

# Long-range interactions between a He(2 $^3S$ ) atom and a He(2 $^3P$ ) atom for like isotopes

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For the interactions between a He(2  $^3S$ ) atom and a He(2  $^3P$ ) atom for like isotopes, we report perturbation theoretic calculations using accurate variational wave functions in Hylleraas coordinates of the coefficients determining the potential energies at large internuclear separations. We evaluate the coefficient  $C_3$  of the first order resonant dipole-dipole energy and the van der Waals coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  for the second order energies arising from the mutual perturbations of instantaneous electric dipole, quadrupole, and octupole interactions. We also evaluate the leading contribution to the third-order energy. We establish definitive values including treatment of the finite nuclear mass for the  ${}^3\text{He}(2 \mathbf{\hat{S}})-{}^3\text{He}(2 \mathbf{\hat{P}})$  and  ${}^4\text{He}(2 \mathbf{\hat{S}})-{}^4\text{He}(2 \mathbf{\hat{P}})$  interactions.

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Recently, there has been considerable interest in the study of helium dimers and ultracold helium collisions associated with metastable helium atoms [1–11]. Molecular lines of the helium dimers associated with the He(2  $^3S$ )-He(2  $^3P$ ) asymptotes have been produced by photoassociation of spin-polarized metastable helium atoms He(2  $^3S_1$ ). In the purely long-range  $0_u^+$  potential well (with a minimum internuclear distance reaching 150 bohrs) associated with the He(2  $^3S_1$ )-He(2  $^3P_0$ ) asymptote, bound states of the helium dimer [1,2,5] can be used in measurements of the  $s$ -wave scattering length for collisions of two  ${}^4\text{He}(2 \mathbf{\hat{S}}_1)$  atoms [4,6]. Molecular lines to the red of the  $D_2$  atomic transition in helium dimers associated with the He(2  $^3S$ )-He(2  $^3P_2$ ) asymptote are of interest for control of the scattering length using an “optical Feshbach resonance” [4,7]. Published data are scarce on the long-range part of the He(2  $^3S$ )-He(2  $^3P$ ) potential energies, which determine the energy level structures of the ultralong-range dimers formed in the photoassociation of ultracold metastable helium atoms.

In this paper, we present perturbation theoretic calculations of the coefficients determining the potential energies at large internuclear separations using accurate variational wave functions in Hylleraas coordinates. We evaluate the coefficient  $C_3$  of the first order resonant dipole-dipole energy, and the van der Waals coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  of the second order energies arising from the mutual perturbations of instantaneous electric dipole, quadrupole, and octupole interactions. We also evaluate for the third order energy the coefficient  $C_9$  of the leading term. We establish definitive values including treatment of the finite nuclear mass for the  ${}^3\text{He}(2 \mathbf{\hat{S}})-{}^3\text{He}(2 \mathbf{\hat{P}})$  and  ${}^4\text{He}(2 \mathbf{\hat{S}})-{}^4\text{He}(2 \mathbf{\hat{P}})$  interactions. Definitive values for the  $C_6$ ,  $C_8$ ,  $C_9$ , and  $C_{10}$  coefficients are established.

In this work, atomic units are used throughout. For the He(2  $^3S$ )-He(2  $^3P$ ) system, the zeroth-order wave function appropriate for the perturbation calculation of the long-range interaction can be written in the form [12],

$$\Psi^{(0)}(M, \pm) = \frac{1}{\sqrt{2}} [\Psi_{n_a}(\boldsymbol{\sigma}) \Psi_{n_b}(1M; \boldsymbol{\rho}) \pm \Psi_{n_a}(\boldsymbol{\rho}) \Psi_{n_b}(1M; \boldsymbol{\sigma})], \quad (1)$$

