296215870(2)	45.797120320(1)	0.4180841809(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	38.4079540763(3)	38.4079540763(3)	16.2404553424(1)	-0.1393613936(1)	0.2787227872(1)	0.2787227872(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	31.0274099057(1)	31.0274099057(1)	31.0274099057(1)	-0.2787769337(1)	-0.2787769337(1)	-0.2787769337(1)
	$\Psi_{2,\Delta}^{(0)}$	23.6361818467(2)	23.6361818467(2)	45.809866023(1)	0.4181654005(2)	0	0
	$\Psi_{3,\Delta}^{(0)}$	38.4186379646(2)	38.4186379646(2)	16.2449537878(1)	-0.1393884668(1)	0.2787769337(1)	0.2787769337(1)
He(2 1S)-He(2 1S)-He(2 1P)							
∞He	$\Psi_{1,\Delta}^{(0)}$	6979.8(2)	6979.8(2)	6979.8(2)	-1118.0223(1)	-1118.0223(1)	-1118.0223(1)
	$\Psi_{2,\Delta}^{(0)}$	8045.0(1)	8045.0(1)	4849.0(2)	1677.0335(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	5914.4(2)	5914.4(2)	9110.4(1)	-559.0111(1)	1118.0223(1)	1118.0223(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	6984.7(1)	6984.7(1)	6984.7(1)	-1118.6941(1)	-1118.6941(1)	-1118.6941(1)
	$\Psi_{2,\Delta}^{(0)}$	8050.5(1)	8050.5(1)	4853.3(2)	1678.0412(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	5919.0(2)	5919.0(2)	9116.2(1)	-559.3470(1)	1118.6941(1)	1118.6941(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	6986.5(2)	6986.5(2)	6986.5(2)	-1118.9140(1)	-1118.9140(1)	-1118.9140(1)
	$\Psi_{2,\Delta}^{(0)}$	8052.3(1)	8052.3(1)	4854.7(2)	1678.3710(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	5920.6(2)	5920.6(2)	9118.1(1)	-559.4570(1)	1118.9140(1)	1118.9140(1)
He(2 3S)-He(2 3S)-He(2 3P)							
∞He	$\Psi_{1,\Delta}^{(0)}$	2593.1622(2)	2593.1622(2)	2593.1622(2)	-329.5477(1)	-329.5477(1)	-329.5477(1)
	$\Psi_{2,\Delta}^{(0)}$	2764.0417(2)	2764.0417(2)	2251.4034(2)	494.3216(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	2422.2828(2)	2422.2828(2)	2934.9211(2)	-164.7738(1)	329.5477(1)	329.5477(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	2594.8134(2)	2594.8134(2)	2594.8134(2)	-329.8292(1)	-329.8292(1)	-329.8292(1)
	$\Psi_{2,\Delta}^{(0)}$	2765.9749(3)	2765.9749(3)	2252.4905(1)	494.7438(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	2423.6520(2)	2423.6520(2)	2937.1361(2)	-164.9146(1)	329.8292(1)	329.8292(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	2595.3540(3)	2595.3540(3)	2595.3540(3)	-329.9214(1)	-329.9214(1)	-329.9214(1)
	$\Psi_{2,\Delta}^{(0)}$	2766.6075(2)	2766.6075(2)	2252.8465(2)	494.8821(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	2424.1002(2)	2424.1002(2)	2937.8612(2)	-164.9607(1)	329.9214(1)	329.9214(1)

interior angles α , β , and γ , we can easily separate them into geometric parameters a , b , and c , and the interaction constants \mathbb{T}_1 , \mathbb{T}_2 , \mathbb{T}_3 , \mathbb{R}_1 , \mathbb{R}_2 , \mathbb{R}_3 , $\mathbb{D}_0(M = 0)$, $\mathbb{D}_0(M = \pm 1)$, $\mathbb{D}_1(M = 0)$, $\mathbb{D}_1(M = \pm 1)$, \mathbb{D}_2 , $\mathbb{Q}_1(M = 0)$, $\mathbb{Q}_1(M = \pm 1)$, \mathbb{Q}_2 , $\mathbb{Q}_3(M = 0)$, $\mathbb{Q}_3(M = \pm 1)$ that are independent of geometrical configuration of the three atoms. For the $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1S)$ system, \mathbb{T}_1 , \mathbb{T}_2 , and \mathbb{T}_3 are connected to the second-order additive dispersion coefficient $C_6^{(IJ)}$. \mathbb{R}_1 , \mathbb{R}_2 , and \mathbb{R}_3 are connected to the second-order additive dispersion coefficient $C_8^{(IJ)}$. For the $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}P)$ system, $\mathbb{D}_0(M = 0)$ and $\mathbb{D}_0(M = \pm 1)$ are connected to the first-order additive coefficient $C_3^{(IJ)}(L, M)$. $\mathbb{D}_1(M = 0)$, $\mathbb{D}_1(M = \pm 1)$, and \mathbb{D}_2 are connected to the second-order additive dispersion coefficient $C_6^{(IJ)}(L, M)$, and $\mathbb{Q}_1(M = 0)$, $\mathbb{Q}_1(M = \pm 1)$, \mathbb{Q}_2 , $\mathbb{Q}_3(M = 0)$, and $\mathbb{Q}_3(M = \pm 1)$ are connected to the second-order additive dispersion coefficient $C_8^{(IJ)}(L, M)$. The values of these interac-

tion constants for two helium isotopes are listed in Tables I and II, respectively. As shown in Eqs. (36) and (37), the nonadditive interaction coefficients are inseparable, because they contain both the expansion coefficients a , b , and c and the interior angles α , β , and γ .

Actually, with these interaction constants, we can easily find the connection between this work and previous studies of long-range interactions for two-body system. For example, if we set $a = 1/\sqrt{2}$, $b = \pm 1/\sqrt{2}$, $c = 0$, our expressions describe the long-range interactions for the two-body $n_0S - n'_0L$ system. For example, for the $\text{He}(1^1S)\text{-He}(2^1S)$ system, the second-order dispersion coefficients $C_6 = \mathbb{T}_1 + \mathbb{T}_3$ and $C_8 = \mathbb{R}_1 + \mathbb{R}_3$. For the $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}P)$ system, the first-order dispersion interaction coefficient $C_3(M) = \mathbb{D}_0(M)$, the second-order dispersion coefficients $C_6(M) = \mathbb{D}_1(M)$ and $C_8(M) = \mathbb{Q}_1(M) + \mathbb{Q}_3(M)$. Similarly, If we set $a = b = 0$,

TABLE VII. The additive and nonadditive dispersion coefficients $C_8^{(IJ)}(1, M=0)$ and $C_8^{(IJJK)}(1, M=0)$ of the $\text{He}(n_0^1S)\text{-He}(n_0^1S)\text{-He}(n_0^1P)$ system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_8^{(12)}(1, M=0)$	$C_8^{(23)}(1, M=0)$	$C_8^{(31)}(1, M=0)$	$C_8^{(12,23)}(1, M=0)$	$C_8^{(23,31)}(1, M=0)$	$C_8^{(31,12)}(1, M=0)$
He(1 ¹ S)-He(1 ¹ S)-He(2 ¹ P)							
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	269.0722(1)	269.0722(1)	269.0722(1)	1.007423570(1)	1.007423570(1)	1.007423570(1)
	$\Psi_{2,\Delta}^{(0)}$	195.5657(1)	195.5657(1)	357.4779(1)	-1.511135354(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	303.5072(1)	303.5072(1)	141.5950(1)	0.5037117851(5)	-1.007423570(1)	-1.007423570(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	269.0392(1)	269.0392(1)	269.0392(1)	1.007830781(1)	1.007830781(1)	1.007830781(1)
	$\Psi_{2,\Delta}^{(0)}$	195.5383(1)	195.5383(1)	357.4056(1)	-1.511746172(2)	0	0
	$\Psi_{3,\Delta}^{(0)}$	303.4498(1)	303.4498(1)	141.5825(1)	0.5039153905(5)	-1.007830781(1)	-1.007830781(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	269.0284(1)	269.0284(1)	269.0284(1)	1.007964062(1)	1.007964062(1)	1.007964062(1)
	$\Psi_{2,\Delta}^{(0)}$	195.5292(1)	195.5292(1)	357.3819(1)	-1.511946094(2)	0	0
	$\Psi_{3,\Delta}^{(0)}$	303.4310(1)	303.4310(1)	141.5784(1)	0.5039820312(5)	-1.007964062(1)	-1.007964062(1)
He(2 ¹ S)-He(2 ¹ S)-He(2 ¹ P)							
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	601051(2)	601051(2)	601051(2)	64166.8492(1)	64166.8492(1)	64166.8492(1)
	$\Psi_{2,\Delta}^{(0)}$	636815(1)	636815(1)	419806(2)	-96250.2737(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	492143(1)	492143(1)	709151(1)	32083.42460(5)	-64166.8492(1)	-64166.8492(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	601351(6)	601351(6)	601351(2)	64203.6588(1)	64203.6588(1)	64203.6588(1)
	$\Psi_{2,\Delta}^{(0)}$	637098(2)	637098(2)	419931(2)	-96305.4883(2)	0	0
	$\Psi_{3,\Delta}^{(0)}$	492320(2)	492320(2)	709488(1)	32101.82942(5)	-64203.6588(1)	-64203.6588(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	601449(2)	601449(2)	601449(2)	64215.7044(1)	64215.7044(1)	64215.7044(1)
	$\Psi_{2,\Delta}^{(0)}$	637193(1)	637193(1)	419971(3)	-96323.5566(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	492379(2)	492379(2)	709599(1)	32107.85225(6)	-64215.7044(1)	-64215.7044(1)
He(2 ³ S)-He(2 ³ S)-He(2 ³ P)							
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	182792.93(1)	182792.93(1)	182792.93(1)	19616.9709(1)	19616.9709(1)	19616.9709(1)
	$\Psi_{2,\Delta}^{(0)}$	173264.08(1)	173264.08(1)	103017.09(1)	-29425.4564(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	126432.75(1)	126432.75(1)	196679.74(1)	9808.4854(1)	-19616.9709(1)	-19616.9709(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	182836.84(1)	182836.84(1)	182836.84(1)	19623.2331(1)	19623.2331(1)	19623.2331(1)
	$\Psi_{2,\Delta}^{(0)}$	173324.04(1)	173324.04(1)	103039.20(1)	-29434.8497(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	126467.48(1)	126467.48(1)	196752.32(1)	9811.6165(1)	-19623.2331(1)	-19623.2331(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	182851.20(1)	182851.20(1)	182851.20(1)	19625.2823(1)	19625.2823(1)	19625.2823(1)
	$\Psi_{2,\Delta}^{(0)}$	173343.67(1)	173343.67(1)	103046.44(1)	-29437.9234(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	126478.85(1)	126478.85(1)	196776.07(1)	9812.6411(1)	-19625.2823(1)	-19625.2823(1)

$c = 1$, our expressions describe the long-range interactions for the two-body $n_0S - n_0^1S$ system, where $C_6 = \mathbb{D}_2$ and $C_8 = \mathbb{Q}_2$.

A. Dispersion coefficients for He(1¹S)-He(1¹S)-He(2¹S)

In this section, we address the dispersion coefficients for the He(1¹S)-He(1¹S)-He(2¹S) system. For the He(1¹S)-He(1¹S)-He(2¹S) system, its degeneracy is not removed by the first-order energy correction but is removed in the second-order energy correction, which leads to an internuclear distance R_{IJ} dependence of atomic states of the three-atom system. Thus, the quantum states of the He(1¹S)-He(1¹S)-He(2¹S) system depend on the geometrical configurations of the three atoms and on the size of those configurations (or the internuclear distance R_{IJ}). Accordingly the dipolar or dispersion interaction coefficients,

for most configurations, are not constant, but change with different internuclear distances R_{IJ} , and the long-range interactions can only be obtained for specific values of R_{IJ} . However, for the very special configuration of an equilateral triangle with $R_{12} = R_{23} = R_{31}$, the dispersion coefficients remain constant, which will be discussed in the following.

