

Calculations of long-range three-body interactions for $\text{Li}(2^2\text{S})\text{-Li}(2^2\text{S})\text{-Li}(2^2\text{P})$

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General formulas for calculating the several leading long-range interactions among three identical atoms where two atoms are in identical S states and the other atom is in a P state are obtained using perturbation theory for the energies up to second order. The first-order (dipolar) interactions depend on the geometrical configurations of the three atoms. In second order, additive and nonadditive dispersion interactions are obtained. The nonadditive interactions depend on the geometrical configurations in marked contrast to the case where all three atoms are in identical S states, for which the nonadditive (also known as triple-dipole or as Axilrod-Muto-Teller) dispersion interactions appear at the third order. The formalism is demonstrated by the calculation of the coefficients for the $\text{Li}(2^2\text{S})\text{-Li}(2^2\text{S})\text{-Li}(2^2\text{P})$ system using variationally generated atomic lithium wave functions in Hylleraas coordinates. The present dipolar coefficients and additive and nonadditive dispersion coefficients may be useful in constructing precise potential energy surfaces for this three lithium atom system.

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I. INTRODUCTION

A considerable number of studies are devoted to investigations of the long-range interactions between three ground state atoms [1–10], but the case of three atoms with one atom in an excited state is less studied. Reliable determinations of long-range interactions for the case of one atom in an excited state might be a consideration for characterizing excited trimers in photoassociation [11–13], in implementing quantum information processing with blockade mechanisms [14,15], and in spectroscopic studies of highly excited bound trimer states [16–19].

In the present work we use perturbation theory up to second order to derive general formulas for calculating the long-range interaction coefficients for three like atoms with two atoms in identical S states and the other atom in an excited P state. We exhibit the additive “dipolar” (or dipole-dipole) interactions and additive dispersion interactions that enter, respectively, in first- and in second-order perturbation theory. (Here, additive means pairwise amongst the three atoms.) In addition, we find that nonadditive dispersion interactions enter in second order and that these contain a dependence on the geometrical configuration of the three atoms. (Nonadditive means that the terms appear collectively amongst the three atoms.) The formalism is demonstrated by the calculation of the coefficients for the $\text{Li}(2^2\text{S})\text{-Li}(2^2\text{S})\text{-Li}(2^2\text{P})$ system using variationally generated atomic lithium wave functions in Hylleraas coordinates. 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 triangle, or equally spaced collinearly. We show that the results are consistent with an available *ab initio* quantum-chemical calculation in the case of the

equilateral triangle and equally spaced collinear configurations of the nuclei.

In general, the long-range interactions [9,20,21] for three-body systems [1,3,8,10] have many applications, such as in studies of atomic three-body recombination [22,23], crystal structure [24], color superfluids [25], Pfaffian states [26], and Efimov effects [27,28]. Three-body recombination is a process in which three atoms collide and two of them form a molecule [22–24,29]. The binding energy among them depends not only on the additive but also on the nonadditive three-body dispersion forces [22]. The nonadditive effects give a successful explanation of the failure of the Cauchy relations for the elastic constants in alkali-metal halide crystals [30]. Furthermore, the importance of these three-body interactions has been considered by many authors in connection with the Pfaffian state [26] and the formation of trions in the color superfluidity [25]. And because of the large spatial extension and tiny binding energies, some properties of Efimov states would be expected to depend on the long-range van der Waals interactions. Recently, some interesting theoretical investigations on the Efimov effect in higher partial waves (P -waves) have been reported [31]. However, additional research is warranted. In this paper, we will focus on the long-range three-body interactions for a system involving one atom in a P state.

In order to emphasize the new aspect of the present analysis, in the remainder of this section we very briefly summarize some related work that places our analysis in context. There are, of course, many studies on the ground and excited potential energy surfaces of three like alkali-metal atom systems for spectroscopy and for chemical dynamics. We will refer to the case of the homonuclear bound molecule as a trimer and to the case of an atom and a bound homonuclear dimer (such as for scattering) as an atom-dimer. A “global” potential energy surface would encompass both of these regimes, but a global potential energy surface might not be necessary for

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description of a particular physical process. For example, in a recent theoretical study of the photoassociation of a $\text{Cs}(6^2S)$ atom and a $\text{Cs}_2(X^1\Sigma_g^+, v=0)$ dimer [32], where two $\text{Cs}(6^2S)$ atoms are already bound up as a diatomic molecule with vibrational quantum number $v=0$, long-range interaction potential energies [33,34] of the (excited) atom-dimer system $\text{Cs}(6^2P)\text{--}\text{Cs}_2(X^1\Sigma_g^+, v=0)$ were used.

Studies on three-lithium-atom system potential energy surfaces include the trimer system [35–37] and treatments of the atom-dimer configuration within the context of a global trimer potential energy surface [38–40]. Motivated by ultracold science, some recent studies on lithium focused on generation of improved global potential energy surfaces for the trimer [41–43] or addressed the atom-dimer configuration in further detail [44–46], with emphasis on the configuration of a $\text{Li}(2^2S)$ atom interacting with a (bound) lithium dimer for applications to scattering processes [44,47,48]. Such investigations on long-range interactions for three-lithium-atom systems continue to support applications to atom-dimer scattering at thermal energies [49] and to atom-dimer photoassociation in the ultracold energy domain [45]. Calculations of trimer excited electronic states are available at various configurations and separations of the atoms [36,39,40,42,45,50]. Cvitaš *et al.* [51] investigated the case of three spin-polarized $\text{Li}(2^2S)$ atoms and considered the connection between the long-range interactions of the atom-dimer and of the atom-atom-atom potential energy surfaces. In contrast to their work, here we consider the atom-atom-atom case where one of the lithium atoms is in the 2^2P excited state. As we will show, our numerical results are consistent with the *ab initio* quantum-chemical excited-state calculations of Ref. [50] for the three atoms in the equilateral configuration or in the equally spaced collinear configuration.

II. THEORETICAL FORMULATION

A. The zeroth-order wave functions

The Hamiltonian for three well-separated (sufficiently far apart that electron exchange can be ignored) lithium atoms can be written as

$$H = H^{(0)} + H', \quad (1)$$

where

$$H^{(0)} = H_1^{(0)} + H_2^{(0)} + H_3^{(0)}, \quad (2)$$

$$H' \equiv V_{123} = V_{12} + V_{23} + V_{31}, \quad (3)$$

with $H_1^{(0)}$, $H_2^{(0)}$, and $H_3^{(0)}$, the unperturbed Hamiltonian of, respectively, atom 1, 2, and 3 and V_{12} , V_{23} , and V_{31} their mutual electrostatic interactions. We label the atoms by I , J , and K , with, respectively, internal coordinates σ , ρ , and ς . When the labels I , J , or K appear, it is understood that cyclic permutation can be used. V_{IJ} can be expanded according to Refs. [3,52]:

$$V_{IJ} = \sum_{l_I l_J} \sum_{m_I m_J} T_{l_I - m_I}(\sigma) T_{l_J m_J}(\rho) W_{l_I l_J}^{m_I - m_J}(IJ). \quad (4)$$

In Eq. (4), the multipole transition operators are

$$T_{l_I - m_I}(\sigma) = \sum_i Q_i \sigma_i^{l_I} Y_{l_I - m_I}(\hat{\sigma}_i), \quad (5)$$

$$T_{l_J m_J}(\rho) = \sum_j q_j \rho_j^{l_J} Y_{l_J m_J}(\hat{\rho}_j), \quad (6)$$

and the geometry factor is

$$W_{l_I l_J}^{m_I - m_J}(IJ) = \frac{4\pi(-1)^{l_J}}{R_{IJ}^{l_I + l_J + 1}} \frac{(l_I + l_J - m_I + m_J)!(l_I, l_J)^{-1/2}}{[(l_I + m_I)!(l_I - m_I)!(l_J + m_J)!(l_J - m_J)!]^{1/2}} P_{l_I + l_J}^{m_I - m_J}(\cos \theta_{IJ}) \exp[i(m_I - m_J)\Phi_{IJ}], \quad (7)$$

where $\mathbf{R}_{IJ} = \mathbf{R}_J - \mathbf{R}_I$ is the relative position vector from atom I to atom J , the notation $(a, b, \dots) = (2a+1)(2b+1)\dots$, 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. Similar expressions result for V_{JK} and V_{KI} . The choice of the z axis is discussed below.

For the $\text{Li}(n_0S)\text{--}\text{Li}(n_0S)\text{--}\text{Li}(n'_0L)$ system where the angular momentum of one atom is L and the associated magnetic quantum number is M , there are three orthogonal eigenvectors for the unperturbed Hamiltonian corresponding to the same energy eigenvalue $E_{n_0 n_0 n'_0}^{(0)} = 2E_{n_0 S}^{(0)} + E_{n'_0 L}^{(0)}$,

$$|\phi_1\rangle = |\varphi_{n'_0}(LM; \sigma) \varphi_{n_0}(0; \rho) \varphi_{n_0}(0; \varsigma)\rangle, \quad (8)$$

$$|\phi_2\rangle = |\varphi_{n_0}(0; \sigma) \varphi_{n'_0}(LM; \rho) \varphi_{n_0}(0; \varsigma)\rangle, \quad (9)$$

$$|\phi_3\rangle = |\varphi_{n_0}(0; \sigma) \varphi_{n_0}(0; \rho) \varphi_{n'_0}(LM; \varsigma)\rangle. \quad (10)$$

According to degenerate perturbation theory, the zeroth-order wave function is a linear combination of the eigenvectors given

in Eqs. (8), (9), and (10),

$$|\Psi^{(0)}\rangle = a|\phi_1\rangle + b|\phi_2\rangle + c|\phi_3\rangle. \quad (11)$$

The expansion coefficients a , b , and c are determined by diagonalizing the perturbation V_{123} in the basis set $\{\phi_1, \phi_2, \phi_3\}$, which depends on the geometrical configuration formed by the three atoms.

B. Choice of coordinates for three atoms

In this work, we set the coordinates for the three atoms as shown in Fig. 1. Specifically, we choose the nucleus of atom 1 as the origin of our coordinate system and the x - y plane as the plane formed by the three atomic nuclei. Furthermore, we set the x -axis to be $\mathbf{R}_{12}$ and the z -axis perpendicular to the x - y plane by the right-hand convention. The interior angles of the triangle formed by the three atoms are denoted as α , β , γ . Noting that [3] $\theta_{12} = \theta_{23} = \theta_{31} = \pi/2$, the associated

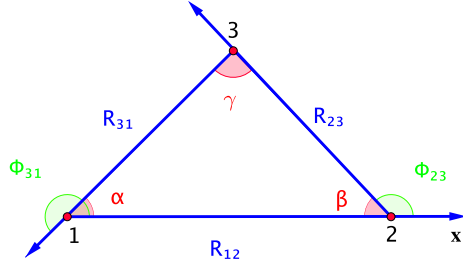


FIG. 1. Coordinate system for the three atoms: the z axis is perpendicular to the plane of the three nuclei and the x axis is parallel to $\mathbf{R}_{12}$. The angles satisfy $\Phi_{12} = 0$, $\Phi_{23} = \pi - \beta$, $\Phi_{31} = \pi + \alpha$. The nuclei lie in the x - y plane.

Legendre functions can be simplified as

$$P_l^m(0) = \frac{1}{2^{l+1}} [1 + (-1)^{l+m}] (-1)^{\frac{l+m}{2}} (l+m)! \times \left[\left(\frac{l+m}{2} \right)! \right]^{-1} \left[\left(\frac{l-m}{2} \right)! \right]^{-1}. \quad (12)$$

The angles Φ_{12} , Φ_{23} , and Φ_{31} satisfy $\Phi_{12} = 0$, $\Phi_{23} = \pi - \beta$, and $\Phi_{31} = \pi + \alpha$, which can be used to simplify the exponential function $\exp[i(m_I - m_J)\Phi_{IJ}]$ in the geometry factor.

C. The connection with other studies

With these eigenvectors and zero-order wave function, we can easily find the connection between this work and preceding studies of long-range interactions. For example, if we eliminate the terms involving particle 3 (with angular momentum L), our formulas describe the long-range interactions for the two-body n_0S - n_0S system. If we set $a = \frac{1}{\sqrt{2}}$, $b = \pm \frac{1}{\sqrt{2}}$, $c = 0$ and remove the terms involving particle 3 (with angular momentum 0), our expressions describe the long-range interactions for the two-body n_0S - n'_0L system. If we set $a = 1$, $b = c = 0$ and $L = 0$, the long-range three-body n_0S - n_0S - n'_0S interaction is described.

We noted earlier that Cvitaš *et al.* [51] considered the connection between the long-range interactions for the atom-dimer and the atom-atom-atom potential energy surfaces in the case of the ground state for the three spin-aligned $\text{Li}(2^2S)$ atoms. They rewrote the distances separating the atoms in terms of Jacobi coordinates $\tilde{r}$, $\tilde{R}$, and $\tilde{\theta}$, where $\tilde{r}$ is the dimer internuclear distance, $\tilde{R}$ is the distance of the third atom from the center of mass of the dimer, and $\tilde{\theta}$ is the angle between $\tilde{r}$ and $\tilde{R}$, and expanded the corresponding results as power series in $\tilde{r}/\tilde{R}$ for $\tilde{r} \ll \tilde{R}$ obtaining the contributions of the atom-atom coefficients to the atom-diatom coefficients. The approximation is suitable because in the n_0S - n_0S - n'_0S system the atom-atom coefficients are constants. However, for the n_0S - n_0S - n'_0L system, we find the atom-atom coefficients depend on the geometrical configuration of the three atoms. In the present case, we can connect the atom-dimer and trimer (atom-atom-atom) systems by adjusting the expansion coefficients in Eq. (11). Thus, if we set $a = b = 0$, $c = 1$, our formulas reduce to the long-range interactions between an atom n'_0L and a diatom n_0S - n_0S . However, unlike the study of Ref. [51], (see also Ref. [38]), we do not include short-range effects (damping), so in our case the limit of an atom-dimer

would still correspond to the two atoms grouped as a dimer sufficiently separated that exchange is negligible. In this work we focus on the long-range interactions for the homonuclear atom-atom-atom lithium system.

In the appendix, the general expressions for the n_0S - n_0S - n'_0L cases are presented up to second order in perturbation theory. In the remainder of the main part of the paper we take $n_0 = 2 = n'_0$, and $L = 1$, to describe the $\text{Li}(2^2S)$ - $\text{Li}(2^2S)$ - $\text{Li}(2^2P)$ system, for which we exhibit and calculate the coefficients.

D. The first-order energy

According to perturbation theory, the first-order energy correction for the $\text{Li}(2^2S)$ - $\text{Li}(2^2S)$ - $\text{Li}(2^2P)$ system is

$$\Delta E^{(1)} = -\frac{C_3^{(12)}(1, M)}{R_{12}^3} - \frac{C_3^{(23)}(1, M)}{R_{23}^3} - \frac{C_3^{(31)}(1, M)}{R_{31}^3}, \quad (13)$$

where

$$C_3^{(IJ)}(1, M) = (A_I^* A_J + A_J^* A_I) \mathbb{D}_0(M), \quad (14)$$

$$A_1 = a, A_2 = b, A_3 = c, \quad (15)$$

and

$$\mathbb{D}_0(M) = \frac{4\pi(-1)^{1+M}}{9(1-M)!(1+M)!} \left| \langle \varphi_{n_0}(0; \sigma) \| T_1(\sigma) \| \varphi_{n'_0}(1; \sigma) \rangle \right|^2. \quad (16)$$

In the above, a , b , c are defined in Eq. (11). It should be mentioned that there exist only additive long-range dipolar interaction terms at this order of perturbation.

