Accurate long-range coefficients for two excited like isotope He atoms: \( \text{He}(2^1P)–\text{He}(2^1P), \text{He}(2^1P)–\text{He}(2^3P), \) and \( \text{He}(2^3P)–\text{He}(2^3P) \)

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Abstract

A general formalism is used to express the long-range potential energies in inverse powers of the separation distance between two like atomic or molecular systems with \( P \) symmetries. The long-range molecular interaction coefficients are calculated for the molecular symmetries \( \Delta, \Pi, \) and \( \Sigma \), arising from the following interactions: \( \text{He}(2^1P)–\text{He}(2^1P), \text{He}(2^1P)–\text{He}(2^3P), \) and \( \text{He}(2^3P)–\text{He}(2^3P) \). The electric quadrupole-quadrupole term, \( C_5 \), the van der Waals (dispersion) term \( C_6 \), and higher-order terms, \( C_8 \), and \( C_{10} \), are calculated \textit{ab initio} using accurate variational wave functions in Hylleraas coordinates with finite nuclear mass effects. A comparison is made with previously published results where available.

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I. INTRODUCTION

Accurate description of the interactions between two excited atoms (or molecules) at long-range is fundamentally important for studies of molecular excited state spectroscopy [1, 2], associative ionization [3, 4], and other collisional processes [5], and is at the heart of several schemes for quantum computation [6, 7]. At sufficiently large separations, the mutual electrostatic interaction energy between the two excited atoms can be accurately described using an expansion of the potential energy in inverse powers of the separation distance $R$. The terms describe the electric quadrupole-quadrupole interaction at order $R^{-5}$ and the instantaneous dipole-dipole (e.g. dispersion) interaction at order $R^{-6}$ [8] and higher order instantaneous multipole-multipole interactions at orders $R^{-8}$ and $R^{-10}$.

Long-range interactions involving few-electron atoms are the only interactions that presently can be rigorously calculated with high accuracy. Different levels of approximation are needed for the calculations of long-range forces for alkali-metal and alkaline-earth atoms. [5, 9, 10]. Sizeable discrepancies between various calculations in the literature can occur, as illustrated in the comparisons of $C_6$ coefficients, for example, given by Zhang et al. [12] for Li (2p)–Li (2p) and given by Yurova [13] for Na(3p)–Na(3p). For helium, it is possible to perform a highly-accurate \textit{ab initio} calculation of atomic properties and long-range interaction coefficients. Such results could become benchmarks for eventual \textit{ab initio} calculations of alkaline-earth atomic interactions. Alkaline-earth and other two-electron excited $P$ atoms are currently being studied as the optimal candidates for frequency-based standards and optical clock experiments [14].

We had previously studied the long-range interaction coefficients $C_n$ (with $n \leq 10$) for all He($n^1S$)–He($n'^1S$) and He($n^1S$)–He($n'^1P$) systems of the energetically lowest five states: He($1^1S$), He($2^3S$), He($2^1S$), He($2^3P$) and He($2^1P$) and the finite nuclear mass effects for like isotopes [15, 16, 17]. In this work, we present results for more complicated set of interactions between two like isotope helium atoms with $P$ symmetries. Degenerate perturbation theory is needed to derive the interaction terms for some of the terms. Section II introduces a general formalism for calculating dispersion coefficients between two like atomic or molecular systems of $P$ symmetry. Section III presents numerical results of dispersion coefficients $C_5$, $C_6$, $C_8$, and $C_{10}$ for the following three systems He($2^1P$)–He($2^1P$), He($2^1P$)–He($2^3P$), and He($2^3P$)–He($2^3P$).
II. FORMULATION

In this work, atomic units are used throughout. At large distances $R$ between two atoms $a$ and $b$, the Coulomb interaction \cite{18}, treated as a perturbation to the two isolated atoms, is

$$ V = \sum_{\ell=0}^{\infty} \sum_{L=0}^{\infty} \frac{V_{\ell L}}{R^{\ell+L+1}}, \quad (1) $$

where

$$ V_{\ell L} = 4\pi(-1)^{\ell} \frac{(\ell + L)_{\ell + \mu} (\ell + L)}{(\ell + L + \mu)} \sum_{\mu} K_{\ell L}^{\mu} T_{\mu}^{(\ell)}(\sigma) T_{-\mu}^{(L)}(\rho). \quad (2) $$

In the above, $T_{\mu}^{(\ell)}(\sigma)$ and $T_{-\mu}^{(L)}(\rho)$ are the atomic multipole tensor operators defined by

$$ T_{\mu}^{(\ell)}(\sigma) = \sum_{i} Q_{i} \sigma_{i}^{\ell} Y_{\ell \mu}(\hat{\sigma}_{i}), \quad (3) $$

and

$$ T_{-\mu}^{(L)}(\rho) = \sum_{j} q_{j} \rho_{j}^{L} Y_{L - \mu}(\hat{\rho}_{j}), \quad (4) $$

and $Q_{i}$ and $\sigma_{i}$ are the charge and the position vector of the $i^{th}$ particle in atom $a$, respectively. Similarly, $q_{j}$ and $\rho_{j}$ are for the $j^{th}$ particle in atom $b$. The coefficient $K_{\ell L}^{\mu}$ in Eq. (2) is

$$ K_{\ell L}^{\mu} = \left[ \frac{(\ell + L) (\ell + L + \mu)}{(\ell + \mu)} \right]^{1/2} \quad (5) $$

and $(\ell, L, \cdots) = (2\ell + 1)(2L + 1) \cdots$.

Since the Coulomb interaction $V$ is cylindrically symmetric about the molecular axis $R$ or $z$ axis \cite{6, 10}, the projection of the total angular momentum of the combined system $a$-$b$ along the $z$ axis (with magnetic quantum number $M$), is conserved. Therefore, states with $M = \pm 2$, $\pm 1$, and $0$ are not mixed with each other, corresponding to the $\Delta$, $\Pi$, and $\Sigma$ molecular states, respectively. The $\Delta$ and $\Pi$ states are degenerate with respect to the sign of $M$ and the degeneracy can not be removed physically in the free combined system $a$-$b$. Therefore, we only study the states with positive $M$ in this work.