where  $\Psi_{n_a}$  is the metastable He(2  $^3S$ ) wave function,  $\Psi_{n_b}$  is the wave function for the He(2  $^3P$ ) atom with magnetic quantum number  $M$ ,  $\boldsymbol{\sigma}$  and  $\boldsymbol{\rho}$  are the collection of coordinates of the two helium atoms in the laboratory reference frame, and the “ $\pm$ ” sign indicates the gerade and ungerade states. The corresponding zeroth-order energy is  $E_{n_a n_b}^{(0)} = E_{n_a}^{(0)} + E_{n_b}^{(0)}$ . At large internuclear distances, the interaction potential between the two helium atoms can be expanded as an infinite series in powers of  $1/R$  [12]

$$V = \sum_{\ell=0}^{\infty} \sum_{L=0}^{\infty} \frac{V_{\ell L}}{R^{\ell+L+1}}, \quad (2)$$

where

$$V_{\ell L} = 4\pi(-1)^L (\ell, L)^{-1/2} \sum_{\mu} K_{\ell L}^{\mu} T_{\mu}^{(\ell)}(\boldsymbol{\sigma}) T_{-\mu}^{(L)}(\boldsymbol{\rho}). \quad (3)$$

$T_{\mu}^{(\ell)}(\boldsymbol{\sigma})$  and  $T_{-\mu}^{(L)}(\boldsymbol{\rho})$  are the atomic multipole tensor operators defined as

$$T_{\mu}^{(\ell)}(\boldsymbol{\sigma}) = \sum_i Q_i \sigma_i^{\ell} Y_{\ell \mu}(\hat{\boldsymbol{\sigma}}_i), \quad (4)$$

and

$$T_{-\mu}^{(L)}(\boldsymbol{\rho}) = \sum_j q_j \rho_j^L Y_{L-\mu}(\hat{\boldsymbol{\rho}}_j), \quad (5)$$

where  $Q_i$  and  $q_j$  are the charges on particles  $i$  and  $j$ . The coefficient  $K_{\ell L}^{\mu}$  is

$$K_{\ell L}^{\mu} = \left[ \binom{\ell+L}{\ell+\mu} \binom{\ell+L}{L+\mu} \right]^{1/2} \quad (6)$$

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

*First order.* According to the perturbation theory, the first-order energy [12] can be written as

$$V^{(1)} = -\frac{C_3(M, \pm)}{R^3}, \quad (7)$$

where

$$C_3(0, \pm) = \pm \frac{8\pi}{9} |\langle \Psi_{n_a}(\boldsymbol{\sigma}) | \sum_i Q_i \sigma_i Y_1(\hat{\boldsymbol{\sigma}}_i) | \Psi_{n_b}(1; \boldsymbol{\sigma}) \rangle|^2, \quad (8)$$

and

$$C_3(\pm 1, \pm) = \mp \frac{4\pi}{9} |\langle \Psi_{n_a}(\boldsymbol{\sigma}) | \sum_i Q_i \sigma_i Y_1(\hat{\boldsymbol{\sigma}}_i) | \Psi_{n_b}(1; \boldsymbol{\sigma}) \rangle|^2. \quad (9)$$

*Second order.* The second-order energy is

$$V^{(2)} = - \sum'_{n_s n_t} \sum_{L_s M_s} \sum_{L_t M_t} \frac{|\langle \Psi^{(0)} | V | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \omega_{n_t}(L_t M_t; \boldsymbol{\rho}) \rangle|^2}{E_{n_s n_t} - E_{n_a n_b}^{(0)}}, \quad (10)$$

where  $\chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \omega_{n_t}(L_t M_t; \boldsymbol{\rho})$  is one of the intermediate states with the energy eigenvalue  $E_{n_s n_t} = E_{n_s}^{(0)} + E_{n_t}^{(0)}$ , and the prime in the summation indicates that the terms with  $E_{n_s n_t} = E_{n_a n_b}^{(0)}$  should be excluded. Substituting (2) into (10), we obtain

$$V^{(2)} = - \sum'_{n_s n_t} \sum_{L_s M_s} \sum_{L_t M_t} \frac{B_1 \pm B_2}{E_{n_s n_t} - E_{n_a n_b}^{(0)}}, \quad (11)$$