E. The second-order energy

The second-order energy correction for the $\text{Li}(2^2S)$ - $\text{Li}(2^2S)$ - $\text{Li}(2^2P)$ system can be written as

$$\Delta E^{(2)} = -\sum_{n \geq 3} \left(\frac{C_{2n}^{(12)}(1, M)}{R_{12}^{2n}} + \frac{C_{2n}^{(23)}(1, M)}{R_{23}^{2n}} + \frac{C_{2n}^{(31)}(1, M)}{R_{31}^{2n}} + \frac{C_{2n}^{(12,23)}(1, M)}{R_{12}^{2n} R_{23}^{2n}} + \frac{C_{2n}^{(23,31)}(1, M)}{R_{23}^{2n} R_{31}^{2n}} + \frac{C_{2n}^{(31,12)}(1, M)}{R_{31}^{2n} R_{12}^{2n}} \right), \quad (17)$$

where the $C_{2n}^{(12)}(1, M)$, $C_{2n}^{(23)}(1, M)$, 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 coefficients. The derivation of these coefficients is given in the appendix. In this work we are only concerned with $n = 3$ and 4 in Eq. (17). The corresponding dispersion coefficients are

$$C_6^{(IJ)}(1, M) = (|A_I|^2 + |A_J|^2) \mathbb{D}_1(M) + |A_K|^2 \mathbb{D}_2, \quad (18)$$

$$C_8^{(IJ)}(1, M) = (|A_I|^2 + |A_J|^2) \mathbb{Q}_1(M) + |A_K|^2 \mathbb{Q}_2 + (A_I^* A_J + A_J^* A_I) \mathbb{Q}_3(M), \quad (19)$$

$$C_6^{(IJ, JK)}(1, M) = \mathbb{Q}_4(A_K, A_I, 1, M, \eta_J), \quad (20)$$

$$C_8^{(IJ, JK)}(1, M) = \mathbb{Q}_4(A_K, A_I, 2, M, \eta_J), \quad (21)$$

with

$$A_1 = a, A_2 = b, A_3 = c, \quad \eta_1 = \alpha, \eta_2 = \beta, \eta_3 = \gamma, \quad (22)$$

where a , b , and c are defined in Eq. (11), α , β , and γ are the interior angles, and the other terms in Eqs. (18)–(21) are given by

$$\mathbb{D}_1(M) = \sum_{n_s n_t L_s} F_1(n_s, n_t, L_s, 1; 1, 1; 1, M), \quad (23)$$

$$\mathbb{D}_2 = \sum_{n_s n_t} F_2(n_s, n_t, 1, 1), \quad (24)$$

$$\begin{aligned} \mathbb{Q}_1(M) = & \sum_{n_s n_t L_s} [F_1(n_s, n_t, L_s, 1; 1, 3; 1, M) \\ & + F_1(n_s, n_t, L_s, 1; 2, 2; 1, M) \\ & + F_1(n_s, n_t, L_s, 1; 3, 1; 1, M) \\ & + F_1(n_s, n_t, L_s, 2; 1, 1; 1, M)], \end{aligned} \quad (25)$$

$$\mathbb{Q}_2 = \sum_{n_s n_t} [F_2(n_s, n_t, 1, 2) + F_2(n_s, n_t, 2, 1)], \quad (26)$$

$$\begin{aligned} \mathbb{Q}_3(M) = & \sum_{n_s n_t} [F_3(n_s, n_t, 1, 1; 2, 2; 1, M) \\ & + F_3(n_s, n_t, 1, 2; 2, 1; 1, M) \\ & + F_3(n_s, n_t, 2, 1; 1, 2; 1, M) \\ & + F_3(n_s, n_t, 2, 2; 1, 1; 1, M)], \end{aligned} \quad (27)$$

and

$$\begin{aligned} \mathbb{Q}_4(A_K, A_I, \lambda, M, \eta_J) \\ = 2 \sum_{n_t M_t} \text{Re}[A_K^* A_I e^{i(M_t - M)\eta_J}] F_4(n_t, \lambda, M_t; 1, M). \end{aligned} \quad (28)$$

In the above (I, J, K) forms a permutation of $(1, 2, 3)$ and the F_i functions are defined by Eqs. (A10)–(A12) and (A13) in the appendix.

F. Three special geometrical configurations

In this work, three special geometrical configurations for the three atoms are considered. The first configuration is the equilateral triangle, where the interatomic separations are the same: $R_{12} = R_{23} = R_{31} = R$. With this configuration, all the diagonal perturbation matrix elements are zero and all the off-diagonal matrix elements are the same. The perturbation matrix with respect to $\{\phi_1, \phi_2, \phi_3\}$ thus becomes

$$H' = H'_{12} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad (29)$$

where

$$\begin{aligned} H'_{12} = & \frac{4\pi}{R^{2L+1}} \frac{(-1)^M [(2L-1)!!]^2}{(2L+1)^2 (L-M)! (L+M)!} \\ & \times \left| \langle \varphi_{n_0}(0; \sigma) \| T_L(\sigma) \| \varphi_{n_0}(L; \sigma) \rangle \right|^2. \end{aligned} \quad (30)$$

Solving the eigenvalue problem of the above matrix, one obtains the eigenvalues: $2H'_{12}$, $-H'_{12}$, $-H'_{12}$, and the corre-

sponding orthonormalized zeroth-order wave functions:

$$\Psi_{1,\Delta}^{(0)} = \frac{1}{\sqrt{3}}|\phi_1\rangle + \frac{1}{\sqrt{3}}|\phi_2\rangle + \frac{1}{\sqrt{3}}|\phi_3\rangle, \quad (31)$$

$$\Psi_{2,\Delta}^{(0)} = \frac{1}{\sqrt{2}}|\phi_1\rangle - \frac{1}{\sqrt{2}}|\phi_3\rangle, \quad (32)$$

$$\Psi_{3,\Delta}^{(0)} = \frac{1}{\sqrt{6}}|\phi_1\rangle - \sqrt{\frac{2}{3}}|\phi_2\rangle + \frac{1}{\sqrt{6}}|\phi_3\rangle, \quad (33)$$

where the symbol Δ denotes the equilateral triangle.

The second special geometrical configuration is the isosceles right triangle such that $R_{12} = \frac{1}{\sqrt{2}}R_{23} = R_{31} = R$. With this configuration, the perturbation matrix has the form,

$$H' = H'_{12} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & \frac{1}{2\sqrt{2}} \\ 1 & \frac{1}{2\sqrt{2}} & 0 \end{pmatrix}. \quad (34)$$

The eigenvalues are $\frac{H'_{12}}{8}(\sqrt{2} + \sqrt{130})$, $\frac{H'_{12}}{8}(\sqrt{2} - \sqrt{130})$, $-\frac{H'_{12}}{2\sqrt{2}}$, and the corresponding orthonormalized zeroth-order wave functions are

$$\begin{aligned} \Psi_{1,\perp}^{(0)} = & \frac{\sqrt{130} - \sqrt{2}}{2\sqrt{65 - \sqrt{65}}}|\phi_1\rangle + \frac{4}{\sqrt{65 - \sqrt{65}}}|\phi_2\rangle \\ & + \frac{4}{\sqrt{65 - \sqrt{65}}}|\phi_3\rangle, \end{aligned} \quad (35)$$

$$\begin{aligned} \Psi_{2,\perp}^{(0)} = & \frac{-(\sqrt{130} + \sqrt{2})}{2\sqrt{65 + \sqrt{65}}}|\phi_1\rangle + \frac{4}{\sqrt{65 + \sqrt{65}}}|\phi_2\rangle \\ & + \frac{4}{\sqrt{65 + \sqrt{65}}}|\phi_3\rangle, \end{aligned} \quad (36)$$

$$\Psi_{3,\perp}^{(0)} = -\frac{1}{\sqrt{2}}|\phi_2\rangle + \frac{1}{\sqrt{2}}|\phi_3\rangle, \quad (37)$$

where the symbol $\perp$ denotes the isosceles right triangle.

The third special geometrical configuration is that the three atoms are in a straight line such that $R_{12} = \frac{1}{2}R_{23} = R_{31} = R$. With this configuration, the perturbation matrix is

$$H' = H'_{12} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & \frac{1}{8} \\ 1 & \frac{1}{8} & 0 \end{pmatrix}. \quad (38)$$

The eigenvalues are $\frac{H'_{12}}{16}(1 + 3\sqrt{57})$, $\frac{H'_{12}}{16}(1 - 3\sqrt{57})$, $-\frac{H'_{12}}{8}$, and the corresponding orthonormalized zeroth-order wave functions are

$$\begin{aligned} \Psi_{1,-}^{(0)} = & \frac{3\sqrt{57} - 1}{\sqrt{1026 - 6\sqrt{57}}}|\phi_1\rangle + \frac{16}{\sqrt{1026 - 6\sqrt{57}}}|\phi_2\rangle \\ & + \frac{16}{\sqrt{1026 - 6\sqrt{57}}}|\phi_3\rangle, \end{aligned} \quad (39)$$

TABLE I. 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 $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$ 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	$\mathbb{D}_0(M=0)$ $\mathbb{Q}_1(M=0)$	$\mathbb{D}_0(M=\pm 1)$ $\mathbb{Q}_1(M=\pm 1)$	$\mathbb{D}_1(M=0)$ $\mathbb{Q}_2$	$\mathbb{D}_1(M=\pm 1)$ $\mathbb{Q}_3(M=0)$	$\mathbb{D}_2$ $\mathbb{Q}_3(M=\pm 1)$
$^\infty\text{Li}$	$-5.500111(1)$ $75804.1(5)$	$2.750054(1)$ $354147(4)$	$1406.68(3)$ $83429(1)$	$1741.06(5)$ $27239.28(1)$	$1393.42(5)$ $-165583.70(1)$
^7Li	$-5.500926(1)$ $75809.6(5)$	$2.750462(1)$ $354206(4)$	$1407.15(5)$ $83456(5)$	$1741.59(4)$ $27242.91(2)$	$1394.05(5)$ $-165615.09(1)$
^6Li	$-5.501062(1)$ $75810.5(5)$	$2.750530(1)$ $354216(4)$	$1407.20(2)$ $83460(5)$	$1741.68(4)$ $27243.52(2)$	$1394.16(5)$ $-165620.32(1)$

$$\Psi_{2,-}^{(0)} = \frac{-(3\sqrt{57}+1)}{\sqrt{1026+6\sqrt{57}}}|\phi_1\rangle + \frac{16}{\sqrt{1026+6\sqrt{57}}}|\phi_2\rangle + \frac{16}{\sqrt{1026+6\sqrt{57}}}|\phi_3\rangle, \quad (40)$$

$$\Psi_{3,-}^{(0)} = -\frac{1}{\sqrt{2}}|\phi_2\rangle + \frac{1}{\sqrt{2}}|\phi_3\rangle, \quad (41)$$

where the symbol $-$ denotes the geometrical configuration of a straight line.

III. RESULTS AND DISCUSSION

In the present work, the atomic wave functions of lithium were constructed variationally using Hylleraas basis sets and the intermediate states were generated by diagonalizing the lithium Hamiltonian, as in Ref. [53]. All relevant matrix elements of the multipole transition operators were thus calculated, including the finite nuclear mass corrections. With these, we calculate the first-order dipolar and second-order long-range dispersion coefficients for the $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$ system.

Table I lists the 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 lithium isotopes, all of which are independent of the geometrical configuration of

the three lithium atoms. However, the quantity $\mathbb{Q}_4$, not listed in Table I, is related to the nonadditive dispersion coefficients and is dependent on the geometrical configuration. $\mathbb{D}_0(M=0)$ and $\mathbb{D}_0(M=\pm 1)$ are connected with 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 with 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 with the second-order additive dispersion coefficient $C_8^{(IJ)}(L, M)$.

With the values in Table I, we can obtain the long-range interaction coefficients for geometrical configurations specified by R_{12} , R_{23} , R_{31} , α , β , and γ as follows: Initially, we obtain the geometric parameters for the configuration under consideration by the method as described in Sec. II F. Then, the long-range interaction coefficients for that configuration are given by Eqs. (13)–(28). In the following, we will discuss the long-range coefficients by explicitly evaluating coefficients for the three elementary geometrical configurations of the atoms in an equilateral triangle, an isosceles triangle, or equally-spaced collinearly, representing, respectively, the symmetries D_{3h} , C_{2v} , and $D_{\infty h}$.

A. Dipolar and dispersion coefficients for an equilateral triangle

Using the coefficients a, b, c of the zeroth-order wave functions Eqs. (31)–(33), for the case where the three atoms

TABLE II. The additive long-range coefficients $C_3^{(IJ)}(1, M)$ of the $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$ 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	$C_3^{(12)}(1, M=0)$	$C_3^{(23)}(1, M=0)$	$C_3^{(31)}(1, M=0)$	$C_3^{(12)}(1, M=\pm 1)$	$C_3^{(23)}(1, M=\pm 1)$	$C_3^{(31)}(1, M=\pm 1)$
$^\infty\text{Li}$	$\Psi_{1,\Delta}^{(0)}$	$-3.6667415(5)$	$-3.6667415(5)$	$-3.6667415(5)$	$1.8333702(3)$	$1.8333702(3)$	$1.8333702(3)$
	$\Psi_{2,\Delta}^{(0)}$	0	0	$5.500110(1)$	0	0	$-2.750054(1)$
	$\Psi_{3,\Delta}^{(0)}$	$3.6667415(5)$	$3.6667415(5)$	$-1.8333702(3)$	$-1.8333702(3)$	$-1.8333702(3)$	$0.9166850(2)$
^7Li	$\Psi_{1,\Delta}^{(0)}$	$-3.667284(1)$	$-3.667284(1)$	$-3.667284(1)$	$1.8336420(5)$	$1.8336420(5)$	$1.8336420(5)$
	$\Psi_{2,\Delta}^{(0)}$	0	0	$5.500925(2)$	0	0	$-2.750462(1)$
	$\Psi_{3,\Delta}^{(0)}$	$3.667284(1)$	$3.667284(1)$	$-1.8336420(5)$	$-1.8336420(5)$	$-1.8336420(5)$	$0.9168210(2)$
^6Li	$\Psi_{1,\Delta}^{(0)}$	$-3.667374(1)$	$-3.667374(1)$	$-3.667374(1)$	$1.833686(1)$	$1.833686(1)$	$1.833686(1)$
	$\Psi_{2,\Delta}^{(0)}$	0	0	$5.501062(1)$	0	0	$-2.750530(1)$
	$\Psi_{3,\Delta}^{(0)}$	$3.667374(1)$	$3.667374(1)$	$-1.833686(1)$	$-1.833686(1)$	$-1.833686(1)$	$0.9168437(2)$

TABLE III. The additive and nonadditive dispersion coefficients $C_6^{(IJ)}(1, M=0)$ and $C_6^{(IJ,K)}(1, M=0)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_6^{(12)}(1, M=0)$	$C_6^{(23)}(1, M=0)$	$C_6^{(31)}(1, M=0)$	$C_6^{(12,23)}(1, M=0)$	$C_6^{(23,31)}(1, M=0)$	$C_6^{(31,12)}(1, M=0)$
$^\infty\text{Li}$	$\Psi_{1,\Delta}^{(0)}$	1402.26(4)	1402.26(4)	1402.26(4)	157.059(5)	157.059(5)	157.059(5)
	$\Psi_{2,\Delta}^{(0)}$	1400.05(4)	1400.05(4)	1406.69(4)	-235.588(7)	0	0
	$\Psi_{3,\Delta}^{(0)}$	1404.46(3)	1404.46(3)	1397.85(5)	78.530(3)	-157.059(5)	-157.059(5)
^7Li	$\Psi_{1,\Delta}^{(0)}$	1402.77(4)	1402.77(4)	1402.77(4)	157.132(5)	157.132(5)	157.132(5)
	$\Psi_{2,\Delta}^{(0)}$	1400.59(4)	1400.59(4)	1407.14(4)	-235.697(7)	0	0
	$\Psi_{3,\Delta}^{(0)}$	1404.95(4)	1404.95(4)	1398.41(4)	78.565(2)	-157.132(5)	-157.132(5)
^6Li	$\Psi_{1,\Delta}^{(0)}$	1402.86(4)	1402.86(4)	1402.86(4)	157.144(5)	157.144(5)	157.144(5)
	$\Psi_{2,\Delta}^{(0)}$	1400.68(4)	1400.68(4)	1407.20(3)	-235.715(7)	0	0
	$\Psi_{3,\Delta}^{(0)}$	1405.02(3)	1405.02(3)	1398.50(4)	78.571(2)	-157.144(5)	-157.144(5)