A. $\Delta$ state

For two like isotope atoms $a$ and $b$ in $P$ symmetry, the zeroth-order wave function for the $\Delta$ state of the combined system $a$-$b$ can be written in the form:

$$ \Psi^{(0)}(\Delta, \beta) = \frac{\alpha}{\sqrt{2}} [\Psi_{n_{a}}(M_{a}; \sigma) \Psi_{n_{b}}(M_{b}; \rho) + \beta \Psi_{n_{a}}(M_{a}; \rho) \Psi_{n_{b}}(M_{b}; \sigma)], \quad (6) $$

3
where $M_a = M_b = 1$ are the magnetic quantum numbers, $\alpha$ is the normalization factor, and $\beta$ describes the symmetry due to the exchange of two initial states $\Psi_{n_a}$ and $\Psi_{n_b}$. If two atoms are both in the same $P$ state, then $\alpha = \sqrt{2}$ and $\beta = 0$; if they are in different $P$ states, then $\alpha = 1$ and $\beta = \pm 1$ \[10\].

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

$$V^{(1)} = -\frac{C_5(\Delta, \beta)}{R^5},$$

where, after some angular momentum algebra, one gets (see also Ref. \[11\]),

$$C_5(\Delta, \beta) = -A_1 + \beta A_2,$$

$$A_1 = \frac{4\pi}{25} \langle \Psi_{n_a}(\sigma) || \sum_i Q_i \sigma_i^2 Y_2(\hat{\sigma}_i) || \Psi_{n_a}(\sigma) \rangle \times \langle \Psi_{n_b}(\rho) || \sum_j q_j \rho_j^2 Y_2(\hat{\rho}_j) || \Psi_{n_b}(\rho) \rangle,$$

$$A_2 = \frac{4\pi}{25} \langle \langle \Psi_{n_a}(\sigma) || \sum_i Q_i \sigma_i^2 Y_2(\hat{\sigma}_i) || \Psi_{n_b}(\sigma) \rangle \rangle^2.$$

The second-order energy is

$$V^{(2)} = -\sum_{n_s n_t}^t \sum_{L_s M_s} \sum_{L_t M_t} \frac{\langle \langle \Psi^{(0)}(\Delta) || V || \chi_{n_s}(L_s M_s; \sigma) \omega_{n_t}(L_t M_t; \rho) \rangle \rangle^2}{E_{n_s n_t} - E^{(0)}_{n_a n_b}},$$

where $\chi_{n_s}(L_s M_s; \sigma) \omega_{n_t}(L_t M_t; \rho)$ is an allowed intermediate state with the energy eigenvalue $E_{n_s n_t} = E_{n_s} + E_{n_t}$, and the prime in the summation indicates that the terms with $E_{n_s n_t} = E^{(0)}_{n_a n_b}$ should be excluded. Substituting Eqs. (11) and (6) into Eq. (11), we obtain

$$V^{(2)} = -\sum_{n_s n_t}^t \sum_{L_s M_s} \sum_{L_t M_t} \frac{B_1 + \beta B_2}{E_{n_s n_t} - E^{(0)}_{n_a n_b}},$$

with

$$B_1 = \langle \langle \Psi_{n_a}(M_a; \sigma) \Psi_{n_b}(M_b; \rho) || V || \chi_{n_s}(L_s M_s; \sigma) \omega_{n_t}(L_t M_t; \rho) \rangle \rangle^2,$$

$$B_2 = \langle \langle \Psi_{n_a}(M_a; \sigma) \Psi_{n_b}(M_b; \rho) || V || \chi_{n_s}(L_s M_s; \sigma) \omega_{n_t}(L_t M_t; \rho) \rangle \rangle \times \langle \langle \Psi_{n_a}(M_a; \rho) \Psi_{n_b}(M_b; \sigma) || V || \chi_{n_s}(L_s M_s; \sigma) \omega_{n_t}(L_t M_t; \rho) \rangle \rangle.$$
with

\[ D_1(\ell, L, \ell', L') = \frac{1}{2\pi} \sum_{L_s L_t} G_1(\ell, L, \ell', L_s, L_t) F_1(\ell, L, \ell', L_s, L_t) \cdot (16) \]

In Eq. (16), \( G_1 \) is the angular-momentum part and \( F_1 \) is the oscillator strength part. Their expressions are

\[ G_1(\ell, L, \ell', L_s, L_t) = (-1)^{L+L'}(\ell, L, \ell', L')^{1/2} \sum_{\mu} K_{\ell L}^{\mu} K_{\ell' L'}^{\mu} \left( \begin{array}{ccc} L_a & \ell & L_s \\ -M_a & \mu & M_a-\mu \end{array} \right) \]

\[ \times \left( \begin{array}{ccc} 1 & L & L_t \\ -M_b & -\mu & M_b+\mu \end{array} \right) \left( \begin{array}{ccc} 1 & \ell' & L_t \\ -M_a & \mu & M_a-\mu \end{array} \right), \quad (17) \]

and

\[ F_1(\ell, L, \ell', L_s, L_t) = \frac{9\pi}{2} \sum_{n_s n_t} \frac{\bar{g}_{n_s n_a n_b}(L_s, 1, 1, \ell, \ell') \bar{g}_{n_t n_a n_b}(L_t, 1, 1, L, L')}{(\Delta E_{n_s n_a} + \Delta E_{n_t n_b}) \Delta E_{n_s n_a} \Delta E_{n_t n_b}}, \quad (18) \]

with

\[ \bar{g}_{n_s n_a n_b}(L_s, L_1, L_2, \ell, \ell') = \frac{8\pi}{(\ell, \ell') \sqrt{(2L_1 + 1)(2L_2 + 1)}} \]

\[ \times \langle \Psi_{n_a}(L_1; \sigma) | \sum_{i} Q_i \sigma_i^{\ell}(\hat{\sigma}_i) | \chi_{n_s}(L_s; \sigma) \rangle \]