1. Zeroth-order wave function for an equilateral triangle

For an equilateral triangle with $R_{12} = R_{23} = R_{31} = R$, the perturbation matrix with respect to $\{\phi_1, \phi_2, \phi_3\}$ thus becomes

$$H' = \begin{pmatrix} A & D & D \\ D & A & D \\ D & D & A \end{pmatrix}, \quad (45)$$

TABLE VIII. The additive and nonadditive dispersion coefficients $C_8^{(JJ)}(1, M = \pm 1)$ and $C_8^{(JJ,JK)}(1, M = \pm 1)$ of the $\text{He}(n_0^i S)\text{-He}(n_0^j S)\text{-He}(n_0^k P)$ system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_8^{(12)}(1, M = \pm 1)$	$C_8^{(23)}(1, M = \pm 1)$	$C_8^{(31)}(1, M = \pm 1)$	$C_8^{(12,23)}(1, M = \pm 1)$	$C_8^{(23,31)}(1, M = \pm 1)$	$C_8^{(31,12)}(1, M = \pm 1)$
He(1 1S)-He(1 1S)-He(2 1P)							
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	3367.9934(1)	3367.9934(1)	3367.9934(1)	-2.707450845(3)	-2.707450845(3)	-2.707450845(3)
	$\Psi_{2,\Delta}^{(0)}$	2568.9867(1)	2568.9867(1)	5202.7801(1)	4.061176267(4)	0	0
	$\Psi_{3,\Delta}^{(0)}$	4324.8490(1)	4324.8490(1)	1691.0556(1)	-1.353725423(2)	2.707450845(3)	2.707450845(3)
^4He	$\Psi_{1,\Delta}^{(0)}$	3370.3905(1)	3370.3905(1)	3370.3905(1)	-2.708545224(3)	-2.708545224(3)	-2.708545224(3)
	$\Psi_{2,\Delta}^{(0)}$	2570.8046(1)	2570.8046(1)	5206.4442(1)	4.062817836(4)	0	0
	$\Psi_{3,\Delta}^{(0)}$	4327.8977(1)	4327.8977(1)	1692.2581(1)	-1.354272611(1)	2.708545224(3)	2.708545224(3)
^3He	$\Psi_{1,\Delta}^{(0)}$	3371.1751(1)	3371.1751(1)	3371.1751(1)	-2.708903418(3)	-2.708903418(3)	-2.708903418(3)
	$\Psi_{2,\Delta}^{(0)}$	2571.3996(1)	2571.3996(1)	5207.6434(1)	4.063355127(4)	0	0
	$\Psi_{3,\Delta}^{(0)}$	4328.8955(1)	4328.8955(1)	1692.6517(1)	-1.354451708(1)	2.708903418(3)	2.708903418(3)
He(2 1S)-He(2 1S)-He(2 1P)							
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	663061(3)	663061(3)	663061(3)	-172448.4071(2)	-172448.4071(2)	-172448.4071(2)
	$\Psi_{2,\Delta}^{(0)}$	1182611(2)	1182611(2)	2509977(5)	258672.6108(4)	0	0
	$\Psi_{3,\Delta}^{(0)}$	2067523(3)	2067523(3)	740156(1)	-86224.2035(1)	172448.4071(2)	172448.4071(2)
^4He	$\Psi_{1,\Delta}^{(0)}$	663476(3)	663476(3)	663476(3)	-172547.3332(3)	-172547.3332(3)	-172547.3332(3)
	$\Psi_{2,\Delta}^{(0)}$	1183287(2)	1183287(2)	2511492(5)	258820.9997(4)	0	0
	$\Psi_{3,\Delta}^{(0)}$	2068757(4)	2068757(4)	740550(2)	-86273.6665(1)	172547.3332(3)	172547.3332(3)
^3He	$\Psi_{1,\Delta}^{(0)}$	663612(3)	663612(3)	663612(3)	-172579.7058(3)	-172579.7058(3)	-172579.7058(3)
	$\Psi_{2,\Delta}^{(0)}$	1183508(2)	1183508(2)	2511988(5)	258869.5588(5)	0	0
	$\Psi_{3,\Delta}^{(0)}$	2069161(4)	2069161(4)	740681(1)	-86289.8528(1)	172579.7058(3)	172579.7058(3)
He(2 3S)-He(2 3S)-He(2 3P)							
$^\infty\text{He}$	$\Psi_{1,\Delta}^{(0)}$	230457.87(2)	230457.87(2)	230457.87(2)	-52720.6094(1)	-52720.6094(1)	-52720.6094(1)
	$\Psi_{2,\Delta}^{(0)}$	371010.24(1)	371010.24(1)	822504.39(2)	79080.9141(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	672006.34(2)	672006.34(2)	220512.21(2)	-26360.3047(1)	52720.6094(1)	52720.6094(1)
^4He	$\Psi_{1,\Delta}^{(0)}$	230514.73(1)	230514.73(1)	230514.73(1)	-52737.4391(1)	-52737.4391(1)	-52737.4391(1)
	$\Psi_{2,\Delta}^{(0)}$	371117.31(2)	371117.31(2)	822695.40(2)	79106.1586(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	672169.37(2)	672169.37(2)	220591.28(2)	-26368.7195(1)	52737.4391(1)	52737.4391(1)
^3He	$\Psi_{1,\Delta}^{(0)}$	230533.34(1)	230533.34(1)	230533.34(1)	-52742.9462(1)	-52742.9462(1)	-52742.9462(1)
	$\Psi_{2,\Delta}^{(0)}$	371152.34(2)	371152.34(2)	822757.90(2)	79114.4192(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	672222.71(2)	672222.71(2)	220617.15(2)	-26371.4731(1)	52742.9462(1)	52742.9462(1)

where

$$A = \Delta_{11} = \Delta_{22} = \Delta_{33}, \quad (46)$$

$$D = \Delta_{12} = \Delta_{12}^* = \Delta_{13} = \Delta_{13}^* = \Delta_{23} = \Delta_{23}^*, \quad (47)$$

where the functions Δ_{IJ} are defined by Eqs. (A3)–(A8) in the Appendix. Solving the eigenvalue problem of the above matrix Eq. (45), one obtains the eigenvalues $A + 2D$, $A - D$, $A - D$, and the corresponding zeroth-order wave functions

$$\Psi_{1,\Delta}^{(0)} = \frac{1}{\sqrt{3}}|\phi_1\rangle + \frac{1}{\sqrt{3}}|\phi_2\rangle + \frac{1}{\sqrt{3}}|\phi_3\rangle, \quad (48)$$

$$\Psi_{2,\Delta}^{(0)} = \frac{1}{\sqrt{2}}|\phi_1\rangle - \frac{1}{\sqrt{2}}|\phi_3\rangle, \quad (49)$$

$$\Psi_{3,\Delta}^{(0)} = \frac{1}{\sqrt{6}}|\phi_1\rangle - \sqrt{\frac{2}{3}}|\phi_2\rangle + \frac{1}{\sqrt{6}}|\phi_3\rangle, \quad (50)$$

where the symbol “ Δ ” denotes the equilateral triangle. Because they have the same eigenvalue $A - D$, the corresponding eigenstates $\Psi_{2,\Delta}^{(0)}$ and $\Psi_{3,\Delta}^{(0)}$ are not unique. Thus, any eigenstates under unitary transformations in the two-dimensional eigenspace belonging to the eigenvalue $A - D$ can be chosen to evaluate the corresponding dipolar and dispersion coefficients, and different quantum states may lead to different coefficients. This phenomenon reflects a kind of quantum three-body effect. In any case, the perturbed Hamiltonian H' would remain unchanged under any unitary transformation in the two-dimensional eigenspace belonging to the eigenvalue $A - D$. Therefore, the total long-range interaction would remain constant under any unitary transformation in this eigenspace. In the present work, we take one set of these eigenfunctions, Eqs. (49) and (50), as an example.

TABLE IX. The additive long-range coefficients $C_3^{(I,J)}(1, M)$ of the $\text{He}(n_0^I S)-\text{He}(n_0^J S)-\text{He}(n_0^0 P)$ system for three different types of the zeroth-order wave functions, where the three atoms form a straight line, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_3^{(12)}(1, M = 0)$	$C_3^{(23)}(1, M = 0)$	$C_3^{(31)}(1, M = 0)$	$\text{He}(1^1 S)-\text{He}(1^1 S)-\text{He}(2^1 P)$	$C_3^{(12)}(1, M = \pm 1)$	$C_3^{(23)}(1, M = \pm 1)$	$C_3^{(31)}(1, M = \pm 1)$
∞He	$\Psi_{1-}^{(0)}$	-0.12507513324(3)	-0.09243639928(2)	-0.12507513324(3)	0.06253756661(1)	0.04621819964(1)	0.06253756661(1)	0.06253756661(1)
	$\Psi_{2-}^{(0)}$	0.12507513324(3)	-0.08461920345(2)	0.12507513324(3)	-0.06253756661(1)	0.04230960172(1)	0.04230960172(1)	-0.06253756661(1)
	$\Psi_{3-}^{(0)}$	0	0.17705560274(4)	0	0	-0.08852780137(2)	-0.08852780137(2)	0
^4He	$\Psi_{1-}^{(0)}$	-0.12508991701(2)	-0.09244732519(2)	-0.12508991701(2)	0.06254495850(1)	0.04622366259(1)	0.04622366259(1)	0.06254495850(1)
	$\Psi_{2-}^{(0)}$	0.12508991701(2)	-0.08462920538(2)	0.12508991701(2)	-0.06254495850(1)	0.04231460269(1)	0.04231460269(1)	-0.06254495850(1)
	$\Psi_{3-}^{(0)}$	0	0.17707653057(4)	0	0	-0.08853826528(2)	-0.08853826528(2)	0
^3He	$\Psi_{1-}^{(0)}$	-0.12509475561(3)	-0.09245090113(2)	-0.12509475561(3)	0.06254737781(2)	0.04622545056(1)	0.04622545056(1)	0.06254737781(2)
	$\Psi_{2-}^{(0)}$	0.12509475561(3)	-0.08463247891(2)	0.12509475561(3)	-0.06254737781(2)	0.04231623945(1)	0.04231623945(1)	-0.06254737781(2)
	$\Psi_{3-}^{(0)}$	0	0.17708338005(4)	0	0	-0.08854169002(2)	-0.08854169002(2)	0
∞He	$\Psi_{1-}^{(0)}$	-6.007961720158(3)	-4.440165955066(3)	-6.007961720158(3)	$\text{He}(2^1 S)-\text{He}(2^1 S)-\text{He}(2^1 P)$	2.220082977532(1)	2.220082977532(1)	3.003980860078(1)
	$\Psi_{2-}^{(0)}$	6.007961720158(3)	-4.064668347556(3)	6.007961720158(3)	-3.003980860078(1)	2.032334173777(1)	2.032334173777(1)	-3.003980860078(1)
	$\Psi_{3-}^{(0)}$	0	8.504834302621(5)	0	0	-4.252417151311(3)	-4.252417151311(3)	0
^4He	$\Psi_{1-}^{(0)}$	-6.010106746250(1)	-4.4417512301165(7)	-6.010106746250(1)	3.0050533731251(5)	2.2208756150583(4)	2.2208756150583(4)	3.0050533731251(5)
	$\Psi_{2-}^{(0)}$	6.010106746250(1)	-4.0661195584758(6)	6.010106746250(1)	-3.0050533731251(5)	2.0330597792379(3)	2.0330597792379(3)	-3.0050533731251(5)
	$\Psi_{3-}^{(0)}$	0	8.507870788593(2)	0	0	-4.2539353942961(6)	-4.2539353942961(6)	0
^3He	$\Psi_{1-}^{(0)}$	-6.010808620995(1)	-4.442269948526(1)	-6.010808620995(1)	3.0054043104976(5)	2.2211349742630(4)	2.2211349742630(4)	3.0054043104976(5)
	$\Psi_{2-}^{(0)}$	6.010808620995(1)	-4.066594409714(1)	6.010808620995(1)	-3.0054043104976(5)	2.0332972048568(3)	2.0332972048568(3)	-3.0054043104976(5)
	$\Psi_{3-}^{(0)}$	0	8.508864358240(2)	0	0	-4.2544321791200(8)	-4.2544321791200(8)	0
∞He	$\Psi_{1-}^{(0)}$	-4.52654274478244(8)	-3.34532773770729(7)	-4.52654274478244(8)	$\text{He}(2^3 S)-\text{He}(2^3 S)-\text{He}(2^3 P)$	1.67266386885365(4)	1.67266386885365(4)	2.26327137239122(4)
	$\Psi_{2-}^{(0)}$	4.52654274478244(8)	-3.06241881615838(6)	4.52654274478244(8)	-2.26327137239122(4)	1.53120940807919(3)	1.53120940807919(3)	-2.26327137239122(4)
	$\Psi_{3-}^{(0)}$	0	6.4077465538656(1)	0	0	-3.20387327693284(7)	-3.20387327693284(7)	0
^4He	$\Psi_{1-}^{(0)}$	-4.5274900548019(1)	-3.34602784431470(8)	-4.5274900548019(1)	2.26374502740096(5)	1.67301392215735(4)	1.67301392215735(4)	2.26374502740096(5)
	$\Psi_{2-}^{(0)}$	4.5274900548019(1)	-3.0630597158896(1)	4.5274900548019(1)	-2.26374502740096(5)	1.53152985794479(4)	1.53152985794479(4)	-2.26374502740096(5)
	$\Psi_{3-}^{(0)}$	0	6.4090875602043(2)	0	0	-3.20454378010215(8)	-3.20454378010215(8)	0
^3He	$\Psi_{1-}^{(0)}$	-4.5277999888255(1)	-3.3462569001183(1)	-4.5277999888255(1)	2.26389999441278(6)	1.67312845005916(4)	1.67312845005916(4)	2.26389999441278(6)
	$\Psi_{2-}^{(0)}$	4.5277999888255(1)	-3.0632694008167(1)	4.5277999888255(1)	-2.26389999441278(6)	1.53163470040838(5)	1.53163470040838(5)	-2.26389999441278(6)
	$\Psi_{3-}^{(0)}$	0	6.4095263009351(2)	0	0	-3.2047631504675(1)	-3.2047631504675(1)	0