TABLE IV. The additive and nonadditive dispersion coefficients $C_6^{(IJ)}(1, M=\pm 1)$ and $C_6^{(IJ,K)}(1, M=\pm 1)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_6^{(12)}(1, M=\pm 1)$	$C_6^{(23)}(1, M=\pm 1)$	$C_6^{(31)}(1, M=\pm 1)$	$C_6^{(12,23)}(1, M=\pm 1)$	$C_6^{(23,31)}(1, M=\pm 1)$	$C_6^{(31,12)}(1, M=\pm 1)$
$^\infty\text{Li}$	$\Psi_{1,\Delta}^{(0)}$	1625.18(5)	1625.18(5)	1625.18(5)	-137.426(4)	-137.426(4)	-137.426(4)
	$\Psi_{2,\Delta}^{(0)}$	1567.24(5)	1567.24(5)	1741.06(5)	206.141(7)	0	0
	$\Psi_{3,\Delta}^{(0)}$	1683.12(5)	1683.12(5)	1509.30(5)	-68.713(2)	137.426(4)	137.426(4)
^7Li	$\Psi_{1,\Delta}^{(0)}$	1625.74(4)	1625.74(4)	1625.74(4)	-137.490(4)	-137.490(4)	-137.490(4)
	$\Psi_{2,\Delta}^{(0)}$	1567.82(4)	1567.82(4)	1741.59(4)	206.235(6)	0	0
	$\Psi_{3,\Delta}^{(0)}$	1683.67(4)	1683.67(4)	1509.89(4)	-68.745(2)	137.490(4)	137.490(4)
^6Li	$\Psi_{1,\Delta}^{(0)}$	1625.84(4)	1625.84(4)	1625.84(4)	-137.500(4)	-137.500(4)	-137.500(4)
	$\Psi_{2,\Delta}^{(0)}$	1567.92(4)	1567.92(4)	1741.68(4)	206.252(7)	0	0
	$\Psi_{3,\Delta}^{(0)}$	1683.76(4)	1683.76(4)	1509.99(4)	-68.750(2)	137.500(4)	137.500(4)

TABLE V. The additive and nonadditive dispersion coefficients $C_8^{(IJ)}(1, M=0)$ and $C_8^{(IJ,K)}(1, M=0)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_8^{(12)}(1, M=0)$	$C_8^{(23)}(1, M=0)$	$C_8^{(31)}(1, M=0)$	$C_8^{(12,23)}(1, M=0)$	$C_8^{(23,31)}(1, M=0)$	$C_8^{(31,12)}(1, M=0)$
$^\infty\text{Li}$	$\Psi_{1,\Delta}^{(0)}$	96505.6(9)	96505.6(9)	96505.6(9)	9858.985(6)	9858.985(6)	9858.985(6)
	$\Psi_{2,\Delta}^{(0)}$	79616.8(9)	79616.8(9)	48564.8(5)	-14788.47(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	58915.7(8)	58915.7(8)	89968(2)	4929.492(3)	-9858.985(6)	-9858.985(6)
^7Li	$\Psi_{1,\Delta}^{(0)}$	96519.5(9)	96519.5(9)	96519.5(9)	9861.200(6)	9861.200(6)	9861.200(6)
	$\Psi_{2,\Delta}^{(0)}$	79631.3(9)	79631.3(9)	48566.4(2)	-14791.80(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	58921.7(8)	58921.7(8)	89987(2)	4930.600(3)	-9861.200(6)	-9861.200(6)
^6Li	$\Psi_{1,\Delta}^{(0)}$	96521.8(9)	96521.8(9)	96521.8(9)	9861.567(5)	9861.567(5)	9861.567(5)
	$\Psi_{2,\Delta}^{(0)}$	79633.7(9)	79633.7(9)	48566.9(4)	-14792.35(1)	0	0
	$\Psi_{3,\Delta}^{(0)}$	58922.7(8)	58922.7(8)	89990(2)	4930.784(3)	-9861.567(5)	-9861.567(5)

TABLE VI. The additive and nonadditive dispersion coefficients $C_8^{(IJ)}(1, M = \pm 1)$ and $C_8^{(IJ, JK)}(1, M = \pm 1)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_8^{(12)}(1, M = \pm 1)$	$C_8^{(23)}(1, M = \pm 1)$	$C_8^{(31)}(1, M = \pm 1)$	$C_8^{(12, 23)}(1, M = \pm 1)$	$C_8^{(23, 31)}(1, M = \pm 1)$	$C_8^{(31, 12)}(1, M = \pm 1)$
$^\infty\text{Li}$	$\Psi_{1,\Delta}^{(0)}$	153520(4)	153520(4)	153520(4)	-26496.02(2)	-26496.02(2)	-26496.02(2)
	$\Psi_{2,\Delta}^{(0)}$	218790(4)	218790(4)	519731(4)	39744.04(3)	0	0
	$\Psi_{3,\Delta}^{(0)}$	419417(4)	419417(4)	118475(3)	-13248.01(1)	26496.02(2)	26496.02(2)
^7Li	$\Psi_{1,\Delta}^{(0)}$	153546(4)	153546(4)	153546(4)	-26501.97(2)	-26501.97(2)	-26501.97(2)
	$\Psi_{2,\Delta}^{(0)}$	218830(3)	218830(3)	519821(4)	39752.95(2)	0	0
	$\Psi_{3,\Delta}^{(0)}$	419491(4)	419491(4)	118500(3)	-13250.98(1)	26501.97(2)	26501.97(2)
^6Li	$\Psi_{1,\Delta}^{(0)}$	153549(3)	153549(3)	153549(3)	-26502.97(2)	-26502.97(2)	-26502.97(2)
	$\Psi_{2,\Delta}^{(0)}$	218838(4)	218838(4)	519838(5)	39754.44(2)	0	0
	$\Psi_{3,\Delta}^{(0)}$	419504(4)	419504(4)	118504(3)	-13251.48(1)	26502.97(2)	26502.97(2)

TABLE VII. The total long-range interaction coefficients of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_3(1, M = 0)$	$C_3(1, M = \pm 1)$	$C_6(1, M = 0)$	$C_6(1, M = \pm 1)$	$C_8(1, M = 0)$	$C_8(1, M = \pm 1)$
$^\infty\text{Li}$	$\Psi_{1,\Delta}^{(0)}$	-11.0002245(15)	5.5001106(9)	4677.95(13)	4463.26(16)	319093.8(27)	381071(12)
	$\Psi_{2,\Delta}^{(0)}$	5.500110(1)	-2.750054(1)	3971.20(12)	5081.68(15)	193009.9(23)	997055(12)
	$\Psi_{3,\Delta}^{(0)}$	5.5001128(13)	-2.7500554(8)	3971.18(12)	5081.67(16)	193010.9(18)	997053(11)

TABLE VIII. The additive long-range coefficients $C_3^{(IJ)}(1, M)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) system for three different types of the zeroth-order wave functions, where the three atoms form an isosceles right triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_3^{(12)}(1, M = 0)$	$C_3^{(23)}(1, M = 0)$	$C_3^{(31)}(1, M = 0)$	$C_3^{(12)}(1, M = \pm 1)$	$C_3^{(23)}(1, M = \pm 1)$	$C_3^{(31)}(1, M = \pm 1)$
$^\infty\text{Li}$	$\Psi_{1,\perp}^{(0)}$	-3.8591328(7)	-3.0911576(6)	-3.8591328(7)	1.9295663(4)	1.5455789(3)	1.9295663(4)
	$\Psi_{2,\perp}^{(0)}$	3.8591328(7)	-2.4089529(4)	3.8591328(7)	-1.9295663(4)	1.2044764(2)	-1.9295663(4)
	$\Psi_{3,\perp}^{(0)}$	0	5.500111(1)	0	0	-2.7500551(6)	0
^7Li	$\Psi_{1,\perp}^{(0)}$	-3.8597053(9)	-3.0916162(7)	-3.8597053(9)	1.9298527(4)	1.5458080(4)	1.9298527(4)
	$\Psi_{2,\perp}^{(0)}$	3.8597053(9)	-2.4093103(5)	3.8597053(9)	-1.9298527(4)	1.2046552(2)	-1.9298527(4)
	$\Psi_{3,\perp}^{(0)}$	0	5.500926(1)	0	0	-2.7504631(7)	0
^6Li	$\Psi_{1,\perp}^{(0)}$	-3.8598006(9)	-3.0916924(8)	-3.8598006(9)	1.9299002(5)	1.5458460(6)	1.9299002(5)
	$\Psi_{2,\perp}^{(0)}$	3.8598006(9)	-2.4093697(6)	3.8598006(9)	-1.9299002(5)	1.2046848(3)	-1.9299002(5)
	$\Psi_{3,\perp}^{(0)}$	0	5.501062(1)	0	0	-2.7505310(7)	0

TABLE IX. The additive and nonadditive dispersion coefficients $C_6^{(IJ)}(1, M=0)$ and $C_6^{(IJ,K)}(1, M=0)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) system for three different types of the zeroth-order wave functions, where the three atoms form an isosceles right triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_6^{(12)}(1, M=0)$	$C_6^{(23)}(1, M=0)$	$C_6^{(31)}(1, M=0)$	$C_6^{(12,23)}(1, M=0)$	$C_6^{(23,31)}(1, M=0)$	$C_6^{(31,12)}(1, M=0)$
$^\infty\text{Li}$	$\Psi_{1,\perp}^{(0)}$	1402.96(4)	1400.87(4)	1402.96(4)	165.300(5)	165.300(5)	132.405(4)
	$\Psi_{2,\perp}^{(0)}$	1403.78(4)	1399.22(4)	1403.78(4)	-165.300(5)	-165.300(5)	103.183(3)
	$\Psi_{3,\perp}^{(0)}$	1400.05(4)	1406.69(4)	1400.05(4)	0	0	-235.588(7)
^7Li	$\Psi_{1,\perp}^{(0)}$	1403.46(4)	1401.40(4)	1403.46(4)	165.376(5)	165.376(5)	132.466(4)
	$\Psi_{2,\perp}^{(0)}$	1404.27(4)	1399.78(4)	1404.27(4)	-165.376(5)	-165.376(5)	103.231(3)
	$\Psi_{3,\perp}^{(0)}$	1400.59(4)	1407.14(4)	1400.59(4)	0	0	-235.697(7)
^6Li	$\Psi_{1,\perp}^{(0)}$	1403.54(4)	1401.49(4)	1403.54(4)	165.389(5)	165.389(5)	132.476(4)
	$\Psi_{2,\perp}^{(0)}$	1404.35(4)	1399.87(4)	1404.35(4)	-165.389(5)	-165.389(5)	103.239(3)
	$\Psi_{3,\perp}^{(0)}$	1400.68(4)	1407.20(3)	1400.68(4)	0	0	-235.715(7)

TABLE X. The additive and nonadditive dispersion coefficients $C_6^{(IJ)}(1, M=\pm 1)$ and $C_6^{(IJ,K)}(1, M=\pm 1)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) system for three different types of the zeroth-order wave functions, where the three atoms form an isosceles right triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_6^{(12)}(1, M=\pm 1)$	$C_6^{(23)}(1, M=\pm 1)$	$C_6^{(31)}(1, M=\pm 1)$	$C_6^{(12,23)}(1, M=\pm 1)$	$C_6^{(23,31)}(1, M=\pm 1)$	$C_6^{(31,12)}(1, M=\pm 1)$
$^\infty\text{Li}$	$\Psi_{1,\perp}^{(0)}$	1643.37(5)	1588.80(5)	1643.37(5)	41.324(1)	41.324(1)	-264.810(8)
	$\Psi_{2,\perp}^{(0)}$	1664.93(5)	1545.68(5)	1664.93(5)	-41.324(1)	-41.324(1)	-206.367(6)
	$\Psi_{3,\perp}^{(0)}$	1567.24(5)	1741.06(5)	1567.24(5)	0	0	471.18(2)
^7Li	$\Psi_{1,\perp}^{(0)}$	1643.94(5)	1589.37(4)	1643.94(5)	41.344(2)	41.344(2)	-264.932(8)
	$\Psi_{2,\perp}^{(0)}$	1665.48(4)	1546.26(4)	1665.48(4)	-41.344(2)	-41.344(2)	-206.462(6)
	$\Psi_{3,\perp}^{(0)}$	1567.83(5)	1741.59(4)	1567.83(5)	0	0	471.40(2)
^6Li	$\Psi_{1,\perp}^{(0)}$	1644.02(4)	1589.48(5)	1644.02(4)	41.348(2)	41.348(2)	-264.954(9)
	$\Psi_{2,\perp}^{(0)}$	1665.59(5)	1546.36(4)	1665.59(5)	-41.348(2)	-41.348(2)	-206.478(6)
	$\Psi_{3,\perp}^{(0)}$	1567.93(5)	1741.68(4)	1567.93(5)	0	0	471.42(1)

TABLE XI. The additive and nonadditive dispersion coefficients $C_8^{(IJ)}(1, M=0)$ and $C_8^{(IJ,K)}(1, M=0)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) system for three different types of the zeroth-order wave functions, where the three atoms form an isosceles right triangle, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_8^{(12)}(1, M=0)$	$C_8^{(23)}(1, M=0)$	$C_8^{(31)}(1, M=0)$	$C_8^{(12,23)}(1, M=0)$	$C_8^{(23,31)}(1, M=0)$	$C_8^{(31,12)}(1, M=0)$
$^\infty\text{Li}$	$\Psi_{1,\perp}^{(0)}$	97059.4(9)	94454(2)	97059.4(9)	14674.28(1)	14674.28(1)	0
	$\Psi_{2,\perp}^{(0)}$	58361.9(9)	92021(2)	58361.9(9)	-14674.28(1)	-14674.28(1)	0
	$\Psi_{3,\perp}^{(0)}$	79617(2)	48564.8(5)	79617(2)	0	0	0
^7Li	$\Psi_{1,\perp}^{(0)}$	97072(1)	94468(1)	97072(1)	14677.57(1)	14677.57(1)	0
	$\Psi_{2,\perp}^{(0)}$	58368.8(9)	92038(2)	58368.8(9)	-14677.57(1)	-14677.57(1)	0
	$\Psi_{3,\perp}^{(0)}$	79631(1)	48566.7(5)	79631(1)	0	0	0
^6Li	$\Psi_{1,\perp}^{(0)}$	97074(1)	94472(2)	97074(1)	14678.12(1)	14678.12(1)	0
	$\Psi_{2,\perp}^{(0)}$	58370(1)	92041(2)	58370(1)	-14678.12(1)	-14678.12(1)	0
	$\Psi_{3,\perp}^{(0)}$	79633(1)	48567.0(5)	79633(1)	0	0	0

TABLE XII. The additive and nonadditive dispersion coefficients $C_8^{(IJ)}(1, M = \pm 1)$ and $C_8^{(IJ,JK)}(1, M = \pm 1)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) system for three different types of the zeroth-order wave functions, where the three atoms form an isosceles right, in atomic units. The numbers in parentheses represent the computational uncertainties.