\[ \times \langle \Psi_{n_b}(L_2; \sigma) | \sum_{i} Q_i \sigma_i^{\ell}(\hat{\sigma}_i) | \chi_{n_s}(L_s; \sigma) \rangle, \quad (19) \]

and \( \Delta E_{n_s n_a} = E_{n_s} - E_{n_a}; etc. \) For the special case where the two initial states \( \Psi_{n_a} \) and \( \Psi_{n_b} \) are the same and \( \ell = \ell' \), \( \bar{g}_{n_s n_a n_a} \) reduces to the absolute value of the \( 2^\ell \)-pole oscillator strength

\[ f_{n_a n_a}^{\ell} = \frac{8\pi \Delta E_{n_s n_a}}{(2\ell + 1)^2(2L_1 + 1)} |\langle \Psi_{n_a}(L_1; \sigma) | \sum_{i} Q_i \sigma_i^{\ell}(\hat{\sigma}_i) | \chi_{n_s}(L_s; \sigma) \rangle|^2. \quad (20) \]

Similarly, we have

\[ \sum_{n_s n_t} \sum_{L_s M_s L_t M_t} \sum_{E_{n_s n_t} - E_{n_a n_b}} = \sum_{\ell \ell' L L'} \frac{B_2}{R^\ell L^\ell L'^{\ell'} + L^{\ell'} + L^{2}}, \quad (21) \]

\[ D_2(\ell, L, \ell', L') = \frac{1}{2\pi} \sum_{L_s L_t} G_2(\ell, L, \ell', L_s, L_t) F_2(\ell, L, \ell', L_s, L_t), \quad (22) \]

with

\[ G_2(\ell, L, \ell', L_s, L_t) = (-1)^{L+L'}(\ell, L, \ell', L')^{1/2} \sum_{\mu} K_{\ell L}^{\mu} K_{\ell' L'}^{\mu - M_a + \mu} \]
Finally, the second-order energy $V^{(2)}$ is

$$
V^{(2)} = - \sum_{n \geq 3} \frac{C_{2n}(\Delta, \beta)}{R^{2n}},
$$

where the dispersion coefficients $C_{2n}(\Delta, \beta)$ are defined by

$$
C_{2n}(\Delta, \beta) = \sum_{\ell, L, \ell', L \geq 1} [D_1(\ell, L, \ell', L') + \beta D_2(\ell, L, \ell', L')] \delta_{\ell + \ell' + L + L' = 2n}.
$$

### B. $\Pi$ state

For the $\Pi$ state, the zeroth-order wave function is in the following form

$$
\Psi^{(0)}(\Pi, \beta, \gamma) = \frac{\alpha}{2} [\Psi_{n_a}(M_a; \sigma) \Psi_{n_b}(M_b; \rho) + \gamma \Psi_{n_a}(M_b; \sigma) \Psi_{n_b}(M_a; \rho)] + \frac{\alpha \beta}{2} [\Psi_{n_a}(M_a; \sigma) \Psi_{n_b}(M_b; \rho) + \gamma \Psi_{n_a}(M_b; \rho) \Psi_{n_b}(M_a; \sigma)],
$$

where $\beta = \pm 1$, $M_a = 0$, and $M_b = 1$. If $n_a = n_b$, $\alpha = \sqrt{2}$ and $\gamma = 0$. If $n_a \neq n_b$, then $\alpha = 1$ and $\gamma = \pm 1$. The first-order energy correction yields

$$
C_5(\Pi, \beta, \gamma) = -\alpha^2 (1 + 2\gamma + \gamma^2) C_5(\Delta, \beta).
$$

The second-order energy correction is

$$
V^{(2)}(\Pi, \beta, \gamma) = - \sum' \sum_{n_{a_1}n_{b_1}} E_{n_{a_1}n_{b_1}} \left| \frac{\langle \Psi^{(0)}(\Pi, \beta, \gamma) \mid V \mid \chi_{n_a}(L_x, M_a; \mathbf{r}) \omega_{n_b}(L_t, M_b; \rho) \rangle}{E_{n_{a_1}n_{b_1}} - E^{(0)}_{n_{a_1}n_{b_1}}} \right|^2.
$$

Introducing a function $g_o$ defined by

$$
g_o(M_a, M_b, M_c, M_d, \ell, L, L_t, L_{t'}, L') = (-1)^{L + L'} (\ell, L, \ell', L')^{1/2} \sum_{\mu \mu' M_s M_{t_s} M_{t_t}} K^\mu_{\ell \ell'} K^\mu_{\ell' \ell} \times \left( \begin{array}{ccc} 1 & \ell & L_s \\ -M_a & \mu & M_s \end{array} \right) \left( \begin{array}{ccc} 1 & L & L_t \\ -M_b & -\mu & M_t \end{array} \right) \left( \begin{array}{ccc} 1 & \ell' & L_s \\ -M_c & \mu' & M_s \end{array} \right) \left( \begin{array}{ccc} 1 & L' & L_t \\ -M_d & -\mu' & M_t \end{array} \right),
$$

(30)
From the above expressions, it is clear that 

\[ f_{\beta \gamma} = 0. \]

\[ \gamma \]

one can write \( V^{(2)}(\Pi, \beta, \gamma) \) as

\[
V^{(2)}(\Pi, \beta, \gamma) = - \sum_{n \geq 3} \frac{C_{2n}(\Pi, \beta, \gamma)}{R^{2n}},
\]

where

\[
C_{2n}(\Pi, \beta, \gamma) = \sum_{\ell, L, \ell', L' \geq 1 \atop \ell + L + \ell' + L' + 2 = 2n} D_{\beta \gamma}(\ell, L, \ell', L'),
\]

\[ D_{\beta \gamma}(\ell, L, \ell', L') = \frac{9a^2}{16} \sum_{L, L'} \left[ f_{1\gamma}(\ell, L, L_{s}, L_{t}, \ell', L') G_{1} + f_{2\gamma}(\ell, L, L_{s}, L_{t}, \ell', L') G_{2} \right], \]