with

$$B_1 = |\langle \Psi_{n_a}(\boldsymbol{\sigma}) \Psi_{n_b}(1M; \boldsymbol{\rho}) | V | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \omega_{n_t}(L_t M_t; \boldsymbol{\rho}) \rangle|^2, \quad (12)$$

and

$$B_2 = \langle \Psi_{n_a}(\boldsymbol{\sigma}) \Psi_{n_b}(1M; \boldsymbol{\rho}) | V | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \omega_{n_t}(L_t M_t; \boldsymbol{\rho}) \rangle \times \langle \Psi_{n_a}(\boldsymbol{\rho}) \Psi_{n_b}(1M; \boldsymbol{\sigma}) | V | \chi_{n_s}(L_s M_s; \boldsymbol{\sigma}) \omega_{n_t}(L_t M_t; \boldsymbol{\rho}) \rangle. \quad (13)$$

$B_2$  in (13) is the exchange interaction of the two states He( $2^3S$ ) and He( $2^3P$ ). After applying the Wigner-Eckart theorem, we have

$$\sum'_{n_s n_t} \sum_{L_s M_s} \sum_{L_t M_t} \frac{B_1}{E_{n_s n_t} - E_{n_a n_b}^{(0)}} = \sum_{LL' L_s L_t} \frac{C_1(L, L', L_s, L_t, M)}{R^{2L_s + L_t + L' + 2}}, \quad (14)$$

with

$$C_1(L, L', L_s, L_t, M) = \frac{1}{2\pi} G'_1(L, L', L_s, L_t, M) F^{(1)}(L, L', L_s, L_t). \quad (15)$$

In (15),  $G'_1$  is the angular-momentum part and  $F^{(1)}$  is the oscillator strength part. Their expressions are

$$G'_1(L, L', L_s, L_t, M) = (-1)^{L+L'} (L, L')^{1/2} \sum_{M_s M_t} K_{L_s L_t}^{-M_s} K_{L_s L_t}^{-M_s} \times \begin{pmatrix} 1 & L & L_t \\ -M & M_s & M_t \end{pmatrix} \begin{pmatrix} 1 & L' & L_s \\ -M & M_s & M_t \end{pmatrix}, \quad (16)$$

and

$$F^{(1)}(L, L', L_s, L_t) = \frac{3\pi}{2} \sum_{n_s n_t} \frac{\bar{g}_{n_s n_a n_b}(L_s, 0, 0, L_s, L_s) \bar{g}_{n_t n_b n_b}(L_t, 1, 1, L, L')}{(\Delta E_{n_s n_a} + \Delta E_{n_t n_b}) |\Delta E_{n_s n_a} \Delta E_{n_t n_b}|}, \quad (17)$$

with

$$\begin{aligned} \bar{g}_{n_s n_a n_b}(L_s, L_1, L_2, \ell, \ell') &= \frac{8\pi}{(\ell, \ell')} \frac{\sqrt{|\Delta E_{n_s n_a} \Delta E_{n_s n_b}|}}{\sqrt{(2L_1 + 1)(2L_2 + 1)}} \\ &\times \langle \Psi_{n_a}(L_1; \boldsymbol{\sigma}) | \sum_i Q_i \sigma_i^\ell Y_\ell(\hat{\boldsymbol{\sigma}}_i) | \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle \\ &\times \langle \Psi_{n_b}(L_2; \boldsymbol{\sigma}) | \sum_i Q_i \sigma_i^{\ell'} Y_{\ell'}(\hat{\boldsymbol{\sigma}}_i) | \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle, \end{aligned} \quad (18)$$

and  $\Delta E_{n_s n_a} = E_{n_s}^{(0)} - E_{n_a}^{(0)}$ , etc. For the special case when 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

$$\begin{aligned} \bar{f}_{n_s n_a}^\ell &= \frac{8\pi \Delta E_{n_s n_a}}{(2\ell + 1)^2 (2L_1 + 1)} \\ &\times |\langle \Psi_{n_a}(L_1; \boldsymbol{\sigma}) | \sum_i Q_i \sigma_i^\ell Y_\ell(\hat{\boldsymbol{\sigma}}_i) | \chi_{n_s}(L_s; \boldsymbol{\sigma}) \rangle|^2. \end{aligned} \quad (19)$$