Atom	State	$C_8^{(12)}(1, M = \pm 1)$	$C_8^{(23)}(1, M = \pm 1)$	$C_8^{(31)}(1, M = \pm 1)$	$C_8^{(12,23)}(1, M = \pm 1)$	$C_8^{(23,31)}(1, M = \pm 1)$	$C_8^{(31,12)}(1, M = \pm 1)$
$^\infty\text{Li}$	$\Psi_{1,\perp}^{(0)}$	161893(4)	142518(4)	161893(4)	-16508.56(1)	-16508.56(1)	0
	$\Psi_{2,\perp}^{(0)}$	411044(4)	129477(3)	411044(4)	16508.56(1)	16508.56(1)	0
	$\Psi_{3,\perp}^{(0)}$	218790(4)	519731(4)	218790(4)	0	0	0
^7Li	$\Psi_{1,\perp}^{(0)}$	161920(4)	142544(4)	161920(4)	-16512.27(1)	-16512.27(1)	0
	$\Psi_{2,\perp}^{(0)}$	411116(3)	129502(3)	411116(3)	16512.27(1)	16512.27(1)	0
	$\Psi_{3,\perp}^{(0)}$	218830(3)	519821(4)	218830(3)	0	0	0
^6Li	$\Psi_{1,\perp}^{(0)}$	161924(4)	142548(4)	161924(4)	-16512.89(1)	-16512.89(1)	0
	$\Psi_{2,\perp}^{(0)}$	411130(4)	129506(3)	411130(4)	16512.89(1)	16512.89(1)	0
	$\Psi_{3,\perp}^{(0)}$	218838(4)	519838(5)	218838(4)	0	0	0

TABLE XIII. The additive long-range coefficients $C_3^{(IJ)}(1, M)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_3^{(12)}(1, M = 0)$	$C_3^{(23)}(1, M = 0)$	$C_3^{(31)}(1, M = 0)$	$C_3^{(12)}(1, M = \pm 1)$	$C_3^{(23)}(1, M = \pm 1)$	$C_3^{(31)}(1, M = \pm 1)$
$^\infty\text{Li}$	$\Psi_{1,-}^{(0)}$	-3.8853730(7)	-2.8714730(6)	-3.8853730(7)	1.9426864(4)	1.4357365(3)	1.9426864(4)
	$\Psi_{2,-}^{(0)}$	3.8853730(7)	-2.6286373(5)	3.8853730(7)	-1.9426864(4)	1.3143187(2)	-1.9426864(4)
	$\Psi_{3,-}^{(0)}$	0	5.500111(1)	0	0	-2.7500551(6)	0
^7Li	$\Psi_{1,-}^{(0)}$	-3.885949(1)	-2.8718991(7)	-3.885949(1)	1.9429746(5)	1.4359496(3)	1.9429746(5)
	$\Psi_{2,-}^{(0)}$	3.885949(1)	-2.6290273(6)	3.885949(1)	-1.9429746(5)	1.3145136(3)	-1.9429746(5)
	$\Psi_{3,-}^{(0)}$	0	5.500926(1)	0	0	-2.7504631(7)	0
^6Li	$\Psi_{1,-}^{(0)}$	-3.886045(1)	-2.8719700(7)	-3.886045(1)	1.9430227(4)	1.4359849(4)	1.9430227(4)
	$\Psi_{2,-}^{(0)}$	3.886045(1)	-2.6290922(6)	3.886045(1)	-1.9430227(4)	1.3145461(3)	-1.9430227(4)
	$\Psi_{3,-}^{(0)}$	0	5.501062(1)	0	0	-2.7505310(7)	0

TABLE XIV. The additive and nonadditive dispersion coefficients $C_6^{(IJ)}(1, M = 0)$ and $C_6^{(IJ,JK)}(1, M = 0)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_6^{(12)}(1, M = 0)$	$C_6^{(23)}(1, M = 0)$	$C_6^{(31)}(1, M = 0)$	$C_6^{(12,23)}(1, M = 0)$	$C_6^{(23,31)}(1, M = 0)$	$C_6^{(31,12)}(1, M = 0)$
$^\infty\text{Li}$	$\Psi_{1,-}^{(0)}$	1403.22(4)	1400.34(4)	1403.22(4)	166.425(6)	166.425(6)	122.995(4)
	$\Psi_{2,-}^{(0)}$	1403.50(3)	1399.76(4)	1403.50(3)	-166.425(6)	-166.425(6)	112.594(4)
	$\Psi_{3,-}^{(0)}$	1400.05(4)	1406.69(4)	1400.05(4)	0	0	-235.588(7)
^7Li	$\Psi_{1,-}^{(0)}$	1403.72(4)	1400.88(4)	1403.72(4)	166.502(6)	166.502(6)	123.052(4)
	$\Psi_{2,-}^{(0)}$	1404.01(4)	1400.30(4)	1404.01(4)	-166.502(6)	-166.502(6)	112.646(4)
	$\Psi_{3,-}^{(0)}$	1400.59(4)	1407.14(4)	1400.59(4)	0	0	-235.697(7)
^6Li	$\Psi_{1,-}^{(0)}$	1403.80(4)	1400.97(4)	1403.80(4)	166.513(5)	166.513(5)	123.060(3)
	$\Psi_{2,-}^{(0)}$	1404.09(4)	1400.39(4)	1404.09(4)	-166.513(5)	-166.513(5)	112.655(4)
	$\Psi_{3,-}^{(0)}$	1400.68(4)	1407.20(3)	1400.68(4)	0	0	-235.715(7)

TABLE XV. The additive and nonadditive dispersion coefficients $C_6^{(IJ)}(1, M = \pm 1)$ and $C_6^{(IJ,K)}(1, M = \pm 1)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_6^{(12)}(1, M = \pm 1)$	$C_6^{(23)}(1, M = \pm 1)$	$C_6^{(31)}(1, M = \pm 1)$	$C_6^{(12,23)}(1, M = \pm 1)$	$C_6^{(23,31)}(1, M = \pm 1)$	$C_6^{(31,12)}(1, M = \pm 1)$
$^\infty\text{Li}$	$\Psi_{1,-}^{(0)}$	1650.30(4)	1574.90(4)	1650.30(4)	416.06(2)	416.06(2)	307.487(9)
	$\Psi_{2,-}^{(0)}$	1657.99(5)	1559.55(4)	1657.99(5)	-416.06(2)	-416.06(2)	281.483(8)
	$\Psi_{3,-}^{(0)}$	1567.24(5)	1741.06(5)	1567.24(5)	0	0	-588.97(2)
^7Li	$\Psi_{1,-}^{(0)}$	1650.88(5)	1575.49(4)	1650.88(5)	416.25(1)	416.25(1)	307.63(1)
	$\Psi_{2,-}^{(0)}$	1658.54(4)	1560.16(5)	1658.54(4)	-416.25(1)	-416.25(1)	281.615(9)
	$\Psi_{3,-}^{(0)}$	1567.83(5)	1741.59(4)	1567.83(5)	0	0	-589.24(2)
^6Li	$\Psi_{1,-}^{(0)}$	1650.96(4)	1575.60(5)	1650.96(4)	416.29(2)	416.29(2)	307.653(9)
	$\Psi_{2,-}^{(0)}$	1658.65(5)	1560.24(4)	1658.65(5)	-416.29(2)	-416.29(2)	281.636(9)
	$\Psi_{3,-}^{(0)}$	1567.93(5)	1741.68(4)	1567.93(5)	0	0	-589.29(2)

TABLE XVI. The additive and nonadditive dispersion coefficients $C_8^{(IJ)}(1, M = 0)$ and $C_8^{(IJ,K)}(1, M = 0)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_8^{(12)}(1, M = 0)$	$C_8^{(23)}(1, M = 0)$	$C_8^{(31)}(1, M = 0)$	$C_8^{(12,23)}(1, M = 0)$	$C_8^{(23,31)}(1, M = 0)$	$C_8^{(31,12)}(1, M = 0)$
$^\infty\text{Li}$	$\Psi_{1,-}^{(0)}$	97037.1(9)	93669(1)	97037.1(9)	20893.68(2)	20893.68(2)	-15441.40(1)
	$\Psi_{2,-}^{(0)}$	58384.2(9)	92803(1)	58384.2(9)	-20893.68(2)	-20893.68(2)	-14135.55(1)
	$\Psi_{3,-}^{(0)}$	79617(1)	48564.8(5)	79617(1)	0	0	29576.95(2)
^7Li	$\Psi_{1,-}^{(0)}$	97049.9(9)	93685(1)	97049.9(9)	20898.36(1)	20898.36(1)	-15444.87(1)
	$\Psi_{2,-}^{(0)}$	58391.4(9)	92821(2)	58391.4(9)	-20898.36(1)	-20898.36(1)	-14138.73(2)
	$\Psi_{3,-}^{(0)}$	79631(1)	48566.7(5)	79631(1)	0	0	29583.60(2)
^6Li	$\Psi_{1,-}^{(0)}$	97052(1)	93689(2)	97052(1)	20899.14(1)	20899.14(1)	-15445.45(1)
	$\Psi_{2,-}^{(0)}$	58392.6(9)	92822(1)	58392.6(9)	-20899.14(1)	-20899.14(1)	-14139.26(2)
	$\Psi_{3,-}^{(0)}$	79633(1)	48567.0(5)	79633(1)	0	0	29584.70(2)

TABLE XVII. The additive and nonadditive dispersion coefficients $C_8^{(IJ)}(1, M = \pm 1)$ and $C_8^{(IJ,K)}(1, M = \pm 1)$ of the Li(2^2S)-Li(2^2S)-Li(2^2P) 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	$C_8^{(12)}(1, M = \pm 1)$	$C_8^{(23)}(1, M = \pm 1)$	$C_8^{(31)}(1, M = \pm 1)$	$C_8^{(12,23)}(1, M = \pm 1)$	$C_8^{(23,31)}(1, M = \pm 1)$	$C_8^{(31,12)}(1, M = \pm 1)$
$^\infty\text{Li}$	$\Psi_{1,-}^{(0)}$	166509(4)	138319(4)	166509(4)	41787.35(3)	41787.35(3)	-30882.81(2)
	$\Psi_{2,-}^{(0)}$	406428(4)	133676(3)	406428(4)	-41787.35(3)	-41787.35(3)	-28271.10(2)
	$\Psi_{3,-}^{(0)}$	218790(4)	519731(4)	218790(4)	0	0	59153.90(3)
^7Li	$\Psi_{1,-}^{(0)}$	166537(4)	138343(3)	166537(4)	41796.72(2)	41796.72(2)	-30889.75(2)
	$\Psi_{2,-}^{(0)}$	406499(3)	133701(3)	406499(3)	-41796.72(2)	-41796.72(2)	-28277.45(2)
	$\Psi_{3,-}^{(0)}$	218830(3)	519821(4)	218830(3)	0	0	59167.19(3)
^6Li	$\Psi_{1,-}^{(0)}$	166540(3)	138347(3)	166540(3)	41798.29(2)	41798.29(2)	-30890.90(2)
	$\Psi_{2,-}^{(0)}$	406513(4)	133707(4)	406513(4)	-41798.29(2)	-41798.29(2)	-28278.51(2)
	$\Psi_{3,-}^{(0)}$	218838(4)	519838(5)	218838(4)	0	0	59169.40(3)

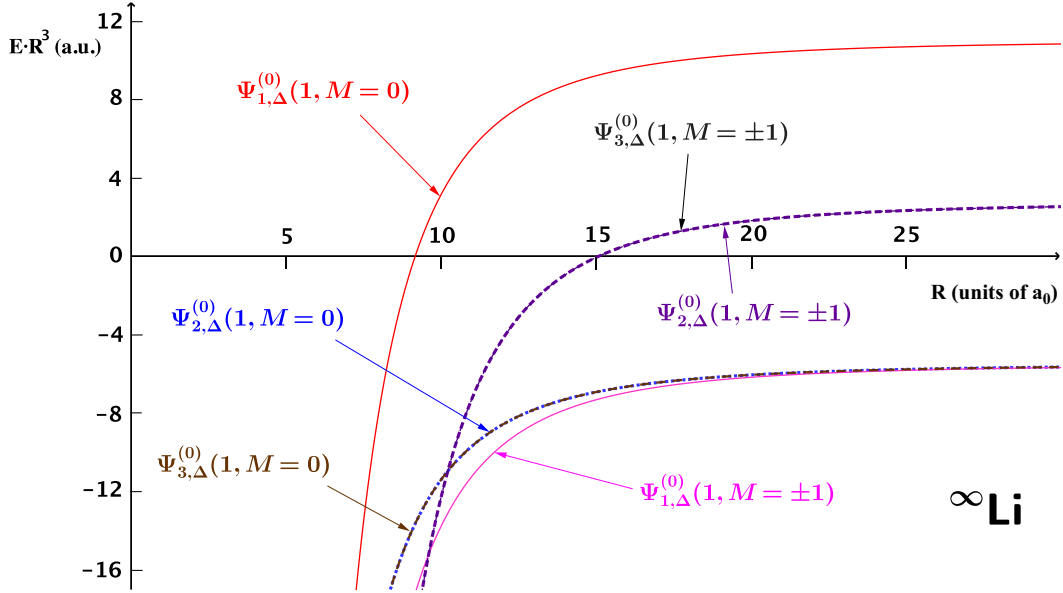


FIG. 2. Long-range potentials (E) multiplied by R^3 for the $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$ system for three different types of the zeroth-order wave functions, where the three atoms form an equilateral triangle and R is the interatomic distance, in atomic units. For each curve labeled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

form an equilateral triangle, the first-order dipolar coefficients are listed in Table II and the second-order additive and nonadditive dispersion coefficients are listed in Tables III–VI.

From Table II, we can see that for the zeroth-order wave function $\Psi_{1,\Delta}^{(0)}$, $C_3^{(12)}(1, M=0)$, $C_3^{(23)}(1, M=0)$, and $C_3^{(31)}(1, M=0)$ are all the same because $a = b = c = 1/\sqrt{3}$; similarly $C_3^{(12)}(1, M=\pm 1)$, $C_3^{(23)}(1, M=\pm 1)$, and $C_3^{(31)}(1, M=\pm 1)$ are all the same. For the zeroth-order wave function $\Psi_{2,\Delta}^{(0)}$, $C_3^{(12)}(1, M)$ and $C_3^{(23)}(1, M)$, whenever $M=0$ or $M=\pm 1$, are zero because $b=0$. For the zeroth-order wave function $\Psi_{3,\Delta}^{(0)}$, $C_3^{(12)}(1, M)$ and $C_3^{(23)}(1, M)$ are the same because $a = c = 1/\sqrt{6}$. The coefficients between $M=0$ and $M=\pm 1$ satisfy the relationship $C_3^{(IJ)}(1, M=0) = -2C_3^{(IJ)}(1, M=\pm 1)$. Also listed in Table II are the values for ^7Li and ^6Li obtained by taking the finite nuclear mass into consideration.

For the leading terms of the second-order long-range interaction, there exist both additive and nonadditive terms as shown in Table III for $C_6^{(IJ)}(1, M=0)$ and $C_6^{(IJ,JK)}(1, M=0)$ and in Table IV for $C_6^{(IJ)}(1, M=\pm 1)$ and $C_6^{(IJ,JK)}(1, M=\pm 1)$, for the $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$ system. For the second zeroth-order wave function $\Psi_{2,\Delta}^{(0)}$, the nonadditive coefficients $C_6^{(23,31)}(1, M)$ and $C_6^{(31,12)}(1, M)$ are zero for $M=0$ or $M=\pm 1$ because $\mathbb{Q}_4(a, b, 1, M, \gamma) = 0$ and $b=0$. For $\Psi_{2,\Delta}^{(0)}$ and $\Psi_{3,\Delta}^{(0)}$, we have $C_6^{(12)}(1, M) = C_6^{(23)}(1, M)$ and $C_6^{(23,31)}(1, M) = C_6^{(31,12)}(1, M)$ for $M=0$ or $M=\pm 1$ because $a = c$.