\[ f_{1\gamma}(\ell, L, L_{s}, L_{t}, \ell', L') = \frac{1}{2}(1 + \gamma^{2}) \left[ g_{0}(0, 1, 0, 1, \ell, L, L_{s}, L_{t}, \ell', L') + g_{0}(1, 0, 1, 0, \ell, L, L_{s}, L_{t}, \ell', L') \right] + \gamma g_{0}(0, 1, 1, 0, \ell, L, L_{s}, L_{t}, \ell', L'), \]

\[ f_{2\gamma}(\ell, L, L_{s}, L_{t}, \ell', L') = \frac{1}{2}(1 + \gamma^{2}) \left[ g_{0}(0, 1, 1, 0, \ell, L, L_{s}, L_{t}, \ell', L') + g_{0}(1, 0, 0, 1, \ell, L, L_{s}, L_{t}, \ell', L') \right] + \gamma g_{0}(0, 1, 0, 1, \ell, L, L_{s}, L_{t}, \ell', L'), \]

\[
G_{1} = \sum_{n_{s}, n_{t}} \left[ \bar{g}_{n_{s}, n_{a} n_{b}}(L_{s}, 1, 1, \ell, \ell') \bar{g}_{n_{t}, n_{a} n_{b}}(L_{t}, 1, 1, L, L') \right.
\left. \left( \Delta E_{n_{s}, n_{a}} + \Delta E_{n_{t}, n_{b}} \right) \left| \Delta E_{n_{s}, n_{a}} \Delta E_{n_{t}, n_{b}} \right| \right]
\left. + \bar{g}_{n_{s}, n_{a} n_{b}}(L_{s}, 1, 1, \ell, \ell') \bar{g}_{n_{t}, n_{a} n_{b}}(L_{t}, 1, 1, L, L') \right]
\left. \left( \Delta E_{n_{s}, n_{a}} + \Delta E_{n_{t}, n_{b}} \right) \left| \Delta E_{n_{s}, n_{a}} \Delta E_{n_{t}, n_{b}} \right| \right]
\]

\[ and \]

\[
G_{2} = \beta \sum_{n_{s}, n_{t}} \left[ \bar{g}_{n_{s}, n_{a} n_{b}}(L_{s}, 1, 1, \ell, \ell') \bar{g}_{n_{t}, n_{a} n_{b}}(L_{t}, 1, 1, L, L') \right.
\left. \left( \Delta E_{n_{s}, n_{a}} + \Delta E_{n_{t}, n_{b}} \right) \left| \Delta E_{n_{s}, n_{a}} \Delta E_{n_{t}, n_{b}} \right| \right]
\left. + \bar{g}_{n_{s}, n_{a} n_{b}}(L_{s}, 1, 1, \ell, \ell') \bar{g}_{n_{t}, n_{a} n_{b}}(L_{t}, 1, 1, L, L') \right]
\left. \left( \Delta E_{n_{s}, n_{a}} + \Delta E_{n_{t}, n_{b}} \right) \left| \Delta E_{n_{s}, n_{a}} \Delta E_{n_{t}, n_{b}} \right| \right]
\]

From the above expressions, it is clear that \( f_{1\gamma} = \gamma f_{2\gamma} \) when \( \gamma = \pm 1 \) and \( G_{2} = \beta G_{1} \) when \( \gamma = 0. \)
C. Σ state

For the Σ state, the possible zeroth-order wave functions for the combined system a-b are

\[
\Psi^{(0)}(\Sigma, \beta) = \frac{\alpha}{\sqrt{2}} [\Psi_{n_a}(M_a; \sigma) \Psi_{n_b}(M_b; \rho) + \beta \Psi_{n_a}(M_a; \rho) \Psi_{n_b}(M_b; \sigma)],
\]

and

\[
\Psi^{(0)}(\Sigma, \beta, \gamma) = \frac{\alpha}{2} [\Psi_{n_a}(M_a; \sigma) \Psi_{n_b}(M_b; \rho) + \gamma \Psi_{n_a}(M_b; \sigma) \Psi_{n_b}(M_a; \rho)]
+ \frac{\alpha \beta}{2} [\Psi_{n_a}(M_b; \rho) \Psi_{n_a}(M_a; \sigma) + \gamma \Psi_{n_a}(M_b; \rho) \Psi_{n_a}(M_a; \sigma)].
\]

In the \(\Psi^{(0)}(\Sigma, \beta)\) state we have \(M_a = M_b = 0\), while in the \(\Psi^{(0)}(\Sigma, \beta, \gamma)\) state, \(M_a = -M_b = 1\), and \(\gamma = \pm 1\). When \(n_a = n_b\), \(\beta = 0\) and \(\alpha = \sqrt{2}\), while otherwise \(\beta = \pm 1\) and \(\alpha = 1\). For the Σ state, there is an additional symmetry with respect to the reflection of wave function on a plane containing the molecular axis. If \(Q\) is the reflection operator \([10]\),

\[
Q \Psi_{n_a}(M_a; r) = (-1)^{M_a} \Psi_{n_a}(-M_a; r),
\]

then

\[
Q \Psi^{(0)}(\Sigma, \beta) = \Psi^{(0)}(\Sigma, \beta),
\]

and

\[
Q \Psi^{(0)}(\Sigma, \beta, \gamma) = \gamma \Psi^{(0)}(\Sigma, \beta, \gamma).
\]

Due to this symmetry, the state \(\Psi^{(0)}(\Sigma, \beta, -1)\) can not be mixed with other two states by the Coulomb interaction \(V\). However, the degenerate perturbation theory is required to remove the degeneracy between \(\Psi^{(0)}(\Sigma, \beta)\) and \(\Psi^{(0)}(\Sigma, \beta, 1)\).