TABLE X. The additive and nonadditive dispersion coefficients $C_6^{(l,j)}$ ($l, M = 0$) and $C_6^{(l,j,\kappa)}$ ($l, M = 0$) of the $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}P)$ system for three different types of the zeroth-order wave functions, where the three atoms form a straight line, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_6^{(2,3)}(1, M = 0)$	$C_6^{(3,1)}(1, M = 0)$	$C_6^{(12,23)}(1, M = 0)$	$C_6^{(23,31)}(1, M = 0)$	$C_6^{(3,1,2)}(1, M = 0)$
∞He	$\Psi_{1,-}^{(0)}$	17.7403887642(2)	24.5033709436(3)	He(1 1S)-He(1 1S)-He(2 1P)		0.3373332400(2)
	$\Psi_{2,-}^{(0)}$	16.3636654802(1)	25.1917325854(2)	0.3373332400(2)	0.3373332400(2)	0.3373332400(2)
	$\Psi_{3,-}^{(0)}$	32.6430764067(3)	17.0520271221(1)	-0.3373332400(2)	-0.3373332400(2)	0.2282217843(1)
^4He	$\Psi_{1,-}^{(0)}$	17.75550520692(5)	24.5242915590(1)	0.3375335775(1)	0.3375335775(1)	0.2494531705(1)
	$\Psi_{2,-}^{(0)}$	16.37760038218(4)	25.21324397142(7)	-0.3375335775(1)	-0.3375335775(1)	0.22835732191(9)
	$\Psi_{3,-}^{(0)}$	32.6709827359(1)	17.0665527946(1)	0	0	-0.4778104925(1)
^3He	$\Psi_{1,-}^{(0)}$	17.7604534647(1)	24.5311397688(1)	0.3375991489(1)	0.3375991489(1)	0.249501629(1)
	$\Psi_{2,-}^{(0)}$	16.3821618715(1)	25.2202855655(2)	-0.3375991489(1)	-0.3375991489(1)	0.228401683(1)
	$\Psi_{3,-}^{(0)}$	32.6801176662(2)	17.0713076681(1)	0	0	-0.4779033149(2)
∞He	$\Psi_{1,-}^{(0)}$	7496.27(4)	5940.58(6)	He(2 1S)-He(2 1S)-He(2 1P)		1000.61509384(5)
	$\Psi_{2,-}^{(0)}$	7812.97(4)	5782.25(7)	1353.92623636(6)	1353.92623636(6)	915.99470407(5)
	$\Psi_{3,-}^{(0)}$	4068.2(1)	7654.62(4)	-1353.92623636(6)	-1353.92623636(6)	-1916.6097979(1)
^4He	$\Psi_{1,-}^{(0)}$	7501.37(5)	5945.01(7)	0	0	1001.21632520(4)
	$\Psi_{2,-}^{(0)}$	7818.18(4)	5786.58(6)	1354.73975890(6)	1354.73975890(6)	916.54509029(5)
	$\Psi_{3,-}^{(0)}$	4071.8(1)	7659.77(4)	-1354.73975890(6)	-1354.73975890(6)	-1917.7614155(1)
^3He	$\Psi_{1,-}^{(0)}$	7503.02(4)	5946.44(6)	0	0	1001.41310708(5)
	$\Psi_{2,-}^{(0)}$	7819.89(4)	5788.00(6)	1355.00602327(7)	1355.00602327(7)	916.72523063(5)
	$\Psi_{3,-}^{(0)}$	4073.0(1)	7661.47(5)	-1355.00602327(7)	-1355.00602327(7)	-1918.1383377(1)
∞He	$\Psi_{1,-}^{(0)}$	2538.4092(2)	2231.7081(2)	He(2 3S)-He(2 3S)-He(2 3P)		294.94085(3)
	$\Psi_{2,-}^{(0)}$	2600.8435(2)	2200.4909(2)	399.08267(3)	399.08267(3)	269.99817(2)
	$\Psi_{3,-}^{(0)}$	1862.5727(2)	2569.6263(2)	-399.08267(3)	-399.08267(3)	-564.93901(4)
^4He	$\Psi_{1,-}^{(0)}$	2540.2072(2)	2233.0985(1)	0	0	295.19278(3)
	$\Psi_{2,-}^{(0)}$	2602.7245(2)	2201.8400(2)	399.42355(3)	399.42355(3)	270.22878(1)
	$\Psi_{3,-}^{(0)}$	1863.4728(2)	2571.4658(2)	-399.42355(3)	-399.42355(3)	-565.42155(3)
^3He	$\Psi_{1,-}^{(0)}$	2540.7957(2)	2233.5538(2)	0	0	295.27524(2)
	$\Psi_{2,-}^{(0)}$	2603.3402(2)	2202.2814(1)	399.53514(2)	399.53514(2)	270.30430(2)
	$\Psi_{3,-}^{(0)}$	1863.7672(1)	2572.0680(2)	-399.53514(2)	-399.53514(2)	-565.57955(4)

TABLE XI. The additive and nonadditive dispersion coefficients $C_6^{(IJ)}(1, M = \pm 1)$ and $C_6^{(IJ,JK)}(1, M = \pm 1)$ of the $\text{He}(n_0^1S)\text{-He}(n_0^1S)\text{-He}(n_0^1P)$ system for three different types of the zeroth-order wave functions, where the three atoms form a straight line, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_6^{(12)}(1, M = \pm 1)$	$C_6^{(23)}(1, M = \pm 1)$	$C_6^{(31)}(1, M = \pm 1)$	$C_6^{(12,23)}(1, M = \pm 1)$	$C_6^{(23,31)}(1, M = \pm 1)$	$C_6^{(31,12)}(1, M = \pm 1)$
He(1 ¹ S)-He(1 ¹ S)-He(2 ¹ P)							
∞He	$\Psi_{1,-}^{(0)}$	34.19493962581(4)	24.58746529725(2)	34.19493962581(4)	0.8433331004(3)	0.8433331004(3)	0.6232627794(3)
	$\Psi_{2,-}^{(0)}$	35.17282432641(4)	22.63169589605(2)	35.17282432641(4)	-0.8433331004(3)	-0.8433331004(3)	0.5705544608(2)
	$\Psi_{3,-}^{(0)}$	23.60958059665(2)	45.7581833555(1)	23.60958059665(2)	0	0	-1.1938172404(4)
^4He	$\Psi_{1,-}^{(0)}$	34.2240114649(2)	24.6083405653(2)	34.2240114649(2)	0.8438339437(3)	0.8438339437(3)	0.6236329263(2)
	$\Psi_{2,-}^{(0)}$	35.2027304431(3)	22.6509026088(1)	35.2027304431(3)	-0.8438339437(3)	-0.8438339437(3)	0.5708933048(2)
	$\Psi_{3,-}^{(0)}$	23.6296215870(2)	45.797120320(1)	23.6296215870(2)	0	0	-1.1945262311(4)
^3He	$\Psi_{1,-}^{(0)}$	34.2335278990(2)	24.6151739190(1)	34.2335278990(2)	0.8439978723(3)	0.8439978723(3)	0.6237540772(1)
	$\Psi_{2,-}^{(0)}$	35.2125199713(2)	22.6571897745(1)	35.2125199713(2)	-0.8439978723(3)	-0.8439978723(3)	0.571004208(2)
	$\Psi_{3,-}^{(0)}$	23.6361818467(2)	45.8098660236(2)	23.6361818467(2)	0	0	-1.1947582873(5)
He(2 ¹ S)-He(2 ¹ S)-He(2 ¹ P)							
∞He	$\Psi_{1,-}^{(0)}$	6517.6(2)	7903.9(1)	6517.6(2)	3384.8155908(1)	3384.8155908(1)	2501.5377345(1)
	$\Psi_{2,-}^{(0)}$	6376.5(2)	8186.1(1)	6376.5(2)	-3384.8155908(1)	-3384.8155908(1)	2289.9867601(1)
	$\Psi_{3,-}^{(0)}$	8045.0(1)	4849.0(1)	8045.0(1)	0	0	-4791.5244947(2)
^4He	$\Psi_{1,-}^{(0)}$	6522.5(2)	7909.3(1)	6522.5(2)	3386.8493973(2)	3386.8493973(2)	2503.0408130(1)
	$\Psi_{2,-}^{(0)}$	6381.4(2)	8191.6(1)	6381.4(2)	-3386.8493973(2)	-3386.8493973(2)	2291.3627258(2)
	$\Psi_{3,-}^{(0)}$	8050.5(1)	4853.3(2)	8050.5(1)	0	0	-4794.4035388(3)
^3He	$\Psi_{1,-}^{(0)}$	6524.0(1)	7911.1(1)	6524.0(1)	3387.5150582(2)	3387.5150582(2)	2503.5327676(1)
	$\Psi_{2,-}^{(0)}$	6382.9(2)	8193.5(1)	6382.9(2)	-3387.5150582(2)	-3387.5150582(2)	2291.81308(1)
	$\Psi_{3,-}^{(0)}$	8052.3(1)	4854.7(2)	8052.3(1)	0	0	-4795.3458442(2)
He(2 ³ S)-He(2 ³ S)-He(2 ³ P)							
∞He	$\Psi_{1,-}^{(0)}$	2519.0393(2)	2741.4083(3)	2519.0393(2)	997.70667(7)	997.70667(7)	737.35211(6)
	$\Psi_{2,-}^{(0)}$	2496.4058(2)	2786.6752(2)	2496.4058(2)	-997.70667(7)	-997.70667(7)	674.99542(4)
	$\Psi_{3,-}^{(0)}$	2764.0417(2)	2251.4034(2)	2764.0417(2)	0	0	-1412.34752(9)
^4He	$\Psi_{1,-}^{(0)}$	2520.5681(2)	2743.3039(2)	2520.5681(2)	998.55888(7)	998.55888(7)	737.98192(5)
	$\Psi_{2,-}^{(0)}$	2497.8973(2)	2788.6456(2)	2497.8973(2)	-998.55888(7)	-998.55888(7)	675.57198(4)
	$\Psi_{3,-}^{(0)}$	2765.9749(3)	2252.4905(1)	2765.9749(3)	0	0	-1413.5539(1)
^3He	$\Psi_{1,-}^{(0)}$	2521.0686(2)	2743.9244(2)	2521.0686(2)	998.8379(1)	998.8379(1)	738.18812(5)
	$\Psi_{2,-}^{(0)}$	2498.3853(1)	2789.2908(3)	2498.3853(1)	-998.8379(1)	-998.8379(1)	675.76074(4)
	$\Psi_{3,-}^{(0)}$	2766.6075(2)	2252.8465(2)	2766.6075(2)	0	0	-1413.9488(1)

2. Dispersion coefficients for an equilateral triangle

With these zeroth-order wave functions Eqs. (48)–(50), the corresponding long-range interaction coefficients $C_6^{(IJ)}$ and $C_8^{(IJ)}$ for the isotopic $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1S)$ systems are listed in Table III. We note that these coefficients $C_6^{(IJ)}$ and $C_8^{(IJ)}$ are all the same and positive for $\Psi_{1,\Delta}^{(0)}$ with the geometric parameter $a = b = c = 1/\sqrt{3}$. For $\Psi_{2,\Delta}^{(0)}$ with the geometric parameter $b = 0, a = -c = 1/\sqrt{2}$, $C_6^{(12)} = C_6^{(23)}$, and $C_8^{(12)} = C_8^{(23)}$. For $\Psi_{3,\Delta}^{(0)}$ with the geometric parameter $b = -\sqrt{2/3}, a = c = 1/\sqrt{6}$, we also have $C_6^{(12)} = C_6^{(23)}$ and $C_8^{(12)} = C_8^{(23)}$. These relationships between these coefficients are due to the different values of geometric parameters. The potential energy curves (E), for the $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1S)$ system, corresponding to the different zeroth-order wave functions, are plotted in Fig. 1.

B. Dipolar and dispersion coefficients for $\text{He}(n_0^1S)\text{-He}(n_0^1S)\text{-He}(n_0^1P)$

In this work, we will present the dipolar and dispersion coefficients for two important configurations: an equilateral triangle and a straight line. In addition, we will also evaluate the dipolar and dispersion coefficients for an isosceles right triangle that will be listed in the Supplemental Material [24].