The long-range dispersion coefficients $C_8^{(IJ)}(1, M)$ and $C_8^{(IJ,JK)}(1, M)$ are listed in Table V for $M=0$ and in Table VI for $M=\pm 1$ for the $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$ system. These coefficients have very similar characteristics as $C_6^{(IJ)}(1, M)$ and $C_6^{(IJ,JK)}(1, M)$. For example, for fixed M , $C_8^{(IJ)}(1, M)$ are all the same for the zeroth-order wave function $\Psi_{1,\Delta}^{(0)}$;

similarly for $C_8^{(IJ,JK)}(1, M)$, they are all the same for $\Psi_{1,\Delta}^{(0)}$. For $\Psi_{2,\Delta}^{(0)}$, $C_8^{(23,31)}(1, M)$ and $C_8^{(31,12)}(1, M)$ are zero because $\mathbb{Q}_4(a, b, 2, M, \gamma) = 0$ and $b=0$. We also have $C_8^{(12)}(1, M) = C_8^{(23)}(1, M)$ and $C_8^{(23,31)}(1, M) = C_8^{(31,12)}(1, M)$ for both $\Psi_{2,\Delta}^{(0)}$ and $\Psi_{3,\Delta}^{(0)}$.

From Tables III–VI, we can also 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. 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 $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$. For example, for the case of $\Psi_{2,\Delta}^{(0)}$, the ratio of $(\frac{C_8^{(12,23)}(1, M=\pm 1)}{R_{12}^4 R_{23}^4}) / (\frac{C_8^{(12)}(1, M=\pm 1)}{R_{12}^8}) \simeq 18\%$. For this configuration the energies $\Delta E^{(1)}$ and $\Delta E^{(2)}$ are given by, respectively, Eqs. (13) and (17), and are listed in Table VII. The curves of potential energy (E) multiplied by R^3 corresponding to the different zeroth-order wave functions are plotted in Fig. 2.

We identify the $\Psi_{1,\Delta}^{(0)}$, $\Psi_{2,\Delta}^{(0)}$, and $\Psi_{3,\Delta}^{(0)}$ states with $M=0$ as trimer states of A symmetry and those with $M=\pm 1$ as trimer states of E symmetry by comparison with the *ab initio* calculations of Ref. [50], where A and E are standard nomenclature labeling D_{3h} symmetry in electronic states. This identification is consistent with the double degeneracy of E symmetry states. In Ref. [50], quantum-chemical calculations were carried out for the ground and excited quartet electronic states of Li_3 . While the emphasis of that work was on the ground electronic state, a plot (Fig. 2 of Ref. [50]) is given of the excited state potential energies corresponding to $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$ for the atoms in an equilateral configuration at atomic separations up to 10^{-9} m ($19a_0$). Six electronic states are given, of which three are identified with

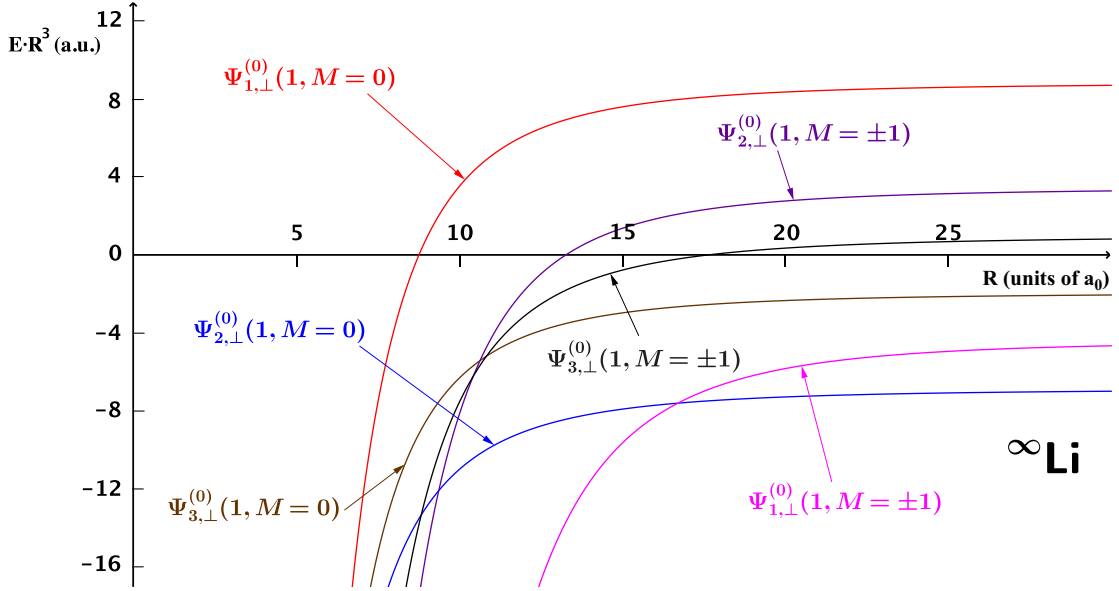


FIG. 3. Long-range potentials (E) multiplied by R^3 for the $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$ system for three different types of the zeroth-order wave functions, where the three atoms form an isosceles right triangle and R is the interatomic distance on the congruent sides, in atomic units. For each curve labeled by a wave function, the plotted curve is the sum of $\Delta E^{(1)}$ and $\Delta E^{(2)}$.

A symmetry and three with E symmetry. At $R \approx 19a_0$, $\Delta E^{(1)}$ is the leading contribution to the long-range interactions and we note that the ordering of the states from lowest to highest energy at the maximum distance is in accord with our results shown in Table VII. At this value of R , our values of $\Delta E^{(1)}$ range from -350 cm^{-1} to 175 cm^{-1} and are entirely consistent with the results shown in Fig. 2 of Ref. [50]. Because the calculation of Ref. [50] includes exchange a more quantitative comparison may be inconclusive. In addition, because our choice of coordinate system (see Fig. 1) doesn't naturally reflect the symmetries of the equilateral triangle, we refrain from making further symmetry assignments.

B. Dipolar and dispersion coefficients for an isosceles right triangle

For the configuration of an isosceles right triangle, the first-order dipolar coefficients are listed in Table VIII and the second-order additive and nonadditive dispersion coefficients are listed in Tables IX–XII.

For this configuration, we have $b = c$ for the first two zeroth-order wave functions $\Psi_{1,\perp}^{(0)}$ and $\Psi_{2,\perp}^{(0)}$, and $b = -c$ and $a = 0$ for the third zeroth-order wave function $\Psi_{3,\perp}^{(0)}$. We can clearly see that $C_3^{(12)}(1, M)$ equals $C_3^{(31)}(1, M)$ for $\Psi_{1,\perp}^{(0)}$ and $\Psi_{2,\perp}^{(0)}$, and $C_3^{(12)}(1, M) = C_3^{(31)}(1, M) = 0$ for $\Psi_{3,\perp}^{(0)}$, as shown in

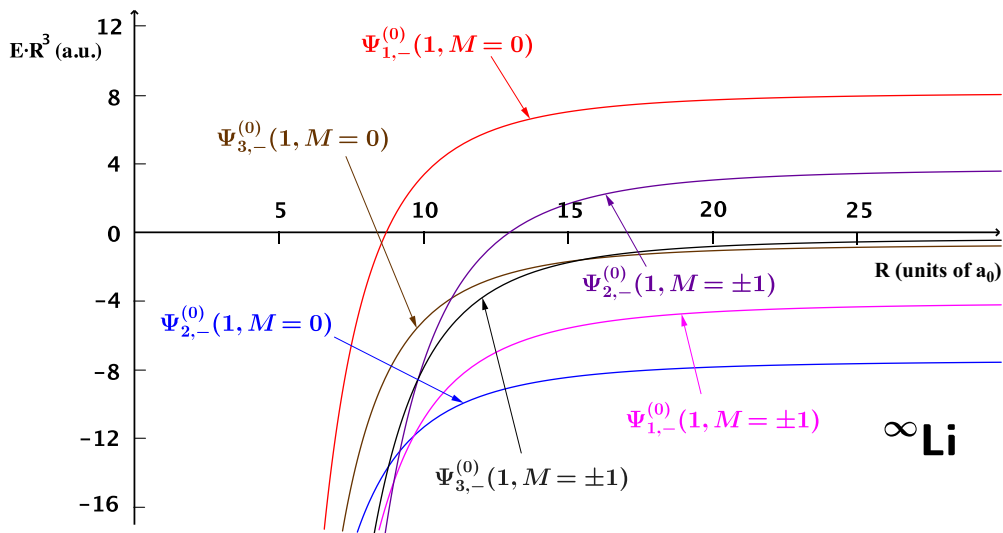


FIG. 4. Long-range potentials (E) multiplied by R^3 for the $\text{Li}(2^2S)\text{-Li}(2^2S)\text{-Li}(2^2P)$ system for three different types of the zeroth-order wave functions, where the three atoms form a straight line and R is the distance between adjacent atoms, in atomic units. For each curve labeled by a wave function, the plotted curve is the sum of $\Delta E^{(1)}$ and $\Delta E^{(2)}$.

Table VIII. Compared to the values in Table II, we can conclude that a change in geometric configuration will influence the long-range coefficients.

The second-order dispersion coefficients $C_6^{(IJ)}$, $C_6^{(IJ,K)}$, $C_8^{(IJ)}$, and $C_8^{(IJ,K)}$ are listed in Tables IX–XII. One can see 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 $\beta=\gamma$. Also $C_8^{(31,12)}(1,M)=0$ and $C_6^{(31,12)}(1,M)\neq 0$ because $\alpha=\pi/2$ and M_t-M can be even or odd in Eq. (28). We find that allowing for finite nuclear mass increases the additive dispersion coefficients, as shown in Tables IX–XII. Similarly to Sec. III A, the nonadditive terms may not be neglected in constructing a three-body potential surface for Li(2^2S)-Li(2^2S)-Li(2^2P). The curves of potential energy (E) multiplied by R^3 resulting from $\Delta E^{(1)}$ and $\Delta E^{(2)}$ for this geometrical structure are shown in Fig. 3.

C. Dipolar and dispersion coefficients for a straight line

For the configuration of three atoms equally spaced and forming a straight line, the long-range dipolar and dispersion coefficients are listed in Tables XIII–XVII. Since the zeroth-order wave function coefficients have $b=c$ in Eqs. (39) and (40), and $a=0$ and $b=-c$ in Eq. (41) the dispersion coefficients have similar characteristics as the case of the isosceles right triangle of Sec. III B. The only differences are the values of three interior angles: $\beta=\gamma=0$ and $\alpha=2\pi$, which leads to the relatively larger nonzero dispersion coefficients $C_8^{(31,12)}(1,M=0)$ and $C_8^{(31,12)}(1,M=\pm 1)$. The corresponding curves of potential energy (E) multiplied by R^3 resulting from $\Delta E^{(1)}$ and $\Delta E^{(2)}$ are shown in Fig. 4.

As in Sec. III A, we can make a comparison with the results of Ref. [50], where, in their Fig. 1, the excited electronic potential energies of Li(2^2S)-Li(2^2S)-Li(2^2P) are given for the equally spaced collinear geometry at values of R up to $19a_0$. We identify $\Psi_{1,-}^{(0)}$, $\Psi_{2,-}^{(0)}$, and $\Psi_{3,-}^{(0)}$ states with $M=0$ as trimer states of Σ symmetry and those with $M=\pm 1$ as trimer states of Π symmetry, corresponding to $D_{\infty h}$ symmetry labels. In the present work, the magnitude of the leading long-range interaction energy $\Delta E^{(1)}$ ranges from -341 cm^{-1} to 170 cm^{-1} and is consistent with the *ab initio* results shown in Fig. 1 of Ref. [50].

IV. CONCLUSION

The long-range additive dipolar and additive dispersion interactions and nonadditive dispersion interactions for the Li(2^2S)-Li(2^2S)-Li(2^2P) system were obtained using perturbation theory. The additive dipolar and additive dispersion

interactions and nonadditive dispersion interactions depend on the geometrical configuration of the atoms.

Here we found that the nonadditive dispersion interactions start to appear at the *second order* in the perturbative treatment, which is different from the case of three S atoms where the geometry dependent nonadditive dispersion interactions start to appear at the *third order*. While the formulas apply to all geometrical configurations, 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 coefficients to high precision using variational wave functions in Hylleraas coordinates. The calculations are in accord with quantum-chemical calculations, where available. Our numerical results might be useful in constructing accurate three-body potential curves and for exploration of schemes to create trimers with ultracold atoms in optical lattices using photoassociation. The formulas listed in the appendix are general for $A(n_0S)$ - $A(n_0S)$ - $A(n'_0L)$, where L is an arbitrary nonzero angular momentum.

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APPENDIX

We consider three like atoms with two atoms in identical S states $|\varphi_{n_0}(0)\rangle$ and the third atom in a non- S state $|\varphi_{n'_0}(LM)\rangle$, where n_0 and n'_0 are the principal quantum numbers, and L and M are the usual angular quantum numbers. In the following, as discussed in Sec. II A, we use σ , ρ , and ς to represent collectively the coordinates of each atom. The three orthonormalized degenerate eigenvectors of the unperturbed Hamiltonian with the energy eigenvalue $E_{n_0S;n_0S;n'_0L}^{(0)} = 2E_{n_0S}^{(0)} + E_{n'_0L}^{(0)}$ are given in Eqs. (8)–(10). The correct zeroth-order wave functions can always be expanded as a linear combination of $\{\phi_1, \phi_2, \phi_3\}$,

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

where a , b , and c are the expansion coefficients with their values depending on the geometrical configuration of the three atoms.

1. The first-order energy correction

According to perturbation theory, the first-order energy correction is

$$\begin{aligned} \Delta E^{(1)} &= \langle \Psi^{(0)} | V_{123} | \Psi^{(0)} \rangle \\ &= |a|^2 \langle \phi_1 | V_{123} | \phi_1 \rangle + |b|^2 \langle \phi_2 | V_{123} | \phi_2 \rangle + |c|^2 \langle \phi_3 | V_{123} | \phi_3 \rangle \\ &\quad + (a^*b + b^*a) \langle \phi_1 | V_{123} | \phi_2 \rangle + (a^*c + c^*a) \langle \phi_1 | V_{123} | \phi_3 \rangle + (b^*c + c^*b) \langle \phi_2 | V_{123} | \phi_3 \rangle \end{aligned}$$

$$\begin{aligned}
 &= (a^*b + b^*a) \frac{4\pi}{R_{12}^{2L+1}} \frac{(-1)^{L+M}(2L)!P_{2L}(\cos\theta_{12})}{(2L+1)^2(L-M)!(L+M)!} \left| \langle \varphi_{n_0}(0; \sigma) \| T_L(\sigma) \| \varphi_{n'_0}(L; \sigma) \rangle \right|^2 \\
 &+ (b^*c + c^*b) \frac{4\pi}{R_{23}^{2L+1}} \frac{(-1)^{L+M}(2L)!P_{2L}(\cos\theta_{23})}{(2L+1)^2(L-M)!(L+M)!} \left| \langle \varphi_{n_0}(0; \rho) \| T_L(\rho) \| \varphi_{n'_0}(L; \rho) \rangle \right|^2 \\
 &+ (c^*a + a^*c) \frac{4\pi}{R_{31}^{2L+1}} \frac{(-1)^{L+M}(2L)!P_{2L}(\cos\theta_{31})}{(2L+1)^2(L-M)!(L+M)!} \left| \langle \varphi_{n_0}(0; \varsigma) \| T_L(\varsigma) \| \varphi_{n'_0}(L; \varsigma) \rangle \right|^2. \tag{A2}
 \end{aligned}$$

2. The second-order energy correction

The second-order energy correction is given by

$$\begin{aligned}
 \Delta E^{(2)} &= - \sum_{n_s n_t n_u} \sum_{L_s L_t L_u} \sum_{M_s M_t M_u} \frac{|\langle \Psi^{(0)} | V_{123} | \chi_{n_s}(L_s M_s; \sigma) \chi_{n_t}(L_t M_t; \rho) \chi_{n_u}(L_u M_u; \varsigma) \rangle|^2}{E_{n_s L_s; n_t L_t; n_u L_u} - E_{n_0 S; n'_0 L}^{(0)}} \\
 &= V_{12}^{(2)} + V_{23}^{(2)} + V_{31}^{(2)} + V_{12,23}^{(2)} + V_{23,31}^{(2)} + V_{31,12}^{(2)}, \tag{A3}
 \end{aligned}$$

where $\chi_{n_s}(L_s M_s; \sigma) \chi_{n_t}(L_t M_t; \rho) \chi_{n_u}(L_u M_u; \varsigma)$ 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 $E_{n_s L_s; n_t L_t; n_u L_u} = E_{n_0 S; n'_0 L}^{(0)}$.