1. The first-order energy

For the \(\Psi^{(0)}(\Sigma, \beta, -1)\) state, the first-order energy is

\[
\langle \Psi^{(0)}(\Sigma, \beta, -1) | V | \Psi^{(0)}(\Sigma, \beta, -1) \rangle = 0.
\]
For $\Psi^{(0)}(\Sigma, \beta)$ and $\Psi^{(0)}(\Sigma, \beta, 1)$, the matrix elements of the Coulomb interaction $V$ are

$$\langle \Psi^{(0)}(\Sigma, \beta) | V | \Psi^{(0)}(\Sigma, \beta) \rangle = -\frac{4C_5(\Delta, \beta)}{R^5}, \quad (44)$$

$$\langle \Psi^{(0)}(\Sigma, \beta) | V | \Psi^{(0)}(\Sigma, \beta, 1) \rangle = -\frac{2\sqrt{2}C_5(\Delta, \beta)}{R^5}, \quad (45)$$

and

$$\langle \Psi^{(0)}(\Sigma, \beta, 1) | V | \Psi^{(0)}(\Sigma, \beta, 1) \rangle = -\frac{2C_5(\Delta, \beta)}{R^5}. \quad (46)$$

The first-order energies are obtained by the diagonalization of the following matrix:

$$-\frac{4C_5(\Delta, \beta)}{R^5} \begin{bmatrix} 1 & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{2} \end{bmatrix}. \quad (47)$$

They are

$$\lambda_1 = 0, \quad (48)$$

$$\lambda_2 = -\frac{6C_5(\Delta, \beta)}{R^5}. \quad (49)$$

Their corresponding normalized eigenvectors are

$$\Psi^{(0)}(\Sigma, \beta; \lambda_1) = -\frac{1}{\sqrt{3}}\Psi^{(0)}(\Sigma, \beta) + \sqrt{\frac{2}{3}}\Psi^{(0)}(\Sigma, \beta, 1), \quad (50)$$

$$\Psi^{(0)}(\Sigma, \beta; \lambda_2) = \sqrt{\frac{2}{3}}\Psi^{(0)}(\Sigma, \beta) + \sqrt{\frac{1}{3}}\Psi^{(0)}(\Sigma, \beta, 1), \quad (51)$$

where we introduce the semicolon to denote the use of the label $\lambda$ now. Thus, $C_5$ for $\Psi^{(0)}(\Sigma, \beta; \lambda_1)$ is zero and $C_5$ for $\Psi^{(0)}(\Sigma, \beta; \lambda_2)$ is

$$C_5(\Sigma, \beta; \lambda_2) = 6 C_5(\Delta, \beta). \quad (52)$$

2. The second-order energy

To be convenient, we use the expression $\Psi^{(0)}(\Sigma, \beta; \lambda_3)$ instead of $\Psi^{(0)}(\Sigma, \beta, -1)$. For the state $\Psi^{(0)}(\Sigma, \beta; \lambda_i)$, the second-order energy correction can be written in the form

$$V^{(2)}(\Sigma, \beta; \lambda_i) = -\sum_{n \geq 3} \frac{C_{2n}(\Sigma, \beta; \lambda_i)}{R^{2n}}, \quad (53)$$
where

\[
C_{2n}(\Sigma, \beta; \lambda_i) = \sum_{\ell, L, \ell', L' \geq 1 \atop \ell + L + \ell' + L' = 2n} D_{\lambda_i}(\ell, L, \ell', L'),
\] (54)

\[
D_{\lambda_i}(\ell, L, \ell', L') = \frac{3\alpha^2}{8} \sum_{L_s L_t} g_{\lambda_i}(\ell, L, L_s, L_t, \ell', L') (G_1 + (2 - i)(2 - i) G_2). \] (55)

and \(g_{\lambda_i}\) are

\[
f_{\lambda_1}(\ell, L, L_s, L_t, \ell', L') = g_0(0, 0, 0, 0, \ell, L, L_s, L_t, \ell', L')
\] (56)

\[
- g_0(0, 0, -1, 1, \ell, L, L_s, L_t, \ell', L') - g_0(0, 0, 1, -1, \ell, L, L_s, L_t, \ell', L')
\]

\[
- g_0(-1, 1, 0, 0, \ell, L, L_s, L_t, \ell', L') + g_0(-1, 1, -1, 1, \ell, L, L_s, L_t, \ell', L')
\]

\[
+ g_0(-1, 1, 1, -1, \ell, L, L_s, L_t, \ell', L') - g_0(1, -1, 0, 0, \ell, L, L_s, L_t, \ell', L')
\]

\[
+ g_0(1, -1, -1, 1, \ell, L, L_s, L_t, \ell', L') + g_0(1, -1, -1, -1, \ell, L, L_s, L_t, \ell', L'),
\]

\[
f_{\lambda_2}(\ell, L, L_s, L_t, \ell', L') = g_0(0, 0, 0, 0, \ell, L, L_s, L_t, \ell', L')
\] (57)

\[
+ 2g_0(0, 0, -1, 1, \ell, L, L_s, L_t, \ell', L') + g_0(0, 0, 1, -1, \ell, L, L_s, L_t, \ell', L')
\]

\[
+ g_0(-1, 1, 0, 0, \ell, L, L_s, L_t, \ell', L') + \frac{1}{2} g_0(-1, 1, -1, 1, \ell, L, L_s, L_t, \ell', L')
\]

\[
+ \frac{1}{2} g_0(-1, 1, 1, -1, \ell, L, L_s, L_t, \ell', L') + g_0(1, -1, 0, 0, \ell, L, L_s, L_t, \ell', L')
\]

\[
+ \frac{1}{2} g_0(1, -1, -1, 1, \ell, L, L_s, L_t, \ell', L') + \frac{1}{2} g_0(1, -1, -1, -1, \ell, L, L_s, L_t, \ell', L'),
\]

and

\[
f_{\lambda_3}(\ell, L, L_s, L_t, \ell', L') =
\]

\[
\frac{3}{2} g_0(-1, 1, -1, 1, \ell, L, L_s, L_t, \ell', L') - g_0(-1, 1, 1, -1, \ell, L, L_s, L_t, \ell', L')
\]

\[
- g_0(1, -1, 1, -1, \ell, L, L_s, L_t, \ell', L') + g_0(1, -1, 1, -1, \ell, L, L_s, L_t, \ell', L').
\]