1. Zeroth-order wave function for an equilateral triangle

For the equilateral triangle with $R_{12} = R_{23} = R_{31} = R$, the perturbation matrix with respect to $\{\phi_1, \phi_2, \phi_3\}$ becomes

$$H' = H'_{12} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad (51)$$

TABLE XII. The additive and nonadditive dispersion coefficients $C_8^{(IJ)}(1, M=0)$ and $C_8^{(IJK)}(1, M=0)$ of the $\text{He}(n_0^i S)\text{-He}(n_0^j S)\text{-He}(n_0^k P)$ system for three different types of the zeroth-order wave functions, where the three atoms form a straight line, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_8^{(12)}(1, M=0)$	$C_8^{(23)}(1, M=0)$	$C_8^{(31)}(1, M=0)$	$C_8^{(12,23)}(1, M=0)$	$C_8^{(23,31)}(1, M=0)$	$C_8^{(31,12)}(1, M=0)$
He(1 1S)-He(1 1S)-He(2 1P)							
$^\infty\text{He}$	$\Psi_{1,-}^{(0)}$	296.0844962(1)	213.77603(5)	296.0844962(1)	2.134984185(2)	2.134984185(2)	-1.577853610(1)
	$\Psi_{2,-}^{(0)}$	276.49490(7)	196.8912(1)	276.49490(7)	-2.134984185(2)	-2.134984185(2)	-1.444417100(2)
	$\Psi_{3,-}^{(0)}$	195.56578(5)	357.4779(1)	195.56578(5)	0	0	3.022270710(3)
^4He	$\Psi_{1,-}^{(0)}$	296.04686(7)	213.75195(5)	296.04686(7)	2.135847167(2)	2.135847167(2)	-1.578491396(2)
	$\Psi_{2,-}^{(0)}$	276.44230(7)	196.86987(4)	276.44230(7)	-2.135847167(2)	-2.135847167(2)	-1.445000948(2)
	$\Psi_{3,-}^{(0)}$	195.53832(5)	357.4056(1)	195.53832(5)	0	0	3.023492343(3)
^3He	$\Psi_{1,-}^{(0)}$	296.03445(7)	213.74400(5)	296.03445(7)	2.136129624(2)	2.136129624(2)	-1.578700145(2)
	$\Psi_{2,-}^{(0)}$	276.42501(7)	196.86284(5)	276.42501(7)	-2.136129624(2)	-2.136129624(2)	-1.445192042(1)
	$\Psi_{3,-}^{(0)}$	195.52927(4)	357.3819(1)	195.52927(4)	0	0	3.023892187(3)
He(2 1S)-He(2 1S)-He(2 1P)							
$^\infty\text{He}$	$\Psi_{1,-}^{(0)}$	576416(2)	647941(2)	576416(2)	135985.7088(2)	135985.7088(2)	-100499.8272(2)
	$\Psi_{2,-}^{(0)}$	516777(2)	662260(1)	516777(2)	-135985.7088(2)	-135985.7088(2)	-92000.7203(1)
	$\Psi_{3,-}^{(0)}$	636815(1)	419806(2)	636815(1)	0	0	192500.5476(3)
^4He	$\Psi_{1,-}^{(0)}$	576705(2)	648259(1)	576705(2)	136063.7177(2)	136063.7177(2)	-100557.4795(2)
	$\Psi_{2,-}^{(0)}$	516966(2)	662582(1)	516966(2)	-136063.7177(2)	-136063.7177(2)	-92053.50(1)
	$\Psi_{3,-}^{(0)}$	637098(2)	419931(2)	637098(2)	0	0	192610.9765(3)
^3He	$\Psi_{1,-}^{(0)}$	576800(2)	648361(2)	576800(2)	136089.2454(2)	136089.2454(2)	-100576.3455(1)
	$\Psi_{2,-}^{(0)}$	517028(2)	662687(1)	517028(2)	-136089.2454(2)	-136089.2454(2)	-92070.7677(1)
	$\Psi_{3,-}^{(0)}$	637193(1)	419971(3)	637193(1)	0	0	192647.1134(3)
He(2 3S)-He(2 3S)-He(2 3P)							
$^\infty\text{He}$	$\Psi_{1,-}^{(0)}$	178708.897(6)	188816.664(8)	178708.897(6)	41573.30041(1)	41573.30041(1)	-30724.622050(6)
	$\Psi_{2,-}^{(0)}$	130516.795(6)	190656.01(1)	130516.795(6)	-41573.30041(1)	-41573.30041(1)	-28126.290775(6)
	$\Psi_{3,-}^{(0)}$	173264.08(1)	103017.090(3)	173264.08(1)	0	0	58850.91282(1)
^4He	$\Psi_{1,-}^{(0)}$	178746.690(5)	188873.006(8)	178746.690(5)	41586.57162(1)	41586.57162(1)	-30734.430098(6)
	$\Psi_{2,-}^{(0)}$	130557.634(5)	190716.156(8)	130557.634(5)	-41586.57162(1)	-41586.57162(1)	-28135.269372(6)
	$\Psi_{3,-}^{(0)}$	173324.043(8)	103039.204(2)	173324.043(8)	0	0	58869.69946(1)
^3He	$\Psi_{1,-}^{(0)}$	178759.057(6)	188891.445(9)	178759.057(6)	41590.914293(8)	41590.914293(8)	-30737.639533(6)
	$\Psi_{2,-}^{(0)}$	130571.000(5)	190735.837(8)	130571.000(5)	-41590.914293(8)	-41590.914293(8)	-28138.207391(6)
	$\Psi_{3,-}^{(0)}$	173343.669(9)	103046.443(2)	173343.669(9)	0	0	58875.84692(1)

where

$$H'_{12} = \frac{4\pi}{R^{2L+1}} \frac{(-1)^M [(2L-1)!!]^2}{(2L+1)^2 (L-M)! (L+M)!} \times \left| \langle \varphi_{n_0}(0; \sigma) \| T_L(\sigma) \| \varphi_{n_0}(L; \sigma) \rangle \right|^2. \quad (52)$$

Solving the eigenvalue problem of the above matrix Eq. (51) for the equilateral triangle, one obtains the eigenvalues $2H'_{12}$, $-H'_{12}$, $-H'_{12}$, and the corresponding orthonormalized zeroth-order wave functions

$$\Psi_{1,\Delta}^{(0)} = \frac{1}{\sqrt{3}} |\phi_1\rangle + \frac{1}{\sqrt{3}} |\phi_2\rangle + \frac{1}{\sqrt{3}} |\phi_3\rangle, \quad (53)$$

$$\Psi_{2,\Delta}^{(0)} = \frac{1}{\sqrt{2}} |\phi_1\rangle - \frac{1}{\sqrt{2}} |\phi_3\rangle, \quad (54)$$

$$\Psi_{3,\Delta}^{(0)} = \frac{1}{\sqrt{6}} |\phi_1\rangle - \sqrt{\frac{2}{3}} |\phi_2\rangle + \frac{1}{\sqrt{6}} |\phi_3\rangle, \quad (55)$$

where the symbol “ Δ ” denotes the equilateral triangle. We note that Eq. (53) corresponds to the “Dicke state” [4].

2. Dipolar and dispersion coefficients for an equilateral triangle

With these zeroth-order wave functions Eqs. (53)–(55), for the isotopic $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1P)$, $\text{He}(2^1S)\text{-He}(2^1S)\text{-He}(2^1P)$, and $\text{He}(2^3S)\text{-He}(2^3S)\text{-He}(2^3P)$ systems, the corresponding long-range interaction coefficients are listed in Tables IV–VIII.

Table IV lists the first-order dipolar coefficients $C_3^{(IJ)}(1, M)$ for the equilateral triangle. We note that these coefficients all satisfy $C_3^{(IJ)}(1, M=0) = -2C_3^{(IJ)}(1, M=\pm 1)$. For $\Psi_{1,\Delta}^{(0)}$ with the geometric parameter $a = b = c = 1/\sqrt{3}$, $C_3^{(IJ)}(1, M=0)$ are all the same and negative; $C_3^{(IJ)}(1, M=\pm 1)$ are all the same and positive. For $\Psi_{2,\Delta}^{(0)}$ with the

TABLE XIII. The additive and nonadditive dispersion coefficients $C_8^{(IJ)}(1, M = \pm 1)$ and $C_8^{(IJ,JK)}(1, M = \pm 1)$ of the $\text{He}(n_0^i S)\text{-He}(n_0^j S)\text{-He}(n_0^k P)$ system for three different types of the zeroth-order wave functions, where the three atoms form a straight line, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_8^{(12)}(1, M = \pm 1)$	$C_8^{(23)}(1, M = \pm 1)$	$C_8^{(31)}(1, M = \pm 1)$	$C_8^{(12,23)}(1, M = \pm 1)$	$C_8^{(23,31)}(1, M = \pm 1)$	$C_8^{(31,12)}(1, M = \pm 1)$
He(1 1S)-He(1 1S)-He(2 1P)							
$^\infty\text{He}$	$\Psi_{1,-}^{(0)}$	3734.26752(8)	2640.58247(6)	3734.26752(8)	4.269968371(4)	4.269968371(4)	-3.155707222(3)
	$\Psi_{2,-}^{(0)}$	3958.5749(1)	2418.46662(5)	3958.5749(1)	-4.269968371(4)	-4.269968371(4)	-2.888834199(3)
	$\Psi_{3,-}^{(0)}$	2568.98676(5)	5202.7801(1)	2568.98676(5)	0	0	6.044541421(6)
^4He	$\Psi_{1,-}^{(0)}$	3736.92490(8)	2642.46139(6)	3736.92490(8)	4.271694335(4)	4.271694335(4)	-3.156982791(3)
	$\Psi_{2,-}^{(0)}$	3961.3633(1)	2420.18732(5)	3961.3633(1)	-4.271694335(4)	-4.271694335(4)	-2.890001895(3)
	$\Psi_{3,-}^{(0)}$	2570.80469(6)	5206.4442(1)	2570.80469(6)	0	0	6.046984686(6)
^3He	$\Psi_{1,-}^{(0)}$	3737.79465(8)	2643.07636(6)	3737.79465(8)	4.272259249(4)	4.272259249(4)	-3.157400290(4)
	$\Psi_{2,-}^{(0)}$	3962.27603(9)	2420.75050(5)	3962.27603(9)	-4.272259249(4)	-4.272259249(4)	-2.890384086(3)
	$\Psi_{3,-}^{(0)}$	2571.3997(1)	5207.6434(1)	2571.3997(1)	0	0	6.047784375(6)
He(2 1S)-He(2 1S)-He(2 1P)							
$^\infty\text{He}$	$\Psi_{1,-}^{(0)}$	677649(3)	696503(2)	677649(3)	271971.4176(4)	271971.4176(4)	-200999.6545(4)
	$\Psi_{2,-}^{(0)}$	2052935(3)	706714(2)	2052935(3)	-271971.4176(4)	-271971.4176(4)	-184001.46(2)
	$\Psi_{3,-}^{(0)}$	1182611(2)	2509977(5)	1182611(2)	0	0	385001.0952(6)
^4He	$\Psi_{1,-}^{(0)}$	678086(3)	696908(3)	678086(3)	272127.4354(4)	272127.4354(4)	-201114.9590(4)
	$\Psi_{2,-}^{(0)}$	2054147(4)	707118(2)	2054147(4)	-272127.4354(4)	-272127.4354(4)	-184106.9942(3)
	$\Psi_{3,-}^{(0)}$	1183287(2)	2511492(5)	1183287(2)	0	0	385221.9532(7)
^3He	$\Psi_{1,-}^{(0)}$	678229(3)	697041(3)	678229(3)	272178.4910(5)	272178.4910(5)	-201152.6912(3)
	$\Psi_{2,-}^{(0)}$	2054544(4)	707250(2)	2054544(4)	-272178.4910(5)	-272178.4910(5)	-184141.5356(3)
	$\Psi_{3,-}^{(0)}$	1183508(2)	2511988(5)	1183508(2)	0	0	385294.2270(7)
He(2 3S)-He(2 3S)-He(2 3P)							
$^\infty\text{He}$	$\Psi_{1,-}^{(0)}$	242087.18(2)	226143.71(2)	242087.18(2)	83146.60083(2)	83146.60083(2)	-61449.24409(1)
	$\Psi_{2,-}^{(0)}$	660377.03(2)	224826.36(1)	660377.03(2)	-83146.60083(2)	-83146.60083(2)	-56252.58154(1)
	$\Psi_{3,-}^{(0)}$	371010.24(1)	822504.39(2)	371010.24(1)	0	0	117701.82562(2)
^4He	$\Psi_{1,-}^{(0)}$	242141.77(1)	226210.21(2)	242141.77(1)	83173.14325(2)	83173.14325(2)	-61468.86023(5)
	$\Psi_{2,-}^{(0)}$	660542.33(2)	224895.80(1)	660542.33(2)	-83173.14325(2)	-83173.14325(2)	-56270.53874(1)
	$\Psi_{3,-}^{(0)}$	371117.31(2)	822695.40(2)	371117.31(2)	0	0	117739.39893(2)
^3He	$\Psi_{1,-}^{(0)}$	242159.65(2)	226231.97(2)	242159.65(2)	83181.82859(2)	83181.82859(2)	-61475.27906(1)
	$\Psi_{2,-}^{(0)}$	660596.40(1)	224918.54(2)	660596.40(1)	-83181.82859(2)	-83181.82859(2)	-56276.41479(2)
	$\Psi_{3,-}^{(0)}$	371152.34(2)	822757.90(2)	371152.34(2)	0	0	117751.69384(2)

geometric parameter $b = 0$, $a = -c = 1/\sqrt{2}$, $C_3^{(12)}(1, M) = C_3^{(23)}(1, M) = 0$; $C_3^{(31)}(1, M = 0)$ appears positive, $C_3^{(31)}(1, M = \pm 1)$ negative. For $\Psi_{3,\Delta}^{(0)}$ with the geometric parameter $b = -\sqrt{2/3}$, $a = c = 1/\sqrt{6}$, $C_3^{(12)}(1, M = 0)$ and $C_3^{(23)}(1, M = 0)$ are the same and positive; $C_3^{(12)}(1, M = \pm 1)$ and $C_3^{(23)}(1, M = \pm 1)$ are the same and negative. While $C_3^{(31)}(1, M = 0)$ appears negative, $C_3^{(31)}(1, M = \pm 1)$ are positive. All these relationships between these coefficients are due to the different values of geometric parameters. These positive or negative signs mean that different states of a fixed system may lead to different types of interaction: attraction or repulsion.