In this paper, we choose the coordinate system defined in Sec. II B and shown in Fig. 1. Thus in the associated Legendre functions, we have all $\cos(\theta_{IJ}) = 0$ due to $\theta_{IJ} = \pi/2$. Also in $\exp[i(m_I - m_J)\Phi_{IJ}]$, etc., $\Phi_{12} = 0$, $\Phi_{23} = \pi - \beta$, and $\Phi_{31} = \pi + \alpha$. 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_{l_1 l'_1} \sum_{M_s M_t M_1} \frac{16\pi^2}{R_{12}^{2L_s+l_1+l'_1+2}} \begin{pmatrix} L & l_1 & L_s \\ -M & m_1 & M_s \end{pmatrix} \begin{pmatrix} L & l'_1 & L_s \\ -M & m_1 & M_s \end{pmatrix} P_{L_t+l_1}^{M_t-m_1}(0) P_{L_t+l'_1}^{M_t-m_1}(0) \\
 &\times \frac{(L_t + l_1 - M_t + m_1)!(L_t + l'_1 - M_t + m_1)!(L_t, L_t)^{-1}(l_1, l'_1)^{-1/2}}{(L_t + M_t)!(L_t - M_t)![(l_1 + m_1)!(l_1 - m_1)!(l'_1 + m_1)!(l'_1 - m_1)!]^{1/2}} \\
 &\times \frac{\langle \varphi_{n'_0}(L; \sigma) \| T_{l_1}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle^* \langle \varphi_{n'_0}(L; \sigma) \| T_{l'_1}(\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^2}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}} \\
 &- |b|^2 \sum_{n_s n_t} \sum_{L_s L_t} \sum_{l_2 l'_2} \sum_{M_s M_t M_2} \frac{16\pi^2}{R_{12}^{2L_s+l_2+l'_2+2}} \begin{pmatrix} L & l_2 & L_t \\ -M & m_2 & M_t \end{pmatrix} \begin{pmatrix} L & l'_2 & L_t \\ -M & m_2 & M_t \end{pmatrix} P_{L_s+l_2}^{M_s-m_2}(0) P_{L_s+l'_2}^{M_s-m_2}(0) \\
 &\times \frac{(L_s + l_2 - M_s + m_2)!(L_s + l'_2 - M_s + m_2)!(L_s, L_s)^{-1}(l_2, l'_2)^{-1/2}}{(L_s + M_s)!(L_s - M_s)![(l_2 + m_2)!(l_2 - m_2)!(l'_2 + m_2)!(l'_2 - m_2)!]^{1/2}} \\
 &\times \frac{|\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle|^2 \langle \varphi_{n'_0}(L; \rho) \| T_{l_2}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle^* \langle \varphi_{n'_0}(L; \rho) \| T_{l'_2}(\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 L}^{(0)}} \\
 &- |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)!} \\
 &\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)}} \\
 &- a^*b \sum_{n_s n_t} \sum_{L_s L_t} \sum_{l_1 l'_1 l'_2} \sum_{M_s M_t M_1 M'_2} \frac{16\pi^2 (-1)^{L_s+l'_2-M_s-M_t}}{R_{12}^{l_1+L_s+L_t+l'_2+2}} \begin{pmatrix} L & l_1 & L_s \\ -M & -m_1 & M_s \end{pmatrix} \begin{pmatrix} L & l'_2 & L_t \\ -M & m'_2 & M_t \end{pmatrix} \\
 &\times \frac{P_{L_t+l_1}^{M_t+m_1}(0) P_{L_s+l'_2}^{M_s-m'_2}(0) (L_t + l_1 - M_t - m_1)!(L_s + l'_2 - M_s + m'_2)!(L_s, L_t)^{-1}(l_1, l'_2)^{-1/2}}{[(L_s + M_s)!(L_s - M_s)!(L_t + M_t)!(L_t - M_t)!(l_1 + m_1)!(l_1 - m_1)!(l'_2 + m'_2)!(l'_2 - m'_2)!]^{1/2}} \\
 &\times \langle \varphi_{n'_0}(L; \sigma) \| T_{l_1}(\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^* \\
 &\times \frac{\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle \langle \varphi_{n'_0}(L; \rho) \| T_{l'_2}(\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 L}^{(0)}}
 \end{aligned}$$

$$\begin{aligned}
& -b^*a \sum_{n_s n_t} \sum_{L_s L_t l'_1 l'_2} \sum_{M_s M_t m'_1 m'_2} \frac{16\pi^2 (-1)^{L_s+l_2-M_s-M_t}}{R_{12}^{l'_1+L_t+L_s+l_2+2}} \begin{pmatrix} L & l'_1 & L_s \\ -M & -m'_1 & M_s \end{pmatrix} \begin{pmatrix} L & l_2 & L_t \\ -M & m_2 & M_t \end{pmatrix} \\
& \times \frac{P_{L_s+l_2}^{M_s-m_2}(0) P_{L_t+l'_1}^{M_t+m'_1}(0) (L_t+l'_1-M_t-m'_1)! (L_s+l_2-M_s+m_2)! (L_s, L_t)^{-1} (l'_1, l_2)^{-1/2}}{[(L_s+M_s)!(L_s-M_s)!(L_t+M_t)!(L_t-M_t)!(l'_1+m'_1)!(l'_1-m'_1)!(l_2+m_2)!(l_2-m_2)!]^{1/2}} \\
& \times \langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle^* \langle \varphi_{n'_0}(L; \rho) \| T_{l_2}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle^* \\
& \times \frac{\langle \varphi_{n'_0}(L; \sigma) \| T_{l'_1}(\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 L}^{(0)}} \\
& = - \left\{ |a|^2 \sum_{n_s n_t} \sum_{L_s L_t l'_1 l'_2} \frac{F_1(n_s, n_t, L_s, L_t; l'_1, l'_2; L, M)}{R_{12}^{2L_t+L_1+l'_1+2}} + |b|^2 \sum_{n_s n_t} \sum_{L_s L_t l_2 l'_2} \frac{F_1(n_t, n_s, L_t, L_s; l_2, l'_2; L, M)}{R_{12}^{2L_s+L_2+l'_2+2}} \right. \\
& + |c|^2 \sum_{n_s n_t} \sum_{L_s L_t} \frac{F_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 l_1 l'_2} \frac{F_3(n_s, n_t, L_s, L_t; l_1, l'_2; L, M)}{R_{12}^{L_s+L_t+l_1+l'_2+2}} \\
& \left. + b^*a \sum_{n_s n_t} \sum_{L_s L_t l'_1 l'_2} \frac{F_3^*(n_s, n_t, L_s, L_t; l'_1, l'_2; L, M)}{R_{12}^{L_s+L_t+l'_1+l'_2+2}} \right\}, \tag{A4} \\
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)!} \\
& \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; \varsigma) \| T_{L_u}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle|^2}{E_{n_t L_t} + E_{n_u L_u} - 2E_{n_0 S}^{(0)}} \\
& - |b|^2 \sum_{n_t n_u} \sum_{L_t L_u l'_2 l'_2} \sum_{M_t M_u m_2} \frac{16\pi^2}{R_{23}^{2L_u+L_2+l'_2+2}} \begin{pmatrix} L & l_2 & L_t \\ -M & m_2 & M_t \end{pmatrix} \begin{pmatrix} L & l'_2 & L_t \\ -M & m_2 & M_t \end{pmatrix} P_{L_u+l'_2}^{M_u-m_2}(0) P_{L_u+l'_2}^{M_u-m_2}(0) \\
& \times \frac{(L_u+l_2-M_u+m_2)!(L_u+l'_2-M_u+m_2)!(L_u, L_u)^{-1} (l_2, l'_2)^{-1/2}}{(L_u+M_u)!(L_u-M_u)!(l_2+m_2)!(l_2-m_2)!(l'_2+m_2)!(l'_2-m_2)!]^{1/2}} \\
& \times \frac{\langle \varphi_{n'_0}(L; \rho) \| T_{l_2}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle^* \langle \varphi_{n'_0}(L; \rho) \| T_{l'_2}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle \langle \varphi_{n_0}(0; \varsigma) \| T_{L_u}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle^2}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}} \\
& - |c|^2 \sum_{n_t n_u} \sum_{L_t L_u l_3 l'_3} \sum_{M_t M_u m_3} \frac{16\pi^2}{R_{23}^{2L_t+L_3+l'_3+2}} \begin{pmatrix} L & l_3 & L_u \\ -M & m_3 & M_u \end{pmatrix} \begin{pmatrix} L & l'_3 & L_u \\ -M & m_3 & M_u \end{pmatrix} P_{L_t+l'_3}^{M_t-m_3}(0) P_{L_t+l'_3}^{M_t-m_3}(0) \\
& \times \frac{(L_t+l_3-M_t+m_3)!(L_t+l'_3-M_t+m_3)!(L_t, L_t)^{-1} (l_3, l'_3)^{-1/2}}{(L_t+M_t)!(L_t-M_t)!(l_3+m_3)!(l_3-m_3)!(l'_3+m_3)!(l'_3-m_3)!]^{1/2}} \\
& \times \frac{|\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2 \langle \varphi_{n'_0}(L; \varsigma) \| T_{l_3}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle^* \langle \varphi_{n'_0}(L; \varsigma) \| T_{l'_3}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}} \\
& - b^*c \sum_{n_t n_u} \sum_{L_t L_u l'_2 l'_3} \sum_{M_t M_u m_2 m'_3} \frac{16\pi^2 (-1)^{L_t+l'_3-M_t-M_u}}{R_{23}^{l'_2+L_u+L_t+l'_3+2}} \begin{pmatrix} L & l_2 & L_t \\ -M & -m_2 & M_t \end{pmatrix} \begin{pmatrix} L & l'_3 & L_u \\ -M & m'_3 & M_u \end{pmatrix} \\
& \times \frac{P_{L_u+l'_2}^{M_u+m_2}(0) P_{L_t+l'_3}^{M_t-m'_3}(0) (L_u+l_2-M_u-m_2)!(L_t+l'_3-M_t+m'_3)!(L_t, L_u)^{-1} (l_2, l'_3)^{-1/2}}{[(l_2+m_2)!(l_2-m_2)!(L_u+M_u)!(L_u-M_u)!(L_t+M_t)!(L_t-M_t)!(l'_3+m'_3)!(l'_3-m'_3)!]^{1/2}} \\
& \times \langle \varphi_{n'_0}(L; \rho) \| T_{l_2}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle^* \langle \varphi_{n_0}(0; \varsigma) \| T_{L_u}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle^* \\
& \times \frac{\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle \langle \varphi_{n'_0}(L; \varsigma) \| T_{l'_3}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}}
\end{aligned}$$

$$\begin{aligned}
 & -c^*b \sum_{n_t n_u} \sum_{L_t L_u l'_2 l'_3} \sum_{M_t M_u m'_2 m'_3} \frac{16\pi^2 (-1)^{L_t+l_3-M_t-M_u}}{R_{23}^{l'_2+L_t+L_u+l_3+2}} \begin{pmatrix} L & l'_2 & L_t \\ -M & -m'_2 & M_t \end{pmatrix} \begin{pmatrix} L & l_3 & L_u \\ -M & m_3 & M_u \end{pmatrix} \\
 & \times \frac{P_{L_t+l_3}^{M_t-m_3}(0) P_{L_u+l'_2}^{M_u+m'_2}(0) (L_u+l'_2-M_u-m'_2)! (L_t+l_3-M_t+m_3)! (L_t, L_u)^{-1} (l'_2, l_3)^{-1/2}}{[(l'_2+m'_2)! (l'_2-m'_2)! (L_u+M_u)! (L_u-M_u)! (L_t+M_t)! (L_t-M_t)! (l_3+m_3)! (l_3-m_3)!]^{1/2}} \\
 & \times \langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle^* \langle \varphi_{n'_0}(L; \varsigma) \| T_{l_3}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle^* \\
 & \times \frac{\langle \varphi_{n'_0}(L; \rho) \| T_{l'_2}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle \langle \varphi_{n_0}(0; \varsigma) \| T_{L_u}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle}{E_{n_t L_t} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}} \\
 & = - \left\{ |a|^2 \sum_{n_t n_u} \sum_{L_t L_u} \frac{F_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 l_2 l'_2} \frac{F_1(n_t, n_u, L_t, L_u; l_2, l'_2; L, M)}{R_{23}^{2L_u+l_2+l'_2+2}} \right. \\
 & + |c|^2 \sum_{n_t n_u} \sum_{L_t L_u l_3 l'_3} \frac{F_1(n_u, n_t, L_u, L_t; l_3, l'_3; L, M)}{R_{23}^{2L_t+l_3+l'_3+2}} + b^*c \sum_{n_t n_u} \sum_{L_t L_u l_2 l'_2} \frac{F_3(n_t, n_u, L_t, L_u; l_2, l'_2; L, M)}{R_{23}^{l_2+L_u+L_t+l'_2+2}} \\
 & \left. + c^*b \sum_{n_s n_t n_u} \sum_{L_s L_t L_u l'_2 l'_3} \frac{F_3^*(n_t, n_u, L_t, L_u; l'_2, l'_3; L, M)}{R_{23}^{L_t+L_u+l'_2+l_3+2}} \right\}, \tag{A5} \\
 V_{31}^{(2)} & = -|a|^2 \sum_{n_s n_u} \sum_{L_s L_u l'_1 l'_2} \sum_{M_s M_u m_1} \frac{16\pi^2}{R_{31}^{2L_u+l_1+l'_1+2}} \begin{pmatrix} L & l_1 & L_s \\ -M & m_1 & M_s \end{pmatrix} \begin{pmatrix} L & l'_1 & L_s \\ -M & m_1 & M_s \end{pmatrix} \\
 & \times \frac{P_{L_u+l_1}^{M_u-m_1}(0) P_{L_u+l'_1}^{M_u-m_1}(0) (L_u+l_1-M_u+m_1)! (L_u+l'_1-M_u+m_1)! (L_u, L_u)^{-1} (l_1, l'_1)^{-1/2}}{(L_u+M_u)! (L_u-M_u)! [(l_1+m_1)! (l_1-m_1)! (l'_1+m_1)! (l'_1-m_1)!]^{1/2}} \\
 & \times \frac{\langle \varphi_{n'_0}(L; \sigma) \| T_{l_1}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle^* \langle \varphi_{n'_0}(L; \sigma) \| T_{l'_1}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle \langle \varphi_{n_0}(0; \varsigma) \| T_{L_u}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle^2}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}} \\
 & - |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; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle|^2 |\langle \varphi_{n_0}(0; \varsigma) \| T_{L_u}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle|^2}{E_{n_s L_s} + E_{n_u L_u} - 2E_{n_0 S}^{(0)}} \\
 & - |c|^2 \sum_{n_s n_u} \sum_{L_s L_u l'_3 l'_2} \sum_{M_s M_u m_3} \frac{16\pi^2}{R_{31}^{2L_s+l_3+l'_3+2}} \begin{pmatrix} L & l_3 & L_u \\ -M & m_3 & M_u \end{pmatrix} \begin{pmatrix} L & l'_3 & L_u \\ -M & m_3 & M_u \end{pmatrix} P_{L_s+l'_3}^{M_s-m_3}(0) P_{L_s+l'_3}^{M_s-m_3}(0) \\
 & \times \frac{(L_s+l_3-M_s+m_3)! (L_s+l'_3-M_s+m_3)! (L_s, L_s)^{-1} (l_3, l'_3)^{-1/2}}{(L_s+M_s)! (L_s-M_s)! [(l_3+m_3)! (l_3-m_3)! (l'_3+m_3)! (l'_3-m_3)!]^{1/2}} \\
 & \times \frac{|\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle|^2 \langle \varphi_{n'_0}(L; \varsigma) \| T_{l_3}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle^* \langle \varphi_{n'_0}(L; \varsigma) \| T_{l'_3}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}} \\
 & - a^*c \sum_{n_s n_u} \sum_{L_s L_u l'_3 l'_1} \sum_{M_s M_u m'_3 m'_1} \frac{16\pi^2 (-1)^{L_u+l_1-M_u-M_s}}{R_{31}^{l'_3+L_s+L_u+l_1+2}} \begin{pmatrix} L & l'_3 & L_u \\ -M & -m'_3 & M_u \end{pmatrix} \begin{pmatrix} L & l_1 & L_s \\ -M & m_1 & M_s \end{pmatrix} \\
 & \times \frac{P_{L_u+l_1}^{M_u-m_1}(0) P_{L_s+l'_3}^{M_s+m'_3}(0) (L_s+l'_3-M_s-m'_3)! (L_u+l_1-M_u+m_1)! (L_u, L_s)^{-1} (l'_3, l_1)^{-1/2}}{[(L_s+M_s)! (L_s-M_s)! (L_u+M_u)! (L_u-M_u)! (l'_3+m'_3)! (l'_3-m'_3)! (l_1+m_1)! (l_1-m_1)!]^{1/2}} \\
 & \times \langle \varphi_{n'_0}(L; \sigma) \| T_{l_1}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle^* \langle \varphi_{n_0}(0; \varsigma) \| T_{L_u}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle^* \\
 & \times \frac{\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle \langle \varphi_{n'_0}(L; \varsigma) \| T_{l'_3}(\varsigma) \| \chi_{n_u}(L_u; \varsigma) \rangle}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}}
 \end{aligned}$$