III. CALCULATIONS AND RESULTS

In the center-of-mass frame, the Hamiltonian of a helium atom can be written in the form

\[
H = -\frac{1}{2\mu_e} \nabla^2_{r_1} - \frac{1}{2\mu_e} \nabla^2_{r_2} - \frac{1}{m_n} \nabla_{r_1} \cdot \nabla_{r_2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}},
\] (59)

where \(m_n\) is the nucleus mass, \(\mu_e\) is the reduced mass between the electron and the nucleus, \(r_1\) and \(r_2\) are the position vectors of the two electrons relative to the nucleus, and \(r_{12}\) is
the distance between them. To calculate dispersion coefficients $C_n$, we variationally evaluate energy eigenvalues and corresponding eigenfunctions of the initial states $\text{He}(2^1P)$ and $\text{He}(2^3P)$ with the correlated Hylleraas basis set

$$\left\{ r_1^i r_2^j r_{12}^{k} e^{-\alpha r_1 - \beta r_2} \mathcal{Y}^{LM}_{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \right\},$$

(60)

where $\mathcal{Y}^{LM}_{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$ is the coupled spherical harmonics for the two electrons forming a common eigenstate of $L^2$ and $L_z$, and $\alpha$ and $\beta$ are two nonlinear parameters, which are optimized by first calculating analytically the first-order derivatives of the variation energy with respect to these parameters and then using Newton’s method to find their roots. The basis set includes all combinations of $i \geq \ell_1$, $j \geq \ell_2$, and $k \geq 0$ with $i + j + k \leq \Omega$, where $\Omega$ is an integer controlling the size of the basis set. Then we generate the spectra of the intermediate states for the $S$, $P$, $D$, $F$, and $G$ symmetries by diagonalizing directly the Hamiltonian of the helium atom in chosen basis sets. In addition, we need to transform the $2\ell$-pole transition operator $T^{\ell}_{\mu}(\sigma)$, defined in Eq. (3), into the center-of-mass coordinates and calculate the reduced matrix elements of dipole, quadrupole, octupole, and hexapole transition operators (for details, refer to Ref. [19]).

Table I shows the convergence study of the nonrelativistic energy of the $\infty \text{He}(2^3P)$ state with the increase of the size of basis set. Compared to the value of Drake et al. [20], our result is accurate to about 15 digits. Table II gives the convergence pattern of $C_6(\Delta, 0)$, $C_6(\Pi, +, 0)$, and $C_6(\Sigma, 0; \lambda_1)$ for $\infty \text{He}(2^3P) - \infty \text{He}(2^3P)$ as the sizes of basis sets, including the initial state and the three intermediate states, increase progressively.

Table III presents the long-range interaction coefficients $C_5$, $C_6$, $C_8$, and $C_{10}$ for the $\text{He}(2^1P) - \text{He}(2^1P)$ system. Table IV shows $C_5$, $C_6$, $C_8$, and $C_{10}$ for the $\text{He}(2^1P) - \text{He}(2^3P)$ system. Table V lists $C_5$, $C_6$, $C_8$, and $C_{10}$ for the $\text{He}(2^3P) - \text{He}(2^3P)$ system. We note that, for the three $\text{He}(n P) - \text{He}(n' P)$ systems, $C_5(\Pi, -, \beta)$, $C_5(\Sigma, \beta; \lambda_1)$, and $C_5(\Sigma, \beta; \lambda_3)$ are zero, $C_5(\Pi, +, \beta)$ and $C_6$ are positive, and both $C_5(\Delta, \beta)$ and $C_5(\Sigma, \beta; \lambda_2)$ are negative. For the $\Psi^{(0)}(\Sigma, \beta; \lambda_3)$ states, $C_8$ and $C_{10}$ are negative in the three tables.

Ovsyannikov obtained expressions for the $C_6$ (dispersion) coefficients between two excited atoms [9] and evaluated the $\text{He}(2^3P_2) - \text{He}(2^3P_2)$ coefficients using the atomic dynamic polarizability obtained with a model potential for the $\text{He}(2^3P)$ atom. The diagonal elements of the long-range interaction were given in the $jj$ representation; after transformation to the $LS$ representation [13] the results of Ref. [9] can be compared with ours. The one signifi-
cant discrepancy is between our results for the summed $C_{\sigma}(\Sigma, 0; \lambda)$ and that of Ref. [9]. In table VI we compare the transformed coefficients of Ref. [9] with the present calculations.

To the best of our knowledge, there are no other published results for the dispersion coefficients for interaction between $\text{He}(2^1P)\text{-He}(2^1P)$ and $\text{He}(2^1P)\text{-He}(2^3P)$.

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TABLE I: Convergence study for the nonrelativistic energy of He(2\(^3\)P) with the infinite nuclear mass. \(N\) denotes the number of terms in the basis set. Units are atomic units.

| \(\Omega\) | \(N\) | \(E(\Omega)\) |
|---|---|---|
| 12 | 910 | \(-2.133\ 164\ 190\ 779\ 194\) |
| 13 | 1120 | \(-2.133\ 164\ 190\ 779\ 246\) |
| 14 | 1360 | \(-2.133\ 164\ 190\ 779\ 279\) |
| 15 | 1632 | \(-2.133\ 164\ 190\ 779\ 281\ 2\) |
| 16 | 1892 | \(-2.133\ 164\ 190\ 779\ 282\ 6\) |
| Drake [20] | \(-2.133\ 164\ 190\ 779\ 283\ 202(5)\) |

TABLE II: Convergence study of \(C_6(\Delta, 0)\), \(C_6(\Pi, +, 0)\), and \(C_6(\Sigma, 0; \lambda_1)\), in atomic units, for \(\infty\)He(2\(^3\)P)\(\infty\)He(2\(^3\)P). \(N_{2\Delta}\), \(N_{3S}\), \(N_{(pp)3P}\), and \(N_{3D}\) denote respectively the sizes of bases for the initial state and the three intermediate states of symmetries \(^3S\), \((pp)^3P\), and \(^3D\).