Table V lists the leading terms of the second-order long-range interaction $C_6^{(IJ)}(1, M = 0)$ and $C_6^{(IJ,JK)}(1, M = 0)$ for the equilateral triangle. Table VI

lists $C_6^{(IJ)}(1, M = \pm 1)$ and $C_6^{(IJ,JK)}(1, M = \pm 1)$. We note that the absolute values of $C_6^{(IJ)}(1, M = 0)$ and $C_6^{(IJ,JK)}(1, M = 0)$ are always a little bit larger than those of $C_6^{(IJ)}(1, M = \pm 1)$ and $C_6^{(IJ,JK)}(1, M = \pm 1)$, respectively. The additive interaction coefficients $C_6^{(IJ)}(1, M)$ are always positive, while the nonadditive interaction coefficients $C_6^{(IJ,JK)}(1, M)$ can be positive, negative, or zero. This is due to the different signs of $\mathbb{Q}_4(a, b, 1, M, \gamma)$ and geometric parameters. For example, for $\Psi_{2,\Delta}^{(0)}$, the nonadditive coefficients $C_6^{(12,23)}(1, M = 0)$ are negative because $\mathbb{Q}_4(a, b, 1, M, \gamma) > 0$ and $a = -c = 1/\sqrt{2}$; the nonadditive coefficients $C_6^{(23,31)}(1, M)$ and $C_6^{(31,12)}(1, M)$ are zero because $\mathbb{Q}_4(a, b, 1, M, \gamma) = 0$ and $b = 0$. The second-order long-range interactions $C_8^{(IJ)}(1, M)$ and $C_8^{(IJ,JK)}(1, M)$ have a very similar characteristic as $C_6^{(IJ)}(1, M)$

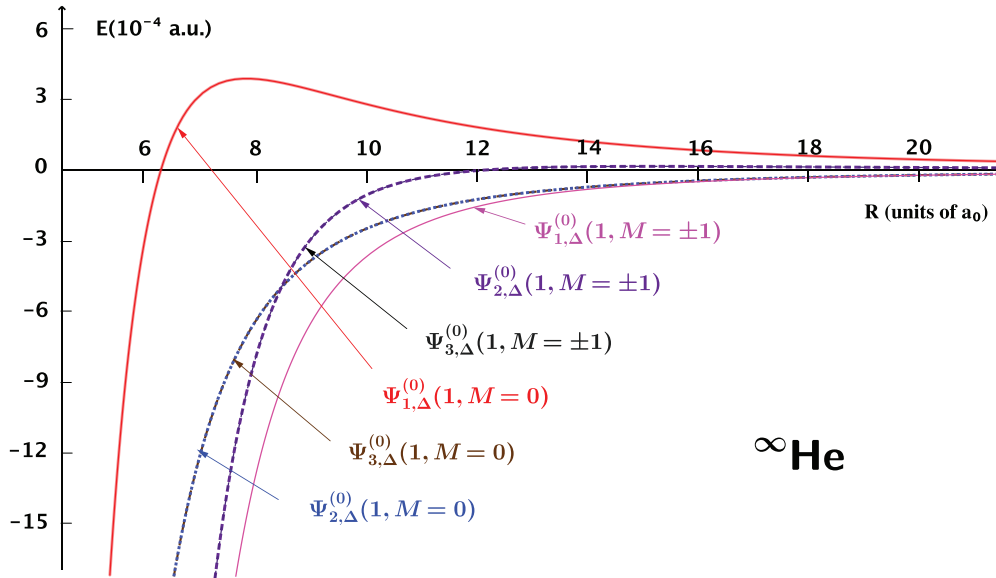


FIG. 2. Long-range potentials for the He(1^1S)-He(1^1S)-He(2^1P) system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. For each curve labeled by a wave function, the plotted curve is the sum of $\Delta E^{(1)}$ and $\Delta E^{(2)}$.

and $C_6^{(IJ,JK)}(1, M)$, respectively. The numerical values are listed in Tables VII and VIII.

From Tables V–VIII, we can see that the dispersion coefficients for the additive terms are always positive, but the dispersion coefficients for the nonadditive terms can be positive or negative or zero. Furthermore, the absolute values of the nonzero nonadditive dispersion coefficients are less than the additive dispersion coefficients by one to two orders of magnitude. However, the nonadditive terms may not be neglected in constructing an accurate potential surface. For example, the ratios of $(\frac{C_8^{(12,23)}(1, M=\pm 1)}{R_{12}^2 R_{23}^2}) / (\frac{C_8^{(12)}(1, M=\pm 1)}{R_{12}^3})$ for the $\Psi_{1,\Delta}^{(0)}$ of

He(1^1S)-He(1^1S)-He(2^1P), He(2^1S)-He(2^1S)-He(2^1P), and He(2^3S)-He(2^3S)-He(2^3P) systems are 0.08%, 26%, and 24%, respectively. The curves of potential energy (E), for the He(1^1S)-He(1^1S)-He(2^1P), He(2^1S)-He(2^1S)-He(2^1P), and He(2^3S)-He(2^3S)-He(2^3P) systems, corresponding to the different zeroth-order wave functions, are plotted in Figs. 2–4, respectively.

3. Zeroth-order wave function for a straight line

For the configuration of three atoms equally spaced and forming a straight line with $R_{12} = \frac{1}{2} R_{23} = R_{31} = R$, the

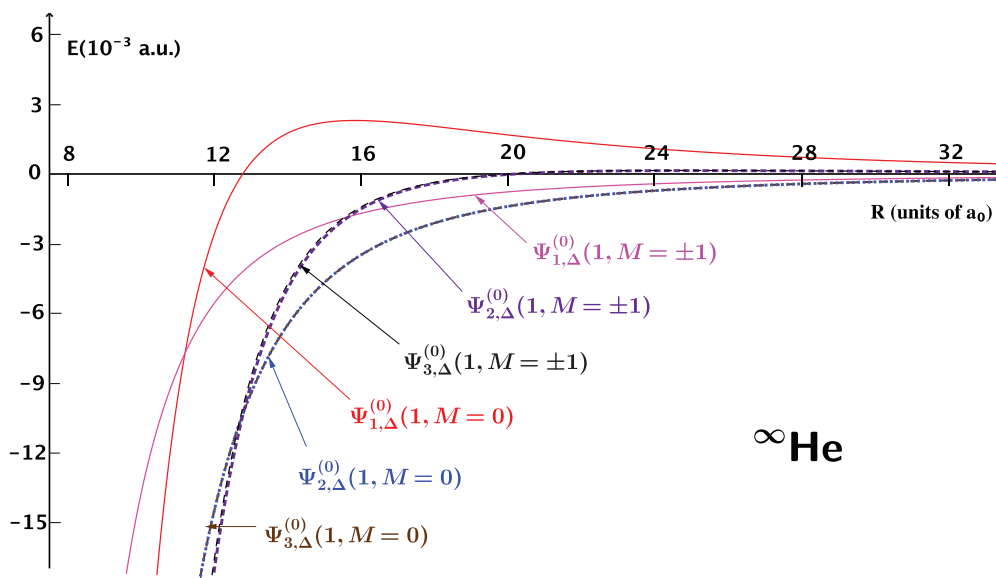


FIG. 3. Long-range potentials for the He(2^1S)-He(2^1S)-He(2^1P) system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. For each curve labeled by a wave function, the plotted curve is the sum of $\Delta E^{(1)}$ and $\Delta E^{(2)}$.

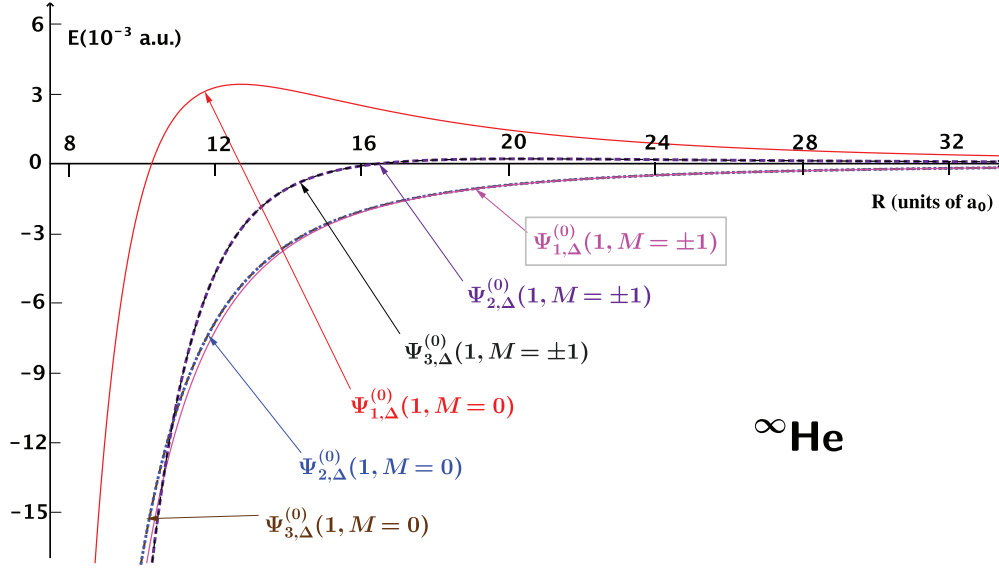


FIG. 4. Long-range potentials for the He(2^3S)-He(2^3S)-He(2^3P) system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle, in atomic units. For each curve labeled by a wave function, the plotted curve is the sum of $\Delta E^{(1)}$ and $\Delta E^{(2)}$.

perturbation matrix with respect to $\{\phi_1, \phi_2, \phi_3\}$ thus becomes

$$H' = H'_{12} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & \frac{1}{8} \\ 1 & \frac{1}{8} & 0 \end{pmatrix}. \quad (56)$$

Solving the eigenvalue problem of the above matrix, one obtains the eigenvalues $\frac{H'_{12}}{16}(1 + 3\sqrt{57})$, $\frac{H'_{12}}{16}(1 - 3\sqrt{57})$, $-\frac{H'_{12}}{8}$, and the corresponding zeroth-order wave functions

$$\begin{aligned} \Psi_{1,-}^{(0)} &= \frac{3\sqrt{57} - 1}{\sqrt{1026 - 6\sqrt{57}}} |\phi_1\rangle + \frac{16}{\sqrt{1026 - 6\sqrt{57}}} |\phi_2\rangle \\ &+ \frac{16}{\sqrt{1026 - 6\sqrt{57}}} |\phi_3\rangle, \end{aligned} \quad (57)$$

$$\begin{aligned} \Psi_{2,-}^{(0)} &= \frac{-(3\sqrt{57} + 1)}{\sqrt{1026 + 6\sqrt{57}}} |\phi_1\rangle + \frac{16}{\sqrt{1026 + 6\sqrt{57}}} |\phi_2\rangle \\ &+ \frac{16}{\sqrt{1026 + 6\sqrt{57}}} |\phi_3\rangle, \end{aligned} \quad (58)$$

$$\Psi_{3,-}^{(0)} = -\frac{1}{\sqrt{2}} |\phi_2\rangle + \frac{1}{\sqrt{2}} |\phi_3\rangle, \quad (59)$$

where the symbol “—” denotes the geometrical configuration of a straight line.

4. Dipolar and dispersion coefficients for a straight line

With these zeroth-order wave functions Eqs. (57)–(59), for the isotopic He(1^1S)-He(1^1S)-He(2^1P), He(2^1S)-He(2^1S)-

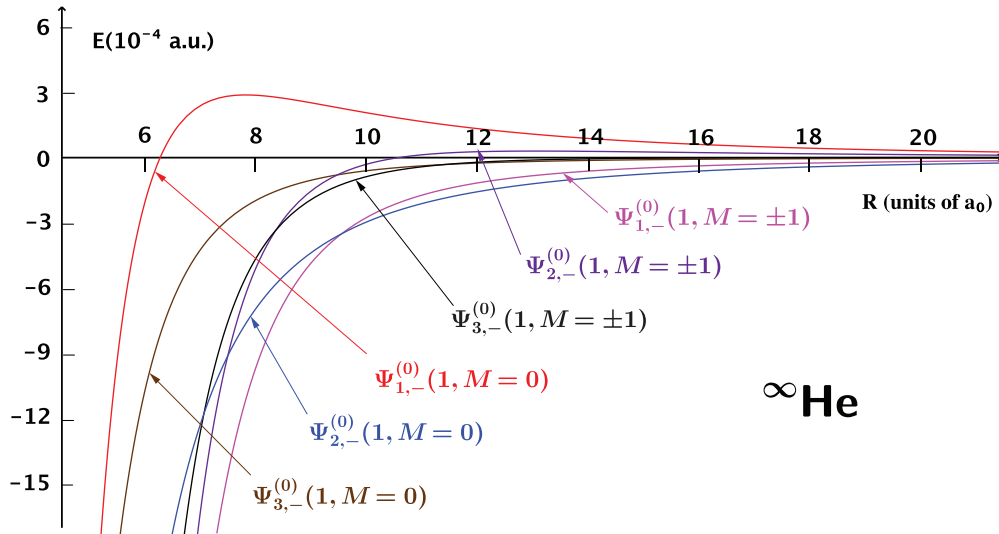


FIG. 5. Long-range potentials for the He(1^1S)-He(1^1S)-He(2^1P) system for three different types of the zeroth-order wave functions, where the three atoms form a straight line, in atomic units. For each curve labeled by a wave function, the plotted curve is the sum of $\Delta E^{(1)}$ and $\Delta E^{(2)}$.