Similarly, we have

$$\sum'_{n_s n_t} \sum_{L_s M_s} \sum_{L_t M_t} \frac{B_2}{E_{n_s n_t} - E_{n_a n_b}^{(0)}} = \sum_{LL' L_s L_t} \frac{C_2(L, L', L_s, L_t, M)}{R^{L_s + L_t + L' + 2}}, \quad (20)$$

$$C_2(L, L', L_s, L_t, M) = \frac{1}{2\pi} G'_2(L, L', L_s, L_t, M) F^{(2)}(L, L', L_s, L_t), \quad (21)$$

with

$$\begin{aligned} G'_2(L, L', L_s, L_t, M) &= (-1)^{L+L_s} (L, L')^{1/2} \sum_{M_s M_t} (-1)^{M_s + M_t} K_{L_s L_t}^{-M_s} K_{L' L_t}^{M_t} \\ &\times \begin{pmatrix} 1 & L & L_t \\ -M & M_s & M_t \end{pmatrix} \begin{pmatrix} 1 & L' & L_s \\ -M & M_t & M_s \end{pmatrix}, \end{aligned} \quad (22)$$

$$F^{(2)}(L, L', L_s, L_t) = \frac{3\pi}{2} \sum'_{n_s n_t} \frac{\bar{g}_{n_s n_a n_b}(L_s, 0, 1, L_s, L') \bar{g}_{n_s n_a n_b}(L_t, 0, 1, L_t, L)}{(\Delta E_{n_s n_a} + \Delta E_{n_t n_b}) \sqrt{|\Delta E_{n_s n_a} \Delta E_{n_s n_b} \Delta E_{n_t n_a} \Delta E_{n_t n_b}|}}. \quad (23)$$

Finally, the second-order energy is

$$V^{(2)} = - \sum_{n \geq 3} \frac{C_{2n}(M, \pm)}{R^{2n}}, \quad (24)$$

where  $C_{2n}(M, \pm)$  are the dispersion coefficients

$$\begin{aligned} C_{2n}(M, \pm) &= \sum_{\substack{LL' L_s L_t \\ L+L'+2L_s+2=2n}} C_1(L, L', L_s, L_t, M) \\ &\pm \sum_{\substack{LL' L_s L_t \\ L+L'+L_s+L_t+2=2n}} C_2(L, L', L_s, L_t, M). \end{aligned} \quad (25)$$

*Third order.* According to the third-order perturbation theory, the third-order energy correction is

$$\begin{aligned} V^{(3)} &= \sum'_{n_u n_v} \sum'_{n_s n_t} \sum_{L_s M_s} \sum_{L_u M_u} \sum_{L_v M_v} \sum_{L_t M_t} \frac{D_1}{(E_{n_s n_t} - E_{n_a n_b}^{(0)}) (E_{n_u n_v} - E_{n_a n_b}^{(0)})} \\ &+ \sum'_{n_u n_v} \sum'_{L_s M_s} \sum_{L_t M_t} \frac{D_2}{(E_{n_s n_t} - E_{n_a n_b}^{(0)})^2}, \end{aligned} \quad (26)$$

where  $D_1$  and  $D_2$  are

$$\begin{aligned} D_1 &= \langle \Psi^{(0)} | V | \chi_{n_s}(L_s M_s; \sigma) \omega_{n_t}(L_t M_t; \rho) \rangle \\ &\times \langle \chi_{n_s}(L_s M_s; \sigma) \omega_{n_t}(L_t M_t; \rho) | V | \chi_{n_u}(L_u M_u; \sigma) \\ &\omega_{n_v}(L_v M_v; \rho) \rangle \langle \chi_{n_u}(L_u M_u; \sigma) \omega_{n_v}(L_v M_v; \rho) | V | \Psi^{(0)} \rangle, \end{aligned} \quad (27)$$

$$D_2 = - \langle \Psi^{(0)} | V | \Psi^{(0)} \rangle | \langle \Psi^{(0)} | V | \chi_{n_s}(L_s M_s; \sigma) \omega_{n_t}(L_t M_t; \rho) \rangle |^2. \quad (28)$$