| \(N_{2\Delta}\) | \(N_{3S}\) | \(N_{(pp)3P}\) | \(N_{3D}\) | \(C_6(\Delta, 0)\) | \(C_6(\Pi, +, 0)\) | \(C_6(\Sigma, 0; \lambda_1)\) |
|---|---|---|---|---|---|---|
| 1360 | 560 | 1230 | 853 | 4083.026\ 993\ 80 | 2324.937\ 567\ 24 | 7296.821\ 324\ 76 |
| 1632 | 680 | 1430 | 1071 | 4083.026\ 997\ 99 | 2324.937\ 572\ 24 | 7296.821\ 330\ 48 |
| 1938 | 816 | 1650 | 1323 | 4083.026\ 998\ 66 | 2324.937\ 572\ 91 | 7296.821\ 331\ 49 |
TABLE III: The long-range interaction coefficients, in atomic units, for the He(2^1P)-He(2^1P) system.

| C_n | ^∞He(2^1P)−∞He(2^1P) | ^4He(2^1P)−^4He(2^1P) | ^3He(2^1P)−^3He(2^1P) |
|-----|------------------------|------------------------|------------------------|
| C_5(Δ, 0) | -227.26160604(2) | -227.31888382(1) | -227.33762037(2) |
| C_5(Π, +, 0) | 909.04642409(1) | 909.27553527(2) | 909.35048146(3) |
| C_5(Π, -, 0) | 0 | 0 | 0 |
| C_5(Σ, 0; λ_1) | 0 | 0 | 0 |
| C_5(Σ, 0; λ_2) | -1363.56963613(1) | -1363.91330289(1) | -1364.02572224(5) |
| C_5(Σ, 0; λ_3) | 0 | 0 | 0 |
| C_6(Δ, 0) | 5578.63(2) | 5584.99(1) | 5587.07(1) |
| C_6(Π, +, 0) | 3606.63(2) | 3610.56(2) | 3611.84(1) |
| C_6(Π, -, 0) | 10831.74(2) | 10844.25(2) | 10848.35(2) |
| C_6(Σ, 0; λ_1) | 9682.78(1) | 9693.98(2) | 9697.63(2) |
| C_6(Σ, 0; λ_2) | 1025.14(2) | 1032.23(2) | 1034.58(3) |
| C_6(Σ, 0; λ_3) | 1966.062(1) | 1968.141(1) | 1968.821(1) |
| C_8(Δ, 0) | 3.61343(3) × 10^6 | 3.61541(2) × 10^6 | 3.61607(3) × 10^6 |
| C_8(Π, +, 0) | 5.163864(4) × 10^7 | 5.168052(3) × 10^7 | 5.169423(3) × 10^7 |
| C_8(Π, -, 0) | 1.7334869(4) × 10^8 | 1.7349273(2) × 10^8 | 1.7353990(4) × 10^8 |
| C_8(Σ, 0; λ_1) | 2.0453997(5) × 10^8 | 2.0471586(3) × 10^8 | 2.0477345(5) × 10^8 |
| C_8(Σ, 0; λ_2) | 7.6324701(1) × 10^8 | 7.6394035(3) × 10^8 | 7.6416728(2) × 10^8 |
| C_8(Σ, 0; λ_3) | -2.992224(2) × 10^6 | -2.996113(3) × 10^6 | -2.997383(2) × 10^6 |
TABLE IV: The long-range interaction coefficients, in atomic units, for the He(2\(^1\)P)-He(2\(^3\)P) system.

| Mass               | \(\infty\text{He}(2\(^1\)P)-\infty\text{He}(2\(^3\)P)\) | \(4\text{He}(2\(^1\)P)-4\text{He}(2\(^3\)P)\) | \(3\text{He}(2\(^1\)P)-3\text{He}(2\(^3\)P)\) |
|--------------------|-------------------------------------------------|-------------------------------------------------|-------------------------------------------------|
| \(C_5(\Delta, \pm)\) | -189.519232605(3) | -189.513470009(3) | -189.511579458(2) |
| \(C_5(\Pi, +, \pm)\) | 758.07693042(3) | 758.05388004(2) | 758.04631785(3) |
| \(C_5(\Pi, -, \pm)\) | 0 | 0 | 0 |
| \(C_5(\Sigma, \pm; \lambda_1)\) | 0 | 0 | 0 |
| \(C_5(\Sigma, \pm; \lambda_2)\) | -1137.11539564(3) | -1137.08082006(2) | -1137.06947676(2) |
| \(C_5(\Sigma, \pm; \lambda_3)\) | 0 | 0 | 0 |
| \(C_6(\Delta, \pm)\) | 5186.93(2) | 5190.06(3) | 5191.91(2) |
| \(C_6(\Pi, +, \pm)\) | 2990.19(1) | 2992.03(2) | 2992.640(2) |
| \(C_6(\Pi, -, \pm)\) | 10353.76(2) | 10359.97(5) | 10362.05(2) |
| \(C_6(\Sigma, \pm; \lambda_1)\) | 9245.11(2) | 9250.65(3) | 9252.52(3) |
| \(C_6(\Sigma, \pm; \lambda_2)\) | 6162.84(4) | 6165.27(3) | 6166.13(4) |
| \(C_6(\Sigma, \pm; \lambda_3)\) | 1505.135(1) | 1506.081(1) | 1506.390(1) |
| \(C_8(\Delta, \pm)\) | -41757.6(6) | -41832.7(4) | -41856.3(4) |
| \(C_8(\Pi, +, \pm)\) | -88728.8(2) | -88801.9(1) | -88825.1(2) |
| \(C_8(\Pi, -, \pm)\) | 993884(3) | 994253(2) | 994375(2) |
| \(C_8(\Sigma, \pm; \lambda_1)\) | 843530(3) | 843832(2) | 843931(2) |
| \(C_8(\Sigma, \pm; \lambda_2)\) | 2139396(4) | 2140392(3) | 2140712(2) |
| \(C_8(\Sigma, \pm; \lambda_3)\) | -11571.12(3) | -11605.17(2) | -11616.32(3) |
| \(C_{10}(\Delta, \pm)\) | 2.32333(4) \(\times 10^6\) | 2.32313(3) \(\times 10^6\) | 2.32312(1) \(\times 10^6\) |
| \(C_{10}(\Pi, +, \pm)\) | 5.236817(3) \(\times 10^7\) | 5.238065(4) \(\times 10^7\) | 5.238463(1) \(\times 10^7\) |
| \(C_{10}(\Pi, -, \pm)\) | 1.224688(2) \(\times 10^8\) | 1.224994(2) \(\times 10^8\) | 1.225094(1) \(\times 10^8\) |
| \(C_{10}(\Sigma, \pm; \lambda_1)\) | 1.435423(2) \(\times 10^8\) | 1.435806(2) \(\times 10^8\) | 1.435933(1) \(\times 10^8\) |
| \(C_{10}(\Sigma, \pm; \lambda_2)\) | 5.737754(2) \(\times 10^8\) | 5.739452(2) \(\times 10^8\) | 5.740007(2) \(\times 10^8\) |
| \(C_{10}(\Sigma, \pm; \lambda_3)\) | -2.018823(3) \(\times 10^6\) | -2.020165(2) \(\times 10^6\) | -2.020604(2) \(\times 10^6\) |
TABLE V: The long-range interaction coefficients, in atomic units, for the He(2^3P)-He(2^3P) system.

