Long-range interactions for He(nS)–He($n'S$) and He(nS)–He($n'P$)

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For helium, long-range interaction coefficients C_3, C_6, C_8, C_9, and C_{10} for all S-S and S-P pairs of the energetically lowest five states ($1\,^1S$, $2\,^3S$, $2\,^1S$, $2\,^3P$, and $2\,^1P$) are calculated precisely using correlated wave functions in Hylleraas coordinates. Finite nuclear isotope mass effects are included.

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In our previous paper [1], we presented precise calculations of long-range interaction coefficients C_3, C_6, C_8, C_9, and C_{10} between two helium atoms in the $2\,^3S$ and $2\,^3P$ states and the finite nuclear mass effects for like isotopes. The purpose of this Brief Report is to extend our calculations to include interactions between all S-S and S-P states of the energetically lowest five states He($1\,^1S$), He($2\,^3S$), He($2\,^1S$), He($2\,^3P$), and He($2\,^1P$). These coefficients are useful in studying ultracold collisions between two helium atoms [2], as well as in serving as a benchmark for other computational methods.

For two like isotope helium atoms a and b, where one is in an S state and the other in an L state with the associate magnetic quantum number M, the zeroth-order wave function for the combined system ab can be written in the form [3]

$$\Psi^{(0)}(M,\beta)=\frac{C}{\sqrt{2}}[\Psi_{n_a}(\boldsymbol{\sigma})\Psi_{n_b}(LM;\boldsymbol{\rho})+\beta\Psi_{n_a}(\boldsymbol{\rho})\Psi_{n_b}(LM;\boldsymbol{\sigma})], \tag{1}$$

where Ψ_{n_a} is the S-state wave function, Ψ_{n_b} is the L-state wave function, $\boldsymbol{\sigma}$ and $\boldsymbol{\rho}$ represent the coordinates of the two helium atoms, C is the normalization factor, and β describes the symmetry due to the exchange of two atoms. If two atoms are both in the same S state, C is $\sqrt{2}$ and β is zero. If they are in different states, C is 1 and β is ± 1.

At large internuclear distances R, the Coulombic interaction operator [3] between two atoms can be expanded as an infinite series in powers of $1/R$

$$V_{\rm op}=\sum_{l=0}^{\infty}\sum_{L=0}^{\infty}\frac{V_{lL}}{R^{l+L+1}}, \tag{2}$$

where

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

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

$$T_{\mu}^{(l)}(\boldsymbol{\sigma})=\sum_i Q_i\sigma_i^l Y_{l\mu}(\hat{\boldsymbol{\sigma}}_i) \tag{4}$$

and

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

where Q_i and q_j are the charges on particles i and j. The coefficient K_{lL}^{μ} is

$$K_{lL}^{\mu}=\left[\binom{l+L}{l+\mu}\binom{l+L}{L+\mu}\right]^{1/2} \tag{6}$$

and $(l,L)=(2l+1)(2L+1)$.

For all S-S systems and for S-P systems with atoms in different spin symmetries, the first order of perturbation theory vanishes and the second-order perturbation in $V_{\rm op}$ gives rise to the long-range interaction potential

$$V=-\frac{C_6(M,\beta)}{R^6}-\frac{C_8(M,\beta)}{R^8}-\frac{C_{10}(M,\beta)}{R^{10}}-\cdots, \tag{7}$$

where $C_6(M,\beta)$, $C_8(M,\beta)$, and $C_{10}(M,\beta)$ are the dispersion coefficients. For resonant S-P systems, where two atoms are in the same spin state, the long-range interaction potential is

$$V=-\frac{C_3(M,\beta)}{R^3}-\frac{C_6(M,\beta)}{R^6}-\frac{C_8(M,\beta)}{R^8}-\frac{C_9(M,\beta)}{R^9}-\frac{C_{10}(M,\beta)}{R^{10}}-\cdots, \tag{8}$$

where $C_3(M,\beta)$ is from the first-order energy correction, $C_6(M,\beta)$, $C_8(M,\beta)$, and $C_{10}(M,\beta)$ are from the second-order energy correction, and $C_9(M,\beta)$ is from the third-order energy correction [1]. The detailed expressions for C_n and their evaluation in Hylleraas coordinates can be found in Ref. [1].