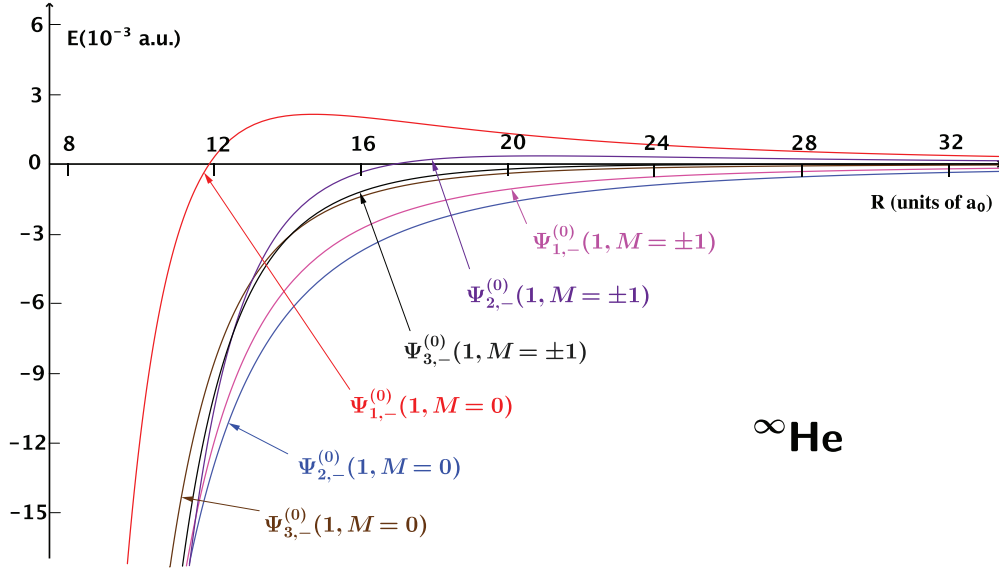


FIG. 6. Long-range potentials for the He(2^1S)-He(2^1S)-He(2^1P) system for three different types of the zeroth-order wave functions, where the three atoms form a straight line, in atomic units. For each curve labeled by a wave function, the plotted curve is the sum of $\Delta E^{(1)}$ and $\Delta E^{(2)}$.

He(2^1P), and He(2^3S)-He(2^3S)-He(2^3P) systems, the corresponding long-range interaction coefficients are listed in Tables IX–XIII.

Table IX lists the first-order dipolar coefficients $C_3^{(31)}(1, M)$ for a straight line. We note that $C_3^{(12)}(1, M) = C_3^{(31)}(1, M)$ for all three zeroth-order wave functions $\Psi_{1,-}^{(0)}$, $\Psi_{2,-}^{(0)}$ with the geometric parameters $b = c$ and $\Psi_{3,-}^{(0)}$ with the geometric parameter $a = 0$. This is why $C_3^{(12)}(1, M) = C_3^{(31)}(1, M) = 0$ for $\Psi_{3,-}^{(0)}$. Similar to the coefficients shown in Table IV, these coefficients also satisfy $C_3^{(IJ)}(1, M = 0) = -2C_3^{(IJ)}(1, M = \pm 1)$. However, the numerical values of these coefficients are totally different. This is because a change in geometric configuration would lead to a change in the quantum state of the three-body system, causing changes in these long-range interaction coefficients.

Tables X–XIII list the second-order dispersion coefficients $C_6^{(IJ)}(1, M)$, $C_6^{(IJ,JK)}(1, M)$, $C_8^{(IJ)}(1, M)$, and $C_8^{(IJ,JK)}(1, M)$ for a straight line. We note that $C_6^{(12)}(1, M) = C_6^{(31)}(1, M)$, $C_6^{(12,23)}(1, M) = C_6^{(23,31)}(1, M)$, $C_8^{(12)}(1, M) = C_8^{(31)}(1, M)$, and $C_8^{(12,23)}(1, M) = C_8^{(23,31)}(1, M)$ because $b = \pm c$, $a = 0$, and $\beta = \gamma$. We find that allowing for finite nuclear mass increases the additive dispersion coefficients, as shown in Tables X–XIII. The nonadditive terms may also not be neglected in constructing a three-body potential surface for He(n_0^1S)-He(n_0^1S)-He(n_0^1P). The curves of potential energy (E) of the He(1^1S)-He(1^1S)-He(2^1P), He(2^1S)-He(2^1S)-He(2^1P), and He(2^3S)-He(2^3S)-He(2^3P) systems, resulting from $\Delta E^{(1)}$ and $\Delta E^{(2)}$ for this geometrical structure, are shown in Figs. 5–7, respectively.

5. Zeroth-order wave function for an isosceles right triangle

For the configuration of three atoms forming an isosceles right triangle with $R_{12} = \frac{1}{\sqrt{2}} R_{23} = R_{31} = R$, the perturbation matrix with respect to $\{\phi_1, \phi_2, \phi_3\}$ thus

becomes

$$H' = H'_{12} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & \frac{1}{2\sqrt{2}} \\ 1 & \frac{1}{2\sqrt{2}} & 0 \end{pmatrix}. \quad (60)$$

Solving the eigenvalue problem of the above matrix, one obtains the eigenvalues, $\frac{H'_{12}}{8}(\sqrt{2} + \sqrt{130})$, $\frac{H'_{12}}{8}(\sqrt{2} - \sqrt{130})$, $-\frac{H'_{12}}{2\sqrt{2}}$, and the corresponding zeroth-order wave functions

$$\begin{aligned} \Psi_{1,\perp}^{(0)} &= \frac{\sqrt{130} - \sqrt{2}}{2\sqrt{65 - \sqrt{65}}} |\phi_1\rangle + \frac{4}{\sqrt{65 - \sqrt{65}}} |\phi_2\rangle \\ &+ \frac{4}{\sqrt{65 - \sqrt{65}}} |\phi_3\rangle, \end{aligned} \quad (61)$$

$$\begin{aligned} \Psi_{2,\perp}^{(0)} &= \frac{-(\sqrt{130} + \sqrt{2})}{2\sqrt{65 + \sqrt{65}}} |\phi_1\rangle + \frac{4}{\sqrt{65 + \sqrt{65}}} |\phi_2\rangle \\ &+ \frac{4}{\sqrt{65 + \sqrt{65}}} |\phi_3\rangle, \end{aligned} \quad (62)$$

$$\Psi_{3,\perp}^{(0)} = -\frac{1}{\sqrt{2}} |\phi_2\rangle + \frac{1}{\sqrt{2}} |\phi_3\rangle, \quad (63)$$

where the symbol “ \perp ” denotes the geometrical configuration of an isosceles right triangle.

6. Dipolar and dispersion coefficients for an isosceles right triangle

The dispersion coefficients of an isosceles right triangle have very similar characteristics to the case of the straight line. Thus the values of dispersion coefficients $C_3^{(IJ)}(1, M)$, $C_6^{(IJ)}(1, M)$, $C_6^{(IJ,JK)}(1, M)$, $C_8^{(IJ)}(1, M)$, and $C_8^{(IJ,JK)}(1, M)$ and the corresponding potential energy curves

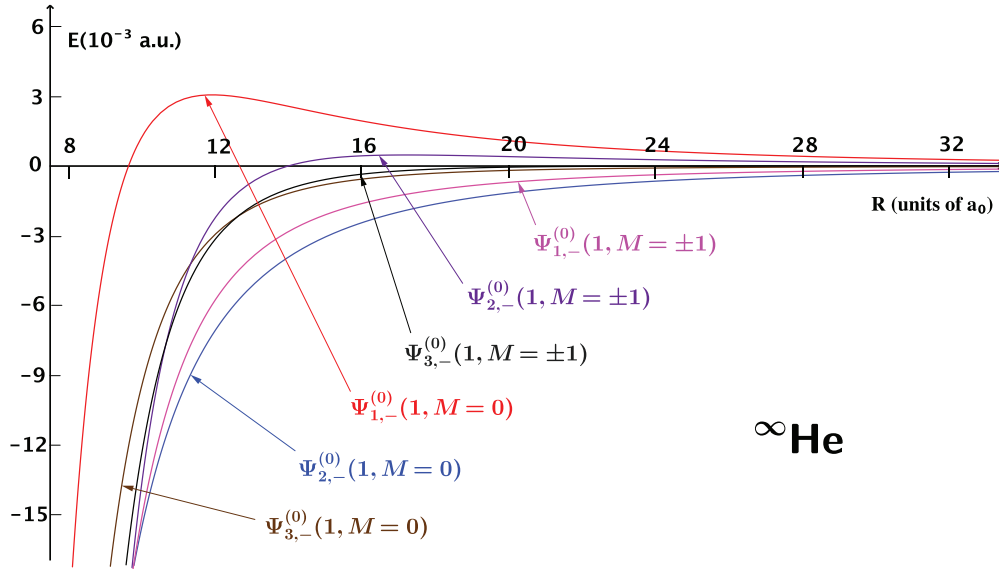


FIG. 7. Long-range potentials for the $\text{He}(2^3S)\text{-He}(2^3S)\text{-He}(2^3P)$ system for three different types of the zeroth-order wave functions, where the three atoms form a straight line, in atomic units. For each curve labeled by a wave function, the plotted curve is the sum of $\Delta E^{(1)}$ and $\Delta E^{(2)}$.

for $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}P)$ are listed in the Supplemental Material [24].

IV. CONCLUSION

The long-range additive dipolar and additive dispersion interactions and nonadditive dispersion interactions C_3 , C_6 , and C_8 for the $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}L)$ systems $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1S)$, $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1P)$, $\text{He}(2^1S)\text{-He}(2^1S)\text{-He}(2^1P)$, and $\text{He}(2^3S)\text{-He}(2^3S)\text{-He}(2^3P)$ were obtained by perturbation theory. We considered configurations of three like-nuclei for the hypothetical infinite mass He nucleus and for the ^3He and the ^4He nucleus.

The coefficients are dependent on the geometrical configuration of the atoms. We note that the geometry-dependent nonadditive dispersion interactions for the degenerate $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}P)$ system start to appear at the *second order* in the perturbative treatment, in contrast to the case of three S atoms where nonadditive dispersion interactions appear at the *third order*. The formulas obtained apply to all geometrical configurations and we demonstrated the methodology for three basic types of geometrical configurations (nuclei forming an equilateral triangle or an isosceles triangle, or nuclei equally spaced and collinear) by calculating these coefficients to high precision using variational wave functions in Hylleraas coordinates. Our numerical results may be useful in constructing accurate three-body potential curves and for applications to scattering and recombination studies.

The present numerical approach differs from widely used “single-electron” approaches (e.g., “model potentials”) used for the calculation of trimer interactions involving three highly excited alkali-metal atoms each in a Rydberg state (see, for example, Ref. [25]) in that we include fully the correlation of the electrons in the He atoms. On the other hand, the electronic structure of metastable triplet He atoms is similar to alkali-metal atoms in the sense of having a single active electron, so a comparison with the theory of Ref. [25] might be possible.

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APPENDIX

In the present work, we take the mutual electrostatic interactions V_{IJ} between pairs of atoms for the $\text{He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)\text{-He}(n_0^{\lambda}S)$ system as a perturbation. According to degenerate perturbation theory, the zeroth-order wave function of the unperturbed system can be written as

$$|\Psi^{(0)}\rangle = a|\phi_1\rangle + b|\phi_2\rangle + c|\phi_3\rangle, \quad (\text{A1})$$

where ϕ_1 , ϕ_2 , and ϕ_3 are three orthogonal eigenvectors corresponding to the same energy eigenvalue $E_{n_0n_0n_0}^{(0)} = 2E_{n_0S}^{(0)} + E_{n_0S}^{(0)}$. With the zeroth-order wave function of Eq. (A1), we can derive general formulas of the dispersion coefficients for the $\text{He}(1^1S)\text{-He}(1^1S)\text{-He}(2^1S)$ system. The values of coefficients a , b , and c can be obtained by the degenerate perturbation theory.