| Mass | $\infty$He(2^3P)$-\infty$He(2^3P) | $^4$He(2^3P)$-^4$He(2^3P) | $^3$He(2^3P)$-^3$He(2^3P) |
|------|----------------------------------|-----------------------------|-----------------------------|
| $C_5(\Delta, 0)$ | $-158.0449076079(7)$ | $-157.99547627265(5)$ | $-157.9793027289(2)$ |
| $C_5(\Pi, +, 0)$ | $632.179630432(3)$ | $631.981905089(1)$ | $631.917210917(2)$ |
| $C_5(\Pi, -, 0)$ | 0 | 0 | 0 |
| $C_5(\Sigma, 0; \lambda_1)$ | 0 | 0 | 0 |
| $C_5(\Sigma, 0; \lambda_2)$ | $-948.269445647(4)$ | $-947.972857636(3)$ | $-947.875816375(3)$ |
| $C_6(\Delta, 0)$ | $4083.0269989(3)$ | $4082.9351409(1)$ | $4082.9049629(7)$ |
| $C_6(\Pi, +, 0)$ | $2324.9375732(4)$ | $2325.2001488(4)$ | $2325.2859848(3)$ |
| $C_6(\Pi, -, 0)$ | $8172.742842(3)$ | $8172.314300(1)$ | $8172.173845(3)$ |
| $C_6(\Sigma, 0; \lambda_1)$ | $7296.821336(5)$ | $7296.447426(2)$ | $7296.324875(5)$ |
| $C_6(\Sigma, 0; \lambda_2)$ | 0 | 0 | 0 |
| $C_6(\Sigma, 0; \lambda_3)$ | 0 | 0 | 0 |
| $C_8(\Delta, 0)$ | $-30170.71(6)$ | $-30168.72(8)$ | $-30168.10(6)$ |
| $C_8(\Pi, +, 0)$ | 17083.8(2) | 17044.4(2) | 17031.5(3) |
| $C_8(\Pi, -, 0)$ | 726869.3(2) | 726728.9(2) | 726682.8(1) |
| $C_8(\Sigma, 0; \lambda_1)$ | 618334.9(1) | 618201.6(2) | 618157.8(1) |
| $C_8(\Sigma, 0; \lambda_2)$ | 1835912.3(2) | 1835108.6(4) | 1834846(1) |
| $C_8(\Sigma, 0; \lambda_3)$ | 1159.1243658(5) | 1159.3780657(5) | 1159.4610336(4) |
| $C_{10}(\Delta, 0)$ | 1537493(3) | 1536725(3) | 1536474(3) |
| $C_{10}(\Pi, +, 0)$ | $3.656172(2) \times 10^7$ | $3.653559(2) \times 10^7$ | $3.652704(2) \times 10^7$ |
| $C_{10}(\Pi, -, 0)$ | $3.6439100(8) \times 10^7$ | $3.6410605(1) \times 10^7$ | $3.6409524(2) \times 10^7$ |
| $C_{10}(\Sigma, 0; \lambda_1)$ | $9.846488(2) \times 10^7$ | $9.842827(2) \times 10^7$ | $9.841629(2) \times 10^7$ |
| $C_{10}(\Sigma, 0; \lambda_2)$ | $3.9464965(4) \times 10^8$ | $3.94483100(3) \times 10^8$ | $3.9442865(4) \times 10^8$ |
| $C_{10}(\Sigma, 0; \lambda_3)$ | $-1.378107(3) \times 10^6$ | $-1.378199(2) \times 10^6$ | $-1.378225(5) \times 10^6$ |
TABLE VI: Comparison of the present results with the available results of Ref. [9] for the $C_6$ coefficients of He($2^3P_2$)–He($2^3P_2$) with infinite nuclear mass. The relation between the present results (LHS) and the results from Ref. [9] (RHS) are given in the first column. The symbols for the dispersion coefficients on the RHS represent values $C_6(M_A, M_B)$ for two atoms in the total angular momentum states $J_A = J_B = 2$ and quantization axis along the inter-nuclear axis.

| Terms                                                                 | Present | Ref. [9] |
|----------------------------------------------------------------------|---------|----------|
| $C_6(\Delta, 0) = C_6(2, 2)$                                         | 4 083   | 4 056    |
| $\frac{1}{2} [C_6(\Pi, +, 0) + C_6(\Pi, -, 0)] = 2C_6(1, 2) - C_6(2, 2)$ | 4 666   | 4 645    |
| $\frac{1}{3} \sum_{i=1}^3 C_6(\Sigma, 0; \lambda_i) = 4C_6(0, 2) + \frac{4}{3}C_6(1, 1) - \frac{20}{3}C_6(1, 2) + \frac{7}{3}C_6(2, 2)$ | 5 608   | 7 026    |