For the He(2<sup>3</sup>S)-He(2<sup>3</sup>P) system, following a procedure similar to the second-order perturbation, the third-order energy correction can be expanded in terms of powers of  $1/R$ ,

$$V^{(3)} = - \frac{C_9(M, \pm)}{R^9} - \frac{C_{11}(M, \pm)}{R^{11}} - \dots \quad (29)$$

In this work, we do not present a complete third order calculation. We only consider the leading term  $C_9(M, \pm)$  of

TABLE I. Convergence characteristics of  $C_6(M, \pm)$ , in atomic units, for the <sup>80</sup>He(2<sup>3</sup>S)-<sup>80</sup>He(2<sup>3</sup>P) system.  $N^{3S}$ ,  $N^{3P}$ ,  $N^{3S^*}$ ,  $N^{3P^*}$ ,  $N_{(pp)}$  <sup>3</sup>P, and  $N^{3D}$  denote, respectively, the sizes of bases for the two initial states and the four intermediate states of symmetries <sup>3</sup>S, <sup>3</sup>P, (pp) <sup>3</sup>P, and <sup>3</sup>D.

$N^{3S}$	$N^{3P}$	$N^{3S^*}$	$N^{3P^*}$	$N_{(pp)}^{3P}$	$N^{3D}$	$C_6(0, \pm)$	$C_6(\pm 1, \pm)$
1330	1360	560	1360	1230	853	2640.233 681	1862.572 368
1540	1632	680	1632	1430	1071	2640.233 694	1862.572 376
1771	1938	816	1938	1650	1323	2640.233 700	1862.572 380

$V^{(3)}$ , which is comparable to the smallest term of  $V^{(2)}$ ,

$$C_9(M, \pm) = C_9^{D_1}(M, \pm) + C_9^{D_2}(M, \pm), \quad (30)$$

where

$$\begin{aligned} C_9^{D_1}(M, \pm) &= \sum_{n_u n_v} \sum_{n_s n_t} \sum_{L_u L_t} \frac{\mp (4\pi)^3 G_{D_1}(L_t, L_u, M)}{(E_{n_s n_t} - E_{n_a n_b}^{(0)}) (E_{n_u n_v} - E_{n_a n_b}^{(0)})} \\ &\times \langle \Psi_{n_a}(\sigma) | \sum_i Q_i \sigma_i Y_1(\hat{\sigma}_i) | \chi_{n_s}(1; \sigma) \rangle \\ &\times \langle \Psi_{n_b}(1; \rho) | \sum_j Q_j \rho_j Y_1(\hat{\rho}_j) | \omega_{n_t}(L_t; \rho) \rangle \\ &\times \langle \chi_{n_s}(1; \sigma) | \sum_i Q_i \sigma_i Y_1(\hat{\sigma}_i) | \chi_{n_u}(L_u; \sigma) \rangle \\ &\times \langle \omega_{n_t}(L_t; \rho) | \sum_j Q_j \rho_j Y_1(\hat{\rho}_j) | \omega_{n_b}(1; \rho) \rangle \\ &\times \langle \chi_{n_u}(L_u; \sigma) | \sum_i Q_i \sigma_i Y_1(\hat{\sigma}_i) | \Psi_{n_b}(1; \sigma) \rangle \\ &\times \langle \omega_{n_v}(1; \rho) | \sum_j Q_j \rho_j Y_1(\hat{\rho}_j) | \Psi_{n_a}(\rho) \rangle, \end{aligned} \quad (31)$$