$$\begin{aligned}
& -c^*a \sum_{n_s n_u} \sum_{L_s L_u l_3 l'_1} \sum_{M_s M_u m_3 m'_1} \frac{16\pi^2 (-1)^{L_u + l'_1 - M_u - M_s}}{R_{31}^{l_3 + L_s + L_u + l'_1 + 2}} \begin{pmatrix} L & l_3 & L_u \\ -M & -m_3 & M_u \end{pmatrix} \begin{pmatrix} L & l'_1 & L_s \\ -M & m'_1 & M_s \end{pmatrix} \\
& \times \frac{P_{L_s + l_3}^{M_s + m_3}(0) P_{L_u + l'_1}^{M_u - m'_1}(0) (L_s + l_3 - M_s - m_3)! (L_u + l'_1 - M_u + m'_1)! (L_u, L_s)^{-1} (l_3, l'_1)^{-1/2}}{[(L_s + M_s)! (L_s - M_s)! (L_u + M_u)! (L_u - M_u)! (l_3 + m_3)! (l_3 - m_3)! (l'_1 + m'_1)! (l'_1 - m'_1)!]^{1/2}} \\
& \times \langle \varphi_{n'_0}(L; \boldsymbol{\varsigma}) \| T_{l_3}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle^* \langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_{L_s}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle^* \\
& \times \frac{\langle \varphi_{n_0}(0; \boldsymbol{\varsigma}) \| T_{L_u}(\boldsymbol{\varsigma}) \| \chi_{n_u}(L_u; \boldsymbol{\varsigma}) \rangle \langle \varphi_{n'_0}(L; \boldsymbol{\sigma}) \| T_{l'_1}(\boldsymbol{\sigma}) \| \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle}{E_{n_s L_s} + E_{n_u L_u} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}} \\
& = - \left\{ |a|^2 \sum_{n_s n_u} \sum_{L_s L_u l_1 l'_1} \frac{F_1(n_s, n_u, L_s, L_u; l_1, l'_1; L, M)}{R_{31}^{2L_u + l_1 + l'_1 + 2}} + |b|^2 \sum_{n_s n_u} \sum_{L_s L_u} \frac{F_2(n_s, n_u, L_s, L_u)}{R_{31}^{2L_s + 2L_u + 2}} \right. \\
& + |c|^2 \sum_{n_s n_u} \sum_{L_s L_u l_3 l'_3} \frac{F_1(n_u, n_s, L_u, L_s; l_3, l'_3; L, M)}{R_{31}^{2L_s + l_3 + l'_3 + 2}} + (a^* c) \sum_{n_s n_u} \sum_{L_s L_u l'_3 l_1} \frac{F_3(n_u, n_s, L_u, L_s; l'_3, l_1; L, M)}{R_{31}^{l'_3 + L_s + L_u + l_1 + 2}} \\
& \left. + (c^* a) \sum_{n_s n_u} \sum_{L_s L_u l_3 l'_1} \frac{F_3^*(n_u, n_s, L_u, L_s; l_3, l'_1; L, M)}{R_{31}^{l_3 + L_s + L_u + l'_1 + 2}} \right\}. \tag{A6}
\end{aligned}$$

Similarly, the three nonadditive terms are

$$\begin{aligned}
V_{12,23}^{(2)} &= - \sum_{n_t L_t M_t} \frac{16\pi^2 (-1)^{L_t + L + M_t - M}}{R_{12}^{L_t + L + 1} R_{23}^{L_t + L + 1}} \frac{[P_{L_t + L}^{M_t - M}(0) (L_t + L - M_t + M)! (L_t, L)^{-1}]^2}{(L_t + M_t)! (L_t - M_t)! (L + M)! (L - M)!} \\
& \times \{ (a^* c) \exp[-i(M_t - M)\beta] + (c^* a) \exp[i(M_t - M)\beta] \} \\
& \times \frac{|\langle \varphi_{n'_0}(L; \boldsymbol{\sigma}) \| T_L(\boldsymbol{\sigma}) \| \chi_{n_0}(0; \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_t L_t} - E_{n'_0 L}^{(0)}} \\
& - \sum_{n_t L_t M_t} \frac{16\pi^2 (-1)^{L_t + L + M_t + M}}{R_{12}^{L_t + L + 1} R_{23}^{L_t + L + 1}} \frac{[P_{L_t + L}^{M_t + M}(0) (L_t + L - M_t - M)! (L_t, L)^{-1}]^2}{(L_t + M_t)! (L_t - M_t)! (L + M)! (L - M)!} \\
& \times \{ (a^* c) \exp[i(M_t + M)\beta] + (c^* a) \exp[-i(M_t + M)\beta] \} \\
& \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_L(\boldsymbol{\sigma}) \| \chi_{n'_0}(L; \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_t L_t} + E_{n'_0 L} - 2E_{n_0 S}^{(0)}} \\
& = - \left\{ \sum_{n_t L_t M_t} \{ (a^* c) \exp[-i(M_t - M)\beta] \} \frac{F_4(n_t, L_t, M_t; L, M)}{R_{12}^{L_t + L + 1} R_{23}^{L_t + L + 1}} \right. \\
& \quad \left. + \sum_{n_t L_t M_t} \{ (c^* a) \exp[i(M_t - M)\beta] \} \frac{F_4(n_t, L_t, M_t; L, M)}{R_{12}^{L_t + L + 1} R_{23}^{L_t + L + 1}} \right\}, \tag{A7} \\
V_{23,31}^{(2)} &= - \sum_{n_u L_u M_u} \frac{16\pi^2 (-1)^{L_u + L + M_u - M}}{R_{23}^{L_u + L + 1} R_{31}^{L_u + L + 1}} \frac{[P_{L_u + L}^{M_u - M}(0) (L_u + L - M_u + M)! (L_u, L)^{-1}]^2}{(L_u + M_u)! (L_u - M_u)! (L + M)! (L - M)!} \\
& \times \{ (a^* b) \exp[i(M_u - M)\gamma] + (b^* a) \exp[-i(M_u - M)\gamma] \} \\
& \times \frac{|\langle \varphi_{n'_0}(L; \boldsymbol{\sigma}) \| T_L(\boldsymbol{\sigma}) \| \chi_{n_0}(0; \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_u L_u} - E_{n'_0 L}^{(0)}} \\
& - \sum_{n_u L_u M_u} \frac{16\pi^2 (-1)^{L_u + L + M_u + M}}{R_{23}^{L_u + L + 1} R_{31}^{L_u + L + 1}} \frac{[P_{L_u + L}^{M_u + M}(0) (L_u + L - M_u - M)! (L_u, L)^{-1}]^2}{(L_u + M_u)! (L_u - M_u)! (L + M)! (L - M)!} \\
& \times \{ (a^* b) \exp[-i(M_u + M)\gamma] + (b^* a) \exp[i(M_u + M)\gamma] \} \\
& \times \frac{|\langle \varphi_{n_0}(0; \boldsymbol{\sigma}) \| T_L(\boldsymbol{\sigma}) \| \chi_{n'_0}(L; \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_u L_u} + E_{n'_0 L} - 2E_{n_0 S}^{(0)}}
\end{aligned}$$

$$\begin{aligned}
&= - \left\{ \sum_{n_u L_u M_u} \{(a^* b) \exp[i(M_u - M)\gamma]\} \frac{F_4(n_u, L_u, M_u; L, M)}{R_{23}^{L_u+L+1} R_{31}^{L_u+L+1}} \right. \\
&\quad \left. + \sum_{n_u L_u M_u} \{(b^* a) \exp[-i(M_u - M)\gamma]\} \frac{F_4(n_u, L_u, M_u; L, M)}{R_{23}^{L_u+L+1} R_{31}^{L_u+L+1}} \right\}, \quad (\text{A8}) \\
V_{31,12}^{(2)} &= - \sum_{n_s L_s M_s} \frac{16\pi^2 (-1)^{L_s+L+M_s-M} [P_{L_s+L}^{M_s-M}(0)(L_s+L-M_s+M)!(L_s, L)^{-1}]^2}{R_{31}^{L_s+L+1} R_{12}^{L_s+L+1}} \frac{1}{(L_s+M_s)!(L_s-M_s)!(L+M)!(L-M)!} \\
&\quad \times \{(b^* c) \exp[i(M_s - M)\alpha] + (c^* b) \exp[-i(M_s - M)\alpha]\} \\
&\quad \times \frac{|\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle|^2 |\langle \varphi_{n'_0}(L; \rho) \| T_L(\rho) \| \chi_{n_0}(0; \rho) \rangle|^2}{E_{n_s L_s} - E_{n'_0 L}^{(0)}} \\
&\quad - \sum_{n_s L_s M_s} \frac{16\pi^2 (-1)^{L_s+L+M_s+M} [P_{L_s+L}^{M_s+M}(0)(L_s+L-M_s-M)!(L_s, L)^{-1}]^2}{R_{31}^{L_s+L+1} R_{12}^{L_s+L+1}} \frac{1}{(L_s+M_s)!(L_s-M_s)!(L+M)!(L-M)!} \\
&\quad \times \{(b^* c) \exp[-i(M_s + M)(\alpha)] + (c^* b) \exp[i(M_s + M)(\alpha)]\} \\
&\quad \times \frac{|\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle|^2 |\langle \varphi_{n'_0}(L; \rho) \| T_L(\rho) \| \chi_{n_0}(0; \rho) \rangle|^2}{E_{n_s L_s} + E_{n'_0 L}^{(0)} - 2E_{n_0 S}^{(0)}} \\
&= - \left\{ \sum_{n_s L_s M_s} \{(b^* c) \exp[i(M_s - M)\alpha]\} \frac{F_4(n_s, L_s, M_s; L, M)}{R_{31}^{L_s+L+1} R_{12}^{L_s+L+1}} \right. \\
&\quad \left. + \sum_{n_s L_s M_s} \{(c^* b) \exp[-i(M_s - M)\alpha]\} \frac{F_4(n_s, L_s, M_s; L, M)}{R_{31}^{L_s+L+1} R_{12}^{L_s+L+1}} \right\}. \quad (\text{A9})
\end{aligned}$$

In the above, the F_i functions are defined by

$$\begin{aligned}
F_1(n_s, n_t, L_s, L_t; l_1, l'_1; L, M) &= G_1(L_s, L_t, l_1, l'_1; L, M) \langle \varphi_{n'_0}(L; \sigma) \| T_{l_1}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle^* \\
&\quad \times \frac{|\langle \varphi_{n'_0}(L; \sigma) \| T_{l'_1}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle| |\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}}, \quad (\text{A10})
\end{aligned}$$

$$F_2(n_s, n_t, L_s, L_t) = G_2(L_s, L_t) \frac{|\langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle|^2 |\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2}{E_{n_s L_s} + E_{n_t L_t} - 2E_{n_0 S}^{(0)}}, \quad (\text{A11})$$

$$\begin{aligned}
F_3(n_s, n_t, L_s, L_t; l_1, l'_2; L, M) &= (-1)^{L_s+l'_2} G_3(L_s, L_t, l_1, l'_2; L, M) \\
&\quad \times \langle \varphi_{n_0}(0; \sigma) \| T_{L_s}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle^* \langle \varphi_{n'_0}(L; \rho) \| T_{l'_2}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle^* \\
&\quad \times \frac{|\langle \varphi_{n'_0}(L; \sigma) \| T_{l_1}(\sigma) \| \chi_{n_s}(L_s; \sigma) \rangle| |\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|}{E_{n_s L_s} + E_{n_t L_t} - E_{n_0 S}^{(0)} - E_{n'_0 L}^{(0)}}. \quad (\text{A12})
\end{aligned}$$

$$\begin{aligned}
F_4(n_t, L_t, M_t; L, M) &= (-1)^{L_t+L+M_t+M} G_4(L_t, M_t; L, M) \left[\frac{|\langle \varphi_{n'_0}(L; \sigma) \| T_L(\sigma) \| \chi_{n_0}(0; \sigma) \rangle|^2 |\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2}{E_{n_t L_t} - E_{n'_0 L}^{(0)}} \right. \\
&\quad \left. + \frac{|\langle \varphi_{n'_0}(L; \sigma) \| T_L(\sigma) \| \chi_{n_0}(0; \sigma) \rangle|^2 |\langle \varphi_{n_0}(0; \rho) \| T_{L_t}(\rho) \| \chi_{n_t}(L_t; \rho) \rangle|^2}{E_{n_t L_t} + E_{n'_0 L}^{(0)} - 2E_{n_0 S}^{(0)}} \right], \quad (\text{A13})
\end{aligned}$$

where $G_1(L_i, L_j, \ell_k, \ell'_k; L, M)$, $G_2(L_i, L_j)$, $G_3(L_i, L_j, \ell_{k_1}, \ell'_{k_2}; L, M)$, and $G_4(L_i, M_i; L, M)$ are further defined by

$$G_1(L_i, L_j, \ell_k, \ell'_k; L, M) = \frac{16\pi^2(\ell_k, \ell'_k)^{-1/2}}{(2L_j + 1)^2} \sum_{M_i M_j m_k} \begin{pmatrix} L & \ell_k & L_i \\ -M & m_k & M_i \end{pmatrix} \begin{pmatrix} L & \ell'_k & L_i \\ -M & m_k & M_i \end{pmatrix} \times \frac{(L_j + \ell_k - M_j + m_k)!(L_j + \ell'_k - M_j + m_k)!P_{L_j + \ell_k}^{M_j - m_k}(0)P_{L_j + \ell'_k}^{M_j - m_k}(0)}{(L_j + M_j)!(L_j - M_j)![(\ell_k + m_k)!(\ell_k - m_k)!(\ell'_k + m_k)!(\ell'_k - m_k)!]^{1/2}}, \quad (\text{A14})$$

$$G_2(L_i, L_j) = 16\pi^2(L_i, L_j)^{-2} \sum_{M_i M_j} \frac{[P_{L_i + L_j}^{M_i + M_j}(0)(L_i + L_j - M_i - M_j)!]^2}{(L_i + M_i)!(L_i - M_i)!(L_j + M_j)!(L_j - M_j)!}, \quad (\text{A15})$$

$$G_3(L_i, L_j, \ell_{k_1}, \ell'_{k_2}; L, M) = \frac{16\pi^2(\ell_{k_1}, \ell'_{k_2})^{-1/2}}{(2L_i + 1)(2L_j + 1)} \sum_{M_i M_j m_{k_1} m'_{k_2}} \begin{pmatrix} L & \ell_{k_1} & L_i \\ -M & -m_{k_1} & M_i \end{pmatrix} \begin{pmatrix} L & \ell'_{k_2} & L_j \\ -M & m'_{k_2} & M_j \end{pmatrix} \times \frac{(-1)^{M_i + M_j} P_{L_j + \ell_{k_1}}^{M_j + m_{k_1}}(0) P_{L_i + \ell'_{k_2}}^{M_i - m'_{k_2}}(0)}{[(L_i + M_i)!(L_i - M_i)!(L_j + M_j)!(L_j - M_j)!]^{1/2}} \times \frac{(L_j + \ell_{k_1} - M_j - m_{k_1})!(L_i + \ell'_{k_2} - M_i + m'_{k_2})!}{[(\ell_{k_1} + m_{k_1})!(\ell_{k_1} - m_{k_1})!(\ell'_{k_2} + m'_{k_2})!(\ell'_{k_2} - m'_{k_2})!]^{1/2}}, \quad (\text{A16})$$

$$G_4(L_i, M_i; L, M) = 16\pi^2 \frac{[P_{L_i + L}^{M_i - M}(0)(L_i + L - M_i + M)!(L_i, L)^{-1}]^2}{(L_i + M_i)!(L_i - M_i)!(L + M)!(L - M)!}. \quad (\text{A17})$$