Tables I and II present dispersion coefficients C_6, C_8, and C_{10} for all six He($n\,^{\lambda}S$)–He($n'\,^{\lambda'}S$) systems with n and $n'=1,2$ and λ and $\lambda'=1,3$. In Table I, we also include the revised values of the dispersion coefficients [3,4] for He($1\,^1S$)–He($1\,^1S$), He($2\,^1S$)–He($2\,^1S$), and He($2\,^3S$)–He($2\,^3S$) for the case of infinite nuclear mass, with some improvement, particularly for C_6. Bishop and Pipin [5] calculated the dispersion coefficients for the system $^{\infty}$He($1\,^1S$)–$^{\infty}$He($2\,^3S$). Their results in atomic units are $C_6=29.082914$, $C_8=1700.2700$, and $C_{10}=136380.30$, which are in agreement with ours at the level of 1, 45, and 10 ppm respectively.

TABLE I. $C_6(0,\beta)$, $C_8(0,\beta)$, and $C_{10}(0,\beta)$, in atomic units, for He($n\,^{\lambda}S$)–He($n'\,^{\lambda'}S$) ($n,n'=1,2$ and $\lambda,\lambda'=1,3$).

System	$C_6(0,\beta)$	$C_8(0,\beta)$	$C_{10}(0,\beta)$
$^{\infty}$He(1 ^1S)–$^{\infty}$He(1 ^1S)	1.460977837725(2)	14.11785737(2)	183.691075(1)
^{4}He(1 ^1S)–^{4}He(1 ^1S)	1.462122853192(3)	14.12578806(2)	183.781468(1)
^{3}He(1 ^1S)–^{3}He(1 ^1S)	1.462497669977(2)	14.12838383(2)	183.811057(2)
$^{\infty}$He(2 ^1S)–$^{\infty}$He(2 ^1S)	11241.04684(4)	817250.26(2)	108167575(3)
^{4}He(2 ^{1}S)–^{4}He(2 ^{1}S)	11247.73927(1)	817626.25(2)	108208732(3)
^{3}He(2 ^1S)–^{3}He(2 ^1S)	11249.92975(4)	817749.27(1)	108222197(1)
$^{\infty}$He(2 ^3S)–$^{\infty}$He(2 ^3S)	3276.67964(5)	210566.54(3)	21786759(1)
^{4}He(2 ^3S)–^{4}He(2 ^3S)	3279.45846(2)	210667.78(1)	21794920(2)
^{3}He(2 ^3S)–^{3}He(2 ^3S)	3280.36825(3)	210700.93(2)	21797593(3)
$^{\infty}$He(1 ^1S)–$^{\infty}$He(2 ^3S)	29.082956(2)	1700.3495(4)	136381.56(2)
^{4}He(1 ^1S)–^{4}He(2 ^3S)	29.104446(2)	1701.1618(1)	136444.57(3)
^{3}He(1 ^1S)–^{3}He(2 ^3S)	29.111482(3)	1701.4278(1)	136465.17(1)
$^{\infty}$He(2 ^1S)–$^{\infty}$He(2 ^3S)	5817.46249(2)	417776.48(2)	49889993(3)
^{4}He(2 ^1S)–^{4}He(2 ^3S)	5821.97285(4)	417978.46(2)	49909416(2)
^{3}He(2 ^1S)–^{3}He(2 ^3S)	5823.44933(4)	418044.56(2)	49915774(4)

Table III shows the contributions to $C_6(M,\beta)$ from different symmetries of intermediate states for He($n\,^{\lambda}S$)–He($n'\,^{\lambda'}P$), except for He(1 ^1S)–He(2 ^3P) and He(2 ^3S)–He(2 ^3P), which have been reported in Refs. [6,1], respectively. From this table, one can see that the contributions from doubly excited $(pp)P$ configurations are much smaller than the contributions from singly excited S and D configurations. It is also interesting to note that only the contributions to $C_6(M,\pm)$ from the symmetries $(^1P,^3S)$ are negative for $^{\infty}$He(2 ^1S)–$^{\infty}$He(2 ^3P). This is because the dominant transitions 2 ^1S–2 ^1P and 2 ^3P–2 ^3S make large negative contributions −10935.32650 and −2733.831626 for $C_6(0,\pm)$ and $C_6(\pm,\pm)$, respectively. For the symmetries $(^3P,^1S)$ for $^{\infty}$He(2 ^3S)–$^{\infty}$He(2 ^1P), the dominant transitions 2 ^3S–2 ^3P and 2 ^1P–2 ^1S contribute 10935.32650 and 2733.831626 for $C_6(0,\pm)$