1. The zeroth-order wave function

According to degenerate perturbation theory, the zeroth-order energy correction is obtained by the perturbation matrix with respect to $\{\phi_1, \phi_2, \phi_3\}$,

$$H' = \begin{pmatrix} \Delta_{11} & \Delta_{12} & \Delta_{13} \\ \Delta_{12}^* & \Delta_{22} & \Delta_{23} \\ \Delta_{13}^* & \Delta_{23}^* & \Delta_{33} \end{pmatrix}, \quad (\text{A2})$$

where

$$\begin{aligned}
 \Delta_{11} &= - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \frac{|\langle \phi_1 | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\zeta}) \rangle|^2}{E_{n_s L_s n_t L_t n_u L_u} - E_{n_0 S; n_0 S; n'_0 S}^{(0)}} \\
 &= - \sum_{n_s n_t} \sum_{L_s L_t} \sum_{M_s M_t} \frac{16\pi^2}{R_{12}^{2L_s+2L_t+2}} \frac{[P_{L_s+L_t}^{M_s+M_t}(0)(L_s+L_t-M_s-M_t)!]^2 (L_s, L_t)^{-2}}{(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!} \\
 &\quad \times \frac{|\langle \varphi_{n'_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}} \\
 &\quad - \sum_{n_t n_u} \sum_{L_t L_u} \sum_{M_t M_u} \frac{16\pi^2}{R_{23}^{2L_t+2L_u+2}} \frac{[P_{L_t+L_u}^{M_t+M_u}(0)(L_t+L_u-M_t-M_u)!]^2 (L_t, L_u)^{-2}}{(L_t+M_t)!(L_t-M_t)!(L_u+M_u)!(L_u-M_u)!} \\
 &\quad \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\zeta}) \| T_{L_u}(\boldsymbol{\zeta}) \| \chi_{n_u}(L_u; \boldsymbol{\zeta}) \rangle|^2}{E_{n_t L_t} + E_{n_u L_u} - 2E_{n_0 S}^{(0)}} \\
 &\quad - \sum_{n_s n_u} \sum_{L_s L_u} \sum_{M_s M_u} \frac{16\pi^2}{R_{31}^{2L_s+2L_u+2}} \frac{[P_{L_u+L_s}^{M_u+M_s}(0)(L_u+L_s-M_u-M_s)!]^2 (L_u, L_s)^{-2}}{(L_u+M_u)!(L_u-M_u)!(L_s+M_s)!(L_s-M_s)!} \\
 &\quad \times \frac{|\langle \varphi_{n'_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\zeta}) \| T_{L_u}(\boldsymbol{\zeta}) \| \chi_{n_u}(L_u; \boldsymbol{\zeta}) \rangle|^2}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S} - E_{n'_0 S}}, \tag{A3}
 \end{aligned}$$

$$\begin{aligned}
 \Delta_{22} &= - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \frac{|\langle \phi_2 | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\zeta}) \rangle|^2}{E_{n_s L_s n_t L_t n_u L_u} - E_{n_0 S; n_0 S; n'_0 S}^{(0)}} \\
 &= - \sum_{n_s n_t} \sum_{L_s L_t} \sum_{M_s M_t} \frac{16\pi^2}{R_{12}^{2L_s+2L_t+2}} \frac{[P_{L_s+L_t}^{M_s+M_t}(0)(L_s+L_t-M_s-M_t)!]^2 (L_s, L_t)^{-2}}{(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!} \\
 &\quad \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n'_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}} \\
 &\quad - \sum_{n_t n_u} \sum_{L_t L_u} \sum_{M_t M_u} \frac{16\pi^2}{R_{23}^{2L_t+2L_u+2}} \frac{[P_{L_t+L_u}^{M_t+M_u}(0)(L_t+L_u-M_t-M_u)!]^2 (L_t, L_u)^{-2}}{(L_t+M_t)!(L_t-M_t)!(L_u+M_u)!(L_u-M_u)!} \\
 &\quad \times \frac{|\langle \varphi_{n'_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\zeta}) \| T_{L_u}(\boldsymbol{\zeta}) \| \chi_{n_u}(L_u; \boldsymbol{\zeta}) \rangle|^2}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}} \\
 &\quad - \sum_{n_s n_u} \sum_{L_s L_u} \sum_{M_s M_u} \frac{16\pi^2}{R_{31}^{2L_s+2L_u+2}} \frac{[P_{L_u+L_s}^{M_u+M_s}(0)(L_u+L_s-M_u-M_s)!]^2 (L_u, L_s)^{-2}}{(L_u+M_u)!(L_u-M_u)!(L_s+M_s)!(L_s-M_s)!} \\
 &\quad \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\zeta}) \| T_{L_u}(\boldsymbol{\zeta}) \| \chi_{n_u}(L_u; \boldsymbol{\zeta}) \rangle|^2}{E_{n_s L_s} + E_{n_u L_u} - 2E_{n_0 S}}, \tag{A4}
 \end{aligned}$$

$$\begin{aligned}
 \Delta_{33} &= - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \frac{|\langle \phi_3 | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\zeta}) \rangle|^2}{E_{n_s L_s n_t L_t n_u L_u} - E_{n_0 S; n_0 S; n'_0 S}^{(0)}} \\
 &= - \sum_{n_s n_t} \sum_{L_s L_t} \sum_{M_s M_t} \frac{16\pi^2}{R_{12}^{2L_s+2L_t+2}} \frac{[P_{L_s+L_t}^{M_s+M_t}(0)(L_s+L_t-M_s-M_t)!]^2 (L_s, L_t)^{-2}}{(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!} \\
 &\quad \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - 2E_{n_0 S}^{(0)}} \\
 &\quad - \sum_{n_t n_u} \sum_{L_t L_u} \sum_{M_t M_u} \frac{16\pi^2}{R_{23}^{2L_t+2L_u+2}} \frac{[P_{L_t+L_u}^{M_t+M_u}(0)(L_t+L_u-M_t-M_u)!]^2 (L_t, L_u)^{-2}}{(L_t+M_t)!(L_t-M_t)!(L_u+M_u)!(L_u-M_u)!}
 \end{aligned}$$

$$\begin{aligned} & \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle|^2 |\langle \varphi_{n'_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle|^2}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}} \\ & - \sum_{n_s n_u} \sum_{L_s L_u} \sum_{M_s M_u} \frac{16\pi^2}{R_{31}^{2L_s+2L_u+2}} \frac{[P_{L_u+L_s}^{M_u+M_s}(0)(L_u+L_s-M_u-M_s)!]^2 (L_u, L_s)^{-2}}{(L_u+M_u)!(L_u-M_u)!(L_s+M_s)!(L_s-M_s)!} \\ & \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle|^2}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S} - E_{n'_0 S}}, \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} \Delta_{12} &= - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \langle \phi_1 | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\varsigma}) \rangle^* \\ & \times \frac{\langle \phi_2 | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\varsigma}) \rangle}{E_{n_s L_s; n_t L_t; n_u L_u} - E_{n_0 S; n_0 S; n'_0 S}^{(0)}} \\ & = - \sum_{n_s n_t} \sum_{L_s L_t} \sum_{M_s M_t} \frac{16\pi^2}{R_{12}^{2L_s+2L_t+2}} \frac{[P_{L_s+L_t}^{M_s+M_t}(0)(L_s+L_t-M_s-M_t)!]^2 (L_s, L_t)^{-2}}{(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!} \\ & \times \langle \varphi_{n'_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle^* \langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle^* \\ & \times \frac{\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle \langle \varphi_{n'_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}}, \end{aligned} \quad (\text{A6})$$

$$\begin{aligned} \Delta_{13} &= - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \langle \phi_1 | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\varsigma}) \rangle^* \\ & \times \frac{\langle \phi_3 | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\varsigma}) \rangle}{E_{n_s L_s; n_t L_t; n_u L_u} - E_{n_0 S; n_0 S; n'_0 S}^{(0)}} \\ & = - \sum_{n_s n_u} \sum_{L_s L_u} \sum_{M_s M_u} \frac{16\pi^2}{R_{31}^{2L_s+2L_u+2}} \frac{[P_{L_u+L_s}^{M_u+M_s}(0)(L_u+L_s-M_u-M_s)!]^2 (L_u, L_s)^{-2}}{(L_u+M_u)!(L_u-M_u)!(L_s+M_s)!(L_s-M_s)!} \\ & \times \langle \varphi_{n'_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle^* \langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle^* \\ & \times \frac{\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle \langle \varphi_{n'_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S} - E_{n'_0 S}}, \end{aligned} \quad (\text{A7})$$

$$\begin{aligned} \Delta_{23} &= - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \langle \phi_2 | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\varsigma}) \rangle^* \\ & \times \frac{\langle \phi_3 | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\varsigma}) \rangle}{E_{n_s L_s; n_t L_t; n_u L_u} - E_{n_0 S; n_0 S; n'_0 S}^{(0)}} \\ & = - \sum_{n_t n_u} \sum_{L_t L_u} \sum_{M_t M_u} \frac{16\pi^2}{R_{23}^{2L_t+2L_u+2}} \frac{[P_{L_t+L_u}^{M_t+M_u}(0)(L_t+L_u-M_t-M_u)!]^2 (L_t, L_u)^{-2}}{(L_t+M_t)!(L_t-M_t)!(L_u+M_u)!(L_u-M_u)!} \\ & \times \langle \varphi_{n'_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle^* \langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle^* \\ & \times \frac{\langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle \langle \varphi_{n'_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}}. \end{aligned} \quad (\text{A8})$$

We solve this eigenvalue problem to get the eigenvalues and corresponding zeroth-order wave functions.

2. The second-order energy correction

The second-order energy correction is given by

$$\Delta E^{(2)} = - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \frac{|\langle \Psi^{(0)} | V_{123} | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \chi_{n_t}(L_t M_t; \boldsymbol{\rho}) \chi_{n_u}(L_u M_u; \boldsymbol{\varsigma}) \rangle|^2}{E_{n_s L_s; n_t L_t; n_u L_u} - E_{n_0 S; n_0 S; n'_0 S}^{(0)}} = V_{12}^{(2)} + V_{23}^{(2)} + V_{31}^{(2)}, \quad (\text{A9})$$

where $\chi_{n_s}(L_s M_s; \sigma) \chi_{n_t}(L_t M_t; \rho) \chi_{n_u}(L_u M_u; \zeta)$ is an intermediate state of the system with the energy eigenvalue $E_{n_s L_s; n_t L_t; n_u L_u} = E_{n_s L_s} + E_{n_t L_t} + E_{n_u L_u}$. It is noted that the above summations should exclude terms with $E_{n_s L_s; n_t L_t; n_u L_u} = E_{n_0 S}^{(0)}$. Then the three additive terms in the second-order energy correction, denoted by $V_{12}^{(2)}$, $V_{23}^{(2)}$, and $V_{31}^{(2)}$, become, respectively,

$$\begin{aligned}
 V_{12}^{(2)} &= -|a|^2 \sum_{n_s n_t} \sum_{L_s L_t} \sum_{M_s M_t} \frac{16\pi^2}{R_{12}^{2L_s+2L_t+2}} \frac{[P_{L_s+L_t}^{M_s+M_t}(0)(L_s+L_t-M_s-M_t)!]^2 (L_s, L_t)^{-2}}{(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!} \\
 &\quad \times \frac{|\langle \varphi_{n_0}'(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle|^2 |\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n_0 S}^{(0)}} \\
 &\quad - |b|^2 \sum_{n_s n_t} \sum_{L_s L_t} \sum_{M_s M_t} \frac{16\pi^2}{R_{12}^{2L_s+2L_t+2}} \frac{[P_{L_s+L_t}^{M_s+M_t}(0)(L_s+L_t-M_s-M_t)!]^2 (L_s, L_t)^{-2}}{(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!} \\
 &\quad \times \frac{|\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle|^2 |\langle \varphi_{n_0}'(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n_0 S}^{(0)}} \\
 &\quad - |c|^2 \sum_{n_s n_t} \sum_{L_s L_t} \sum_{M_s M_t} \frac{16\pi^2}{R_{12}^{2L_s+2L_t+2}} \frac{[P_{L_s+L_t}^{M_s+M_t}(0)(L_s+L_t-M_s-M_t)!]^2 (L_s, L_t)^{-2}}{(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!} \\
 &\quad \times \frac{|\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle|^2 |\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - 2E_{n_0 S}^{(0)}} \\
 &\quad - a^* b \sum_{n_s n_t} \sum_{L_s L_t} \sum_{M_s M_t} \frac{16\pi^2}{R_{12}^{2L_s+2L_t+2}} \frac{[P_{L_s+L_t}^{M_s+M_t}(0)(L_s+L_t-M_s-M_t)!]^2 (L_s, L_t)^{-2}}{(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!} \\
 &\quad \times \frac{\langle \varphi_{n_0}'(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle^* \langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle^*}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n_0 S}^{(0)}} \\
 &\quad \times \frac{\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle \langle \varphi_{n_0}'(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n_0 S}^{(0)}} \\
 &\quad - b^* a \sum_{n_s n_t} \sum_{L_s L_t} \sum_{M_s M_t} \frac{16\pi^2}{R_{12}^{2L_s+2L_t+2}} \frac{[P_{L_s+L_t}^{M_s+M_t}(0)(L_s+L_t-M_s-M_t)!]^2 (L_s, L_t)^{-2}}{(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!} \\
 &\quad \times \frac{\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle^* \langle \varphi_{n_0}'(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle^*}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n_0 S}^{(0)}} \\
 &\quad \times \frac{\langle \varphi_{n_0}'(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle \langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n_0 S}^{(0)}} \\
 &= - \left\{ |a|^2 \sum_{n_s n_t} \sum_{L_s L_t} \frac{K_1(n_s, n_t, L_s, L_t)}{R_{12}^{2L_s+2L_t+2}} + |b|^2 \sum_{n_s n_t} \sum_{L_s L_t} \frac{K_1(n_t, n_s, L_t, L_s)}{R_{12}^{2L_s+2L_t+2}} \right. \\
 &\quad \left. + |c|^2 \sum_{n_s n_t} \sum_{L_s L_t} \frac{K_2(n_s, n_t, L_s, L_t)}{R_{12}^{2L_s+2L_t+2}} + a^* b \sum_{n_s n_t} \sum_{L_s L_t} \frac{K_3(n_s, n_t, L_s, L_t)}{R_{12}^{2L_s+2L_t+2}} + b^* a \sum_{n_s n_t} \sum_{L_s L_t} \frac{K_3^*(n_s, n_t, L_s, L_t)}{R_{12}^{2L_s+2L_t+2}} \right\}, \quad (\text{A10}) \\
 V_{23}^{(2)} &= -|a|^2 \sum_{n_t n_u} \sum_{L_t L_u} \sum_{M_t M_u} \frac{16\pi^2}{R_{23}^{2L_t+2L_u+2}} \frac{[P_{L_t+L_u}^{M_t+M_u}(0)(L_t+L_u-M_t-M_u)!]^2 (L_t, L_u)^{-2}}{(L_t+M_t)!(L_t-M_t)!(L_u+M_u)!(L_u-M_u)!} \\
 &\quad \times \frac{|\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2 |\langle \varphi_{n_0}(0; \zeta) \| T_{L_u}(\zeta) \| \chi_{n_u}(L_u; \zeta) \rangle|^2}{E_{n_t L_t} + E_{n_u L_u} - 2E_{n_0 S}^{(0)}} \\
 &\quad - |b|^2 \sum_{n_t n_u} \sum_{L_t L_u} \sum_{M_t M_u} \frac{16\pi^2}{R_{23}^{2L_t+2L_u+2}} \frac{[P_{L_t+L_u}^{M_t+M_u}(0)(L_t+L_u-M_t-M_u)!]^2 (L_t, L_u)^{-2}}{(L_t+M_t)!(L_t-M_t)!(L_u+M_u)!(L_u-M_u)!} \\
 &\quad \times \frac{|\langle \varphi_{n_0}'(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2 |\langle \varphi_{n_0}(0; \zeta) \| T_{L_u}(\zeta) \| \chi_{n_u}(L_u; \zeta) \rangle|^2}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n_0 S}^{(0)}}
 \end{aligned}$$