Then the second-order energy correction is simplified as

$$\Delta E^{(2)} = - \sum_{n \geq 3} \left(\frac{C_{2n}^{(12)}(L, M)}{R_{12}^{2n}} + \frac{C_{2n}^{(23)}(L, M)}{R_{23}^{2n}} + \frac{C_{2n}^{(31)}(L, M)}{R_{31}^{2n}} + \frac{C_{2n}^{(12, 23)}(L, M)}{R_{12}^n R_{23}^n} + \frac{C_{2n}^{(23, 31)}(L, M)}{R_{23}^n R_{31}^n} + \frac{C_{2n}^{(31, 12)}(L, M)}{R_{31}^n R_{12}^n} \right), \quad (\text{A18})$$

where $C_{2n}^{(IJ)}(L, M)$ and $C_{2n}^{(IJ, JK)}(L, M)$ are, respectively, the additive and nonadditive dispersion coefficients. These coefficients can be expressed as

$$\begin{aligned} C_{2n}^{(12)}(L, M) &= |a|^2 \sum_{n_s n_t} \sum_{\substack{L_s L_t l_1 l'_1 \\ 2L_t + l_1 + l'_1 + 2 = 2n}} F_1(n_s, n_t, L_s, L_t; l_1, l'_1; L, M) \\ &+ |b|^2 \sum_{n_s n_t} \sum_{\substack{L_s L_t l_2 l'_2 \\ 2L_s + l_2 + l'_2 + 2 = 2n}} F_1(n_t, n_s, L_t, L_s; l_2, l'_2; L, M) \\ &+ |c|^2 \sum_{n_s n_t} \sum_{\substack{L_s L_t \\ 2L_s + 2L_t + 2 = 2n}} F_2(n_s, n_t, L_s, L_t) \\ &+ a^* b \sum_{n_s n_t} \sum_{\substack{L_s L_t l_1 l'_2 \\ L_s + L_t + l_1 + l'_2 + 2 = 2n}} F_3(n_s, n_t, L_s, L_t; l_1, l'_2; L, M) \\ &+ b^* a \sum_{n_s n_t} \sum_{\substack{L_s L_t l'_1 l_2 \\ L_s + L_t + l'_1 + l_2 + 2 = 2n}} F_3^*(n_s, n_t, L_s, L_t; l'_1, l_2; L, M), \quad (\text{A19}) \\ C_{2n}^{(23)}(L, M) &= |a|^2 \sum_{n_t n_u} \sum_{\substack{L_t L_u \\ 2L_t + 2L_u + 2 = 2n}} F_2(n_t, n_u, L_t, L_u) \\ &+ |b|^2 \sum_{n_t n_u} \sum_{\substack{L_t L_u l_2 l'_2 \\ 2L_u + l_2 + l'_2 + 2 = 2n}} F_1(n_t, n_u, L_t, L_u; l_2, l'_2; L, M) \\ &+ |c|^2 \sum_{n_t n_u} \sum_{\substack{L_t L_u l_3 l'_3 \\ 2L_t + l_3 + l'_3 + 2 = 2n}} F_1(n_u, n_t, L_u, L_t; l_3, l'_3; L, M) \end{aligned}$$

$$\begin{aligned}
& + b^* c \sum_{n_t n_u} \sum_{\substack{L_t L_u l_2 l'_3 \\ L_u + L_t + l_2 + l'_3 + 2 = 2n}} F_3(n_t, n_u, L_t, L_u; l_2, l'_3; L, M) \\
& + c^* b \sum_{n_t n_u} \sum_{\substack{L_s L_t L_u l'_2 l'_3 \\ L_t + L_u + l'_2 + l'_3 + 2 = 2n}} F_3^*(n_t, n_u, L_t, L_u; l'_2, l'_3; L, M), \tag{A20}
\end{aligned}$$

$$\begin{aligned}
C_{2n}^{(31)}(L, M) & = |a|^2 \sum_{n_s n_u} \sum_{\substack{L_s L_u l_1 l'_1 \\ 2L_u + l_1 + l'_1 + 2 = 2n}} F_1(n_s, n_u, L_s, L_u; l_1, l'_1; L, M) \\
& + |b|^2 \sum_{n_s n_u} \sum_{\substack{L_s L_u \\ 2L_s + 2L_u + 2 = 2n}} F_2(n_s, n_u, L_s, L_u) \\
& + |c|^2 \sum_{n_s n_u} \sum_{\substack{L_s L_u l_3 l'_3 \\ 2L_s + l_3 + l'_3 + 2 = 2n}} F_1(n_u, n_s, L_u, L_s; l_3, l'_3; L, M) \\
& + (a^* c) \sum_{n_s n_u} \sum_{\substack{L L_s L_u l'_3 l_1 \\ L_s + L_u + l_1 + l'_3 + 2 = 2n}} F_3^*(n_u, n_s, L_u, L_s; l'_3, l_1; L, M) \\
& + (c^* a) \sum_{n_s n_u} \sum_{\substack{L_s L_u l_3 l'_1 \\ L_s + L_u + l'_1 + l_3 + 2 = 2n}} F_3(n_u, n_s, L_u, L_s; l_3, l'_1; L, M), \tag{A21}
\end{aligned}$$

$$\begin{aligned}
C_{2n}^{(12,23)}(L, M) & = \sum_{\substack{n_t L_t M_t \\ L_t + L + 1 = n}} \{(a^* c) \exp[-i(M_t - M)\beta]\} F_4(n_t, L_t, M_t; L, M) \\
& + \sum_{\substack{n_t L_t M_t \\ L_t + L + 1 = n}} \{(c^* a) \exp[i(M_t - M)\beta]\} F_4(n_t, L_t, M_t; L, M), \tag{A22}
\end{aligned}$$

$$\begin{aligned}
C_{2n}^{(23,31)}(L, M) & = \sum_{\substack{n_u L_u M_u \\ L_u + L + 1 = n}} \{(a^* b) \exp[i(M_u - M)\gamma]\} F_4(n_u, L_u, M_u; L, M) \\
& + \sum_{\substack{n_u L_u M_u \\ L_u + L + 1 = n}} \{(b^* a) \exp[-i(M_u - M)\gamma]\} F_4(n_u, L_u, M_u; L, M), \tag{A23}
\end{aligned}$$

$$\begin{aligned}
C_{2n}^{(31,12)}(L, M) & = \sum_{\substack{n_s L_s M_s \\ L_s + L + 1 = n}} \{(b^* c) \exp[i(M_s - M)\alpha]\} F_4(n_s, L_s, M_s; L, M) \\
& + \sum_{\substack{n_s L_s M_s \\ L_s + L + 1 = n}} \{(c^* b) \exp[-i(M_s - M)\alpha]\} F_4(n_s, L_s, M_s; L, M). \tag{A24}
\end{aligned}$$

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- [1] B. M. Axilrod and E. Teller, *J. Chem. Phys.* **11**, 299 (1943).
[2] B. M. Axilrod, *J. Chem. Phys.* **19**, 719 (1951).
[3] R. J. Bell, *J. Phys. B* **3**, L101 (1970).
[4] D. E. Stogryn, *Molec. Phys.* **22**, 81 (1971).
[5] R. Moszynski, P. E. S. Wormer, B. Jeziorski, and A. van der Avoird, *J. Chem. Phys.* **103**, 8058 (1995).
[6] S. A. C. McDowell, A. Kumar, and W. J. Meath, *Molec. Phys.* **87**, 845 (1996).
[7] X. Li and K. L. C. Hunt, *J. Chem. Phys.* **105**, 4076 (1996).
[8] M. Marinescu and A. F. Starace, *Phys. Rev. A* **55**, 2067 (1997).
[9] Z. C. Yan, A. Dalgarno, and J. F. Babb, *Phys. Rev. A* **55**, 2882 (1997).
[10] L. Y. Tang, Z. C. Yan, T. Y. Shi, J. F. Babb, and J. Mitroy, *J. Chem. Phys.* **136**, 104104 (2012).
[11] K. M. Jones, E. Tiesinga, P. D. Lett, and P. S. Julienne, *Rev. Mod. Phys.* **78**, 483 (2006).
[12] A. Safavi-Naini, J. von Stecher, B. Capogrosso-Sansone, and S. T. Rittenhouse, *Phys. Rev. Lett.* **109**, 135302 (2012).
[13] W. Zhang, R. Li, W. X. Zhang, C. B. Duan, and T. C. Scott, *Phys. Rev. A* **90**, 033622 (2014).
[14] T. Pohl and P. R. Berman, *Phys. Rev. Lett.* **102**, 013004 (2009).
[15] D. Barredo, S. Ravets, H. Labuhn, L. Béguin, A. Vernier, F. Nogrette, T. Lahaye, and A. Browaeys, *Phys. Rev. Lett.* **112**, 183002 (2014).
[16] F. Shen, J. Gao, A. A. Senin, C. J. Zhu, J. R. Allen, Z. H. Lu, Y. Xiao, and J. G. Eden, *Phys. Rev. Lett.* **99**, 143201 (2007).
[17] I. C. H. Liu, J. Stanojevic, and J. M. Rost, *Phys. Rev. Lett.* **102**, 173001 (2009).

- [18] N. Samboy and R. Côté, *Phys. Rev. A* **87**, 032512 (2013).
- [19] M. Kiffner, W. Li, and D. Jaksch, *Phys. Rev. Lett.* **111**, 233003 (2013).
- [20] Z. C. Yan, J. F. Babb, A. Dalgarno, and G. W. F. Drake, *Phys. Rev. A* **54**, 2824 (1996).
- [21] Z. C. Yan and G. W. F. Drake, *Phys. Rev. A* **52**, R4316 (1995).
- [22] P. Soldán, M. T. Cvitaš, J. M. Hutson, P. Honvault, and J. M. Launay, *Phys. Rev. Lett.* **89**, 153201 (2002).
- [23] P. Soldán, M. T. Cvitaš, and J. M. Hutson, *Phys. Rev. A* **67**, 054702 (2003).
- [24] V. F. Lotrich and K. Szalewicz, *Phys. Rev. Lett.* **79**, 1301 (1997).
- [25] A. Rapp, G. Zaránd, C. Honerkamp, and W. Hofstetter, *Phys. Rev. Lett.* **98**, 160405 (2007).
- [26] B. Paredes, T. Keilmann, and J. I. Cirac, *Phys. Rev. A* **75**, 053611 (2007).
- [27] N. Gross, Z. Shotan, S. Kokkelmans, and L. Khaykovich, *Phys. Rev. Lett.* **103**, 163202 (2009).
- [28] S. E. Pollack, D. Dries, and R. G. Hulet, *Science* **326**, 1683 (2009).
- [29] A. J. Daley, J. M. Taylor, S. Diehl, M. Baranov, and P. Zoller, *Phys. Rev. Lett.* **102**, 040402 (2009).
- [30] M. Bulski and G. Chałasiński, *J. Chem. Phys.* **86**, 937 (1987).
- [31] K. Helfrich and H. W. Hammer, *J. Phys. B* **44**, 215301 (2011).
- [32] J. Pérez-Ríos, M. Lepers, and O. Dulieu, *Phys. Rev. Lett.* **115**, 073201 (2015).
- [33] M. Lepers, O. Dulieu, and V. Kokoouline, *Phys. Rev. A* **82**, 042711 (2010).
- [34] M. Lepers, R. Vexiau, N. Bouloufa, O. Dulieu, and V. Kokoouline, *Phys. Rev. A* **83**, 042707 (2011).
- [35] T. C. Thompson, G. Izmirlian Jr., S. J. Lemon, D. G. Truhlar, and C. A. Mead, *J. Chem. Phys.* **82**, 5597 (1985).
- [36] H. G. Krämer, M. Keil, C. B. Suarez, W. Demtröder, and W. Meyer, *Chem. Phys. Lett.* **299**, 212 (1999).
- [37] W. Meyer, M. Keil, A. Kudell, M. A. Baig, J. Zhu, and W. Demtröder, *J. Chem. Phys.* **115**, 2590 (2001).
- [38] A. J. C. Varandas and A. A. C. C. Pais, *J. Chem. Soc., Faraday Trans.* **89**, 1511 (1993).
- [39] M. Ehara and K. Yamashita, *Theor. Chem. Acc.* **102**, 226 (1999).
- [40] E. N. Ghassemi, J. Larson, and Å. Larson, *J. Chem. Phys.* **140**, 154304 (2014).
- [41] D. A. Brue, X. Li, and G. A. Parker, *J. Chem. Phys.* **123**, 091101 (2005).
- [42] X. Li, D. A. Brue, and G. A. Parker, *J. Chem. Phys.* **129**, 124305 (2008).
- [43] J. N. Byrd, J. A. Montgomery, H. H. Michels, and R. Côté, *Int. J. Quantum Chem.* **109**, 3112 (2009).
- [44] M. T. Cvitaš, P. Soldán, J. M. Hutson, P. Honvault, and J. M. Launay, *Phys. Rev. Lett.* **94**, 033201 (2005).
- [45] J. N. Byrd, J. A. Montgomery, H. H. Michels, and R. Côté, *Int. J. Quantum Chem.* **109**, 3626 (2009).
- [46] J. N. Byrd, H. H. Michels, J. A. Montgomery Jr., and R. Côté, *Chem. Phys. Lett.* **529**, 23 (2012).
- [47] G. Quémener, J.-M. Launay, and P. Honvault, *Phys. Rev. A* **75**, 050701 (2007).
- [48] X. Li, G. A. Parker, P. Brumer, I. Thanopoulos, and M. Shapiro, *J. Chem. Phys.* **128**, 124314 (2008).
- [49] S. Copping, P. Matei, and B. Stewart, *J. Chem. Phys.* **128**, 241103 (2008).
- [50] M. T. Cvitaš, P. Soldán, J. M. Hutson, P. Honvault, and J.-M. Launay, *J. Chem. Phys.* **127**, 074302 (2007).
- [51] M. T. Cvitaš, P. Soldán, and J. M. Hutson, *Mol. Phys.* **104**, 23 (2006).
- [52] P. R. Fontana, *Phys. Rev.* **123**, 1865 (1961).
- [53] L. Y. Tang, Z. C. Yan, T. Y. Shi, and J. F. Babb, *Phys. Rev. A* **79**, 062712 (2009).