$$\begin{aligned} G_{D_1}(L_t, L_u, M) &= \sum_{M_t M_u M_z} \frac{(-1)^{M_z + L_t + L_u - M_u}}{81} K_{11}^{-M_z} K_{11}^{M_z - M_u} K_{11}^{M_u - M} \\ &\times \begin{pmatrix} 1 & 1 & L_t \\ -M & M_z & M_t \end{pmatrix} \begin{pmatrix} 1 & 1 & L_u \\ -M_z & M_z - M_u & M_u \end{pmatrix} \\ &\times \begin{pmatrix} L_t & 1 & 1 \\ -M_t & M_u - M_z & M - M_u \end{pmatrix} \\ &\times \begin{pmatrix} L_u & 1 & 1 \\ -M_u & M_u - M & M \end{pmatrix}, \end{aligned} \quad (32)$$

$$C_9^{D_2}(M, \pm) = \frac{-C_3(M, \pm)}{2\pi} \sum_{L_t} G'_1(1, 1, 1, L_t, M) F^{D_2}(L_t), \quad (33)$$

$$F^{D_2}(L_t) = \frac{3\pi}{2} \sum_{n_s n_t} \frac{\bar{g}_{n_s n_a n_b}(1, 0, 0, 1, 1) \bar{g}_{n_t n_b n_b}(L_t, 1, 1, 1, 1)}{(\Delta E_{n_s n_a} + \Delta E_{n_t n_b})^2 |\Delta E_{n_s n_a} \Delta E_{n_t n_b}|}. \quad (34)$$

*Hamiltonian.* The nonrelativistic Hamiltonian for a helium atom in a laboratory frame is

TABLE II. Contributions to  $C_6(M, \pm)$ , in atomic units for the  ${}^{\infty}\text{He}(2\ ^3S)\text{-}{}^{\infty}\text{He}(2\ ^3P)$  system from  $(^3P, {}^3S)$ ,  $(^3P, (pp) {}^3P)$ , and  $(^3P, {}^3D)$  symmetries.

Symmetries	$C_6(0, \pm)$	$C_6(\pm 1, \pm)$
$(^3P, {}^3S)$	684.091969(2)	171.0229919(1)
$(^3P, (pp) {}^3P)$	1.31648932(2)	3.29122329(3)
$(^3P, {}^3D)$	1954.825248(4)	1688.258168(3)

$$H = -\frac{1}{2m_n}\nabla_{R_n}^2 - \frac{1}{2m_e}\nabla_{R_1}^2 - \frac{1}{2m_e}\nabla_{R_2}^2 + \frac{q_n q_e}{|\mathbf{R}_n - \mathbf{R}_1|} + \frac{q_n q_e}{|\mathbf{R}_n - \mathbf{R}_2|} + \frac{q_e^2}{|\mathbf{R}_1 - \mathbf{R}_2|}, \quad (35)$$

where  $m_n$  and  $m_e$  are the masses of the nucleus and electron, respectively,  $q_n$  and  $q_e$  are their charges, and  $\mathbf{R}_n$ ,  $\mathbf{R}_1$ , and  $\mathbf{R}_2$  are the corresponding position vectors relative to the laboratory frame. We introduce the following transformation:

$$\mathbf{r}_1 = \mathbf{R}_1 - \mathbf{R}_n, \quad (36)$$

$$\mathbf{r}_2 = \mathbf{R}_2 - \mathbf{R}_n, \quad (37)$$

$$\mathbf{X} = \frac{1}{M_T}(m_n\mathbf{R}_n + m_e\mathbf{R}_1 + m_e\mathbf{R}_2), \quad (38)$$

where  $M_T = m_n + 2m_e$  is the total mass of helium atom and  $\mathbf{X}$  is the position vector for the center of mass of helium. In the center-of-mass frame, the Hamiltonian becomes

TABLE III.  $C_3(M, \pm)$ ,  $C_6(M, \pm)$ ,  $C_8(M, \pm)$ ,  $C_9(M, \pm)$ , and  $C_{10}(M, \pm)$ , in atomic units, for the  ${}^{\infty}\text{He}(2\ ^3S)\text{-}{}^{\infty}\text{He}(2\ ^3P)$  system.

Mass	${}^{\infty}\text{He-}{}^{\infty}\text{He}$	${}^4\text{He-}{}^4\text{He}$	${}^3\text{He-}{}^3\text{He}$
$C_3(0, \pm)$	$\pm 12.8154931075(4)$	$\pm 12.8181751205(4)$	$\pm 12.8190526019(4)$
$C_3(\pm 1, \pm)$	$\mp 6.4077465536(2)$	$\mp 6.4090875603(2)$	$\mp 6.4095263011(2)$
$C_6(0, \pm)$	2640.2338(1)	2641.5083(2)	2641.9255(3)
$C_6(\pm 1, \pm)$	1862.5724(1)	1863.4726(2)	1863.7674(4)
$C_8(0, +)$	311901.2(4)	311955.4(5)	311972.8(1)
$C_8(0, -)$	1541993(2)	1542352(1)	1542470(1)
$C_8(\pm 1, +)$	168906.5(4)	168921.6(3)	168926.5(2)
$C_8(\pm 1, -)$	103017.3(3)	103039.5(4)	103046.7(3)
$C_9(0, \pm)$	$\pm 512059.227(6)$	$\pm 512572.343(6)$	$\pm 512740.318(6)$
$C_9(\pm 1, \pm)$	$\mp 117073.536(2)$	$\mp 117199.211(2)$	$\mp 117240.354(2)$
$C_{10}(0, +)$	$2.922482(3) \times 10^7$	$2.922304(5) \times 10^7$	$2.922244(3) \times 10^7$
$C_{10}(0, -)$	$1.857456(3) \times 10^8$	$1.8574503(3) \times 10^8$	$1.8574492(3) \times 10^8$
$C_{10}(\pm 1, +)$	$1.611301(3) \times 10^7$	$1.611325(3) \times 10^7$	$1.611334(5) \times 10^7$
$C_{10}(\pm 1, -)$	$2.40597(3) \times 10^6$	$2.40608(1) \times 10^6$	$2.40613(2) \times 10^6$

$$H = -\frac{1}{2\mu_e}\nabla_{\mathbf{r}_1}^2 - \frac{1}{2\mu_e}\nabla_{\mathbf{r}_2}^2 - \frac{1}{m_n}\nabla_{\mathbf{r}_1} \cdot \nabla_{\mathbf{r}_2} + \frac{q_n q_e}{r_1} + \frac{q_n q_e}{r_2} + \frac{q_e^2}{r_{12}}, \quad (39)$$

where  $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$  and  $\mu_e = m_e m_n / (m_e + m_n)$  is the reduced mass between the electron and the nucleus. The eigenvalue spectrum and corresponding eigenfunctions are obtained by diagonalizing the Hamiltonian (39) in the correlated Hylleraas basis set [12]

$$\{r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2} \mathcal{Y}_{\ell_1 \ell_2}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)\}, \quad (40)$$

where  $\mathcal{Y}_{\ell_1 \ell_2}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$  is the coupled spherical harmonics for the two electrons forming a common eigenstate of  $\mathbf{L}^2$  and  $L_z$ . Except for some truncations, all terms are included in the basis such that

$$i + j + k \leq \Omega, \quad (41)$$

with  $\Omega$  being an integer. As  $\Omega$  increases, the size of the basis set is increased progressively.

It is necessary to transform the transition operator,

$$T_\ell = q_n R_n^\ell Y_{\ell 0}(\hat{\mathbf{R}}_n) + q_e R_1^\ell Y_{\ell 0}(\hat{\mathbf{R}}_1) + q_e R_2^\ell Y_{\ell 0}(\hat{\mathbf{R}}_2), \quad (42)$$

into the center-of-mass coordinates [13]. The transformed  $T_\ell$  with  $\ell = 1, 2$ , and 3 for the dipole, quadrupole, and octupole moments for a neutral helium are

$$T_1 = -\sum_{j=1}^2 r_j Y_{10}(\hat{\mathbf{r}}_j), \quad (43)$$

$$T_2 = -\left(1 - 2\frac{m_e}{M_T}\right) \sum_{j=1}^2 r_j^2 Y_{20}(\hat{\mathbf{r}}_j) + \sqrt{\frac{30}{\pi}} \frac{m_e}{M_T} r_1 r_2 (\hat{\mathbf{r}}_1 \otimes \hat{\mathbf{r}}_2)_0^{(2)}, \quad (44)$$

TABLE IV. Comparison  $C_3(M, \pm)$  and  $C_6(M, \pm)$  for the  ${}^4\text{He}(2^3S)$ - ${}^4\text{He}(2^3P)$  system.

Author	$C_3(0, \pm)$	$C_3(\pm 1, \pm)$	$C_6(0, \pm)$	$C_6(\pm 1, \pm)$
Venturi <i>et al.</i> [5]	$\pm 12.82044$	$\mp 6.41022$	2620.76	1846.60
Léonard <i>et al.</i> [2]	$\pm 12.810(6)$	$\mp 6.405(3)$		
This work	$\pm 12.8181751205(4)$	$\mp 6.4090875603(2)$	2641.5083(2)	1863.4726(2)

$$T_3 = - \left[ 1 - 3 \frac{m_e}{M_T} + 3 \left( \frac{m_e}{M_T} \right)^2 \right] \sum_{j=1}^2 r_j^3 Y_{30}(\hat{\mathbf{r}}_j) \\ + \frac{3}{2} \sqrt{\frac{35}{2\pi}} \left[ \frac{m_e}{M_T} - 3 \left( \frac{m_e}{M_T} \right)^2 \right] \{ r_1^2 r_2 ((\hat{\mathbf{r}}_1 \otimes \hat{\mathbf{r}}_1)^{(2)} \otimes \hat{\mathbf{r}}_2)_0^{(3)} \\ + r_2^2 r_1 ((\hat{\mathbf{r}}_2 \otimes \hat{\mathbf{r}}_2)^{(2)} \otimes \hat{\mathbf{r}}_1)_0^{(3)} \}. \quad (45)$$

It is noted that for the case of infinite nuclear mass, the above operators reduce to

$$T_\ell^\omega = - \sum_{j=1}^2 r_j^\ell Y_{\ell 0}(\hat{\mathbf{r}}_j). \quad (46)$$

For the finite nuclear mass case, however,  $T_\ell$  cannot be obtained by a simple mass scaling from  $T_\ell^\omega$ , except  $T_1$  which does not contain  $m_e/M_T$  explicitly for a neutral system.

Table I gives the convergence pattern of  $C_6(M, \pm)$  for the case of infinite nuclear mass as the sizes of the basis sets, including the two initial states and the four intermediate states, increase progressively. Table II lists the contributions to  $C_6(M, \pm)$  from three pairs of intermediate symmetries ( ${}^3P, {}^3S$ ), ( ${}^3P, (pp){}^3P$ ) doubly excited states, and ( ${}^3P, {}^3D$ ). Our final results for  $C_3(M, \pm)$ ,  $C_6(M, \pm)$ ,  $C_8(M, \pm)$ ,

$C_9(M, \pm)$ , and  $C_{10}(M, \pm)$  are presented in Table III. To our knowledge, no definitive calculations have been reported for the dispersion coefficients  $C_6(M, \pm)$ ,  $C_8(M, \pm)$ ,  $C_9(M, \pm)$ , and  $C_{10}(M, \pm)$ . Table IV is a comparison with the existing values of  $C_3(M, \pm)$  and  $C_6(M, \pm)$ . Our values for  $C_3(M, \pm)$  differ from those given in Refs. [2,5]. The origins of these discrepancies are uncertain. Drake [14] tabulated the oscillator strengths of helium, including  ${}^3\text{He}$  and  ${}^4\text{He}$ . In order to extract the square of the transition matrix element connecting  $2^3S$  and  $2^3P$ , besides some numerical constants, the tabulated value should be multiplied by  $1+2m_e/m_n$  and divided by the transition energy corrected for the finite nuclear mass. Our results are in perfect agreement with the values obtained by Drake. For  $C_6(M, \pm)$ , our values differ from the values used in the work of Venturi *et al.* [5] at the level of 0.8 and 0.9%, respectively, for  $C_6(0, \pm)$  and  $C_6(\pm 1, \pm)$ .

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