$$\begin{aligned}
& -|c|^2 \sum_{n_t n_u} \sum_{L_t L_u} \sum_{M_t M_u} \frac{16\pi^2}{R_{23}^{2L_t+2L_u+2}} \frac{[P_{L_t+L_u}^{M_t+M_u}(0)(L_t+L_u-M_t-M_u)!]^2 (L_t, L_u)^{-2}}{(L_t+M_t)!(L_t-M_t)!(L_u+M_u)!(L_u-M_u)!} \\
& \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle|^2 |\langle \varphi_{n'_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle|^2}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}} \\
& - b^* c \sum_{n_t n_u} \sum_{L_t L_u} \sum_{M_t M_u} \frac{16\pi^2}{R_{23}^{2L_t+2L_u+2}} \frac{[P_{L_t+L_u}^{M_t+M_u}(0)(L_t+L_u-M_t-M_u)!]^2 (L_t, L_u)^{-2}}{(L_t+M_t)!(L_t-M_t)!(L_u+M_u)!(L_u-M_u)!} \\
& \times \langle \varphi_{n'_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle^* \langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle^* \\
& \times \frac{\langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle \langle \varphi_{n'_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}} \\
& - c^* b \sum_{n_t n_u} \sum_{L_t L_u} \sum_{M_t M_u} \frac{16\pi^2}{R_{23}^{2L_t+2L_u+2}} \frac{[P_{L_t+L_u}^{M_t+M_u}(0)(L_t+L_u-M_t-M_u)!]^2 (L_t, L_u)^{-2}}{(L_t+M_t)!(L_t-M_t)!(L_u+M_u)!(L_u-M_u)!} \\
& \times \langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle^* \langle \varphi_{n'_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle^* \\
& \times \frac{\langle \varphi_{n'_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle \langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}} \\
& = - \left\{ |a|^2 \sum_{n_t n_u} \sum_{L_t L_u} \frac{K_2(n_t, n_u, L_t, L_u)}{R_{23}^{2L_t+2L_u+2}} + |b|^2 \sum_{n_t n_u} \sum_{L_t L_u} \frac{K_1(n_t, n_u, L_t, L_u)}{R_{23}^{2L_t+2L_u+2}} \right. \\
& \left. + |c|^2 \sum_{n_t n_u} \sum_{L_t L_u} \frac{K_1(n_u, n_t, L_u, L_t)}{R_{23}^{2L_t+2L_u+2}} + b^* c \sum_{n_t n_u} \sum_{L_t L_u} \frac{K_3(n_t, n_u, L_t, L_u)}{R_{23}^{2L_t+2L_u+2}} + c^* b \sum_{n_t n_u} \sum_{L_t L_u} \frac{K_3^*(n_t, n_u, L_t, L_u)}{R_{23}^{2L_t+2L_u+2}} \right\}, \quad (\text{A11}) \\
V_{31}^{(2)} & = -|a|^2 \sum_{n_s n_u} \sum_{L_s L_u} \sum_{M_s M_u} \frac{16\pi^2}{R_{31}^{2L_s+2L_u+2}} \frac{[P_{L_u+L_s}^{M_u+M_s}(0)(L_u+L_s-M_u-M_s)!]^2 (L_u, L_s)^{-2}}{(L_u+M_u)!(L_u-M_u)!(L_s+M_s)!(L_s-M_s)!} \\
& \times \frac{|\langle \varphi_{n'_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle|^2}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S} - E_{n'_0 S}} \\
& - |b|^2 \sum_{n_s n_u} \sum_{L_s L_u} \sum_{M_s M_u} \frac{16\pi^2}{R_{31}^{2L_s+2L_u+2}} \frac{[P_{L_u+L_s}^{M_u+M_s}(0)(L_u+L_s-M_u-M_s)!]^2 (L_u, L_s)^{-2}}{(L_u+M_u)!(L_u-M_u)!(L_s+M_s)!(L_s-M_s)!} \\
& \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle|^2}{E_{n_s L_s} + E_{n_u L_u} - 2E_{n_0 S}} \\
& - |c|^2 \sum_{n_s n_u} \sum_{L_s L_u} \sum_{M_s M_u} \frac{16\pi^2}{R_{31}^{2L_s+2L_u+2}} \frac{[P_{L_u+L_s}^{M_u+M_s}(0)(L_u+L_s-M_u-M_s)!]^2 (L_u, L_s)^{-2}}{(L_u+M_u)!(L_u-M_u)!(L_s+M_s)!(L_s-M_s)!} \\
& \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle|^2}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S} - E_{n'_0 S}} \\
& - c^* a \sum_{n_s n_u} \sum_{L_s L_u} \sum_{M_s M_u} \frac{16\pi^2}{R_{31}^{2L_s+2L_u+2}} \frac{[P_{L_u+L_s}^{M_u+M_s}(0)(L_u+L_s-M_u-M_s)!]^2 (L_u, L_s)^{-2}}{(L_u+M_u)!(L_u-M_u)!(L_s+M_s)!(L_s-M_s)!} \\
& \times \langle \varphi_{n'_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle^* \langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle^* \\
& \times \frac{\langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle \langle \varphi_{n'_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S} - E_{n'_0 S}} \\
& - a^* c \sum_{n_s n_u} \sum_{L_s L_u} \sum_{M_s M_u} \frac{16\pi^2}{R_{31}^{2L_s+2L_u+2}} \frac{[P_{L_u+L_s}^{M_u+M_s}(0)(L_u+L_s-M_u-M_s)!]^2 (L_u, L_s)^{-2}}{(L_u+M_u)!(L_u-M_u)!(L_s+M_s)!(L_s-M_s)!}
\end{aligned}$$

$$\begin{aligned}
 & \times \langle \varphi_{n'_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle^* \langle \varphi_{n_0}(0; \boldsymbol{\zeta}) \| T_{L_u}(\boldsymbol{\zeta}) \| \chi_{n_u}(L_u; \boldsymbol{\zeta}) \rangle^* \\
 & \times \frac{\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle \langle \varphi_{n'_0}(0; \boldsymbol{\zeta}) \| T_{L_u}(\boldsymbol{\zeta}) \| \chi_{n_u}(L_u; \boldsymbol{\zeta}) \rangle}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S} - E_{n'_0 S}} \\
 & = - \left\{ |a|^2 \sum_{n_s n_u} \sum_{L_s L_u} \frac{K_1(n_s, n_u, L_s, L_u)}{R_{31}^{2L_u+2L_s+2}} + |b|^2 \sum_{n_s n_u} \sum_{L_s L_u} \frac{K_2(n_s, n_u, L_s, L_u)}{R_{31}^{2L_s+2L_u+2}} + |c|^2 \sum_{n_s n_u} \sum_{L_s L_u} \frac{K_1(n_u, n_s, L_u, L_s)}{R_{31}^{2L_s+2L_u+2}} \right. \\
 & \left. + a^* c \sum_{n_s n_u} \sum_{L_s L_u} \frac{K_3(n_u, n_s, L_u, L_s)}{R_{31}^{2L_s+2L_u+2}} + c^* a \sum_{n_s n_u} \sum_{L_s L_u} \frac{K_3^*(n_u, n_s, L_u, L_s)}{R_{31}^{2L_s+2L_u+2}} \right\}. \tag{A12}
 \end{aligned}$$

In the above, the K_i functions are defined by

$$K_1(n_s, n_t, L_s, L_t) = G_1(L_s, L_t) \frac{|\langle \varphi_{n'_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}}, \tag{A13}$$

$$K_2(n_s, n_t, L_s, L_t) = G_1(L_s, L_t) \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2 |\langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - 2E_{n_0 S}^{(0)}}, \tag{A14}$$

$$\begin{aligned}
 K_3(n_s, n_t, L_s, L_t) &= G_1(L_s, L_t) \langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle^* \langle \varphi_{n'_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle^* \\
 & \times \frac{\langle \varphi_{n'_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle \langle \varphi_{n_0}(0; \boldsymbol{\rho}) \| T_{L_t}(\boldsymbol{\rho}) \| \chi_{n_t}(L_t; \boldsymbol{\rho}) \rangle}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n'_0 S}^{(0)}}, \tag{A15}
 \end{aligned}$$

where $G_1(L_i, L_j)$ is further defined by

$$G_1(L_i, L_j) = 16\pi^2 (L_i, L_j)^{-2} \sum_{M_i M_j} \frac{[P_{L_i+L_j}^{M_i+M_j}(0)(L_i + L_j - M_i - M_j)!]^2}{(L_i + M_i)!(L_i - M_i)!(L_j + M_j)!(L_j - M_j)!}. \tag{A16}$$

Then the second-order energy correction is simplified to

$$\Delta E^{(2)} = - \sum_{n \geq 3} \left(\frac{C_{2n}^{(12)}}{R_{12}^{2n}} + \frac{C_{2n}^{(23)}}{R_{23}^{2n}} + \frac{C_{2n}^{(31)}}{R_{31}^{2n}} \right), \tag{A17}$$

where $C_{2n}^{(IJ)}$ are the additive dispersion coefficients. These coefficients can be expressed as

$$\begin{aligned}
 C_{2n}^{(12)}(L, M) &= |a|^2 \sum_{n_s n_t} \sum_{L_s L_t} K_1(n_s, n_t, L_s, L_t) + |b|^2 \sum_{n_s n_t} \sum_{L_s L_t} K_1(n_t, n_s, L_t, L_s) \\
 & + |c|^2 \sum_{n_s n_t} \sum_{L_s L_t} K_2(n_s, n_t, L_s, L_t) + a^* b \sum_{n_s n_t} \sum_{L_s L_t} K_3(n_s, n_t, L_s, L_t) + b^* a \sum_{n_s n_t} \sum_{L_s L_t} K_3^*(n_s, n_t, L_s, L_t), \tag{A18}
 \end{aligned}$$

$$\begin{aligned}
 C_{2n}^{(23)}(L, M) &= |a|^2 \sum_{n_t n_u} \sum_{L_t L_u} K_2(n_t, n_u, L_t, L_u) + |b|^2 \sum_{n_t n_u} \sum_{L_t L_u} K_1(n_t, n_u, L_t, L_u) \\
 & + |c|^2 \sum_{n_t n_u} \sum_{L_t L_u} K_1(n_u, n_t, L_u, L_t) + b^* c \sum_{n_t n_u} \sum_{L_t L_u} K_3(n_t, n_u, L_t, L_u) + c^* b \sum_{n_t n_u} \sum_{L_t L_u} K_3^*(n_t, n_u, L_t, L_u), \tag{A19}
 \end{aligned}$$

$$\begin{aligned}
 C_{2n}^{(31)}(L, M) &= |a|^2 \sum_{n_s n_u} \sum_{L_s L_u} K_1(n_s, n_u, L_s, L_u) + |b|^2 \sum_{n_s n_u} \sum_{L_s L_u} K_2(n_s, n_u, L_s, L_u) \\
 & + |c|^2 \sum_{n_s n_u} \sum_{L_s L_u} K_1(n_u, n_s, L_u, L_s) + a^* c \sum_{n_s n_u} \sum_{L_s L_u} K_3^*(n_u, n_s, L_u, L_s) + c^* a \sum_{n_s n_u} \sum_{L_s L_u} K_3(n_u, n_s, L_u, L_s). \tag{A20}
 \end{aligned}$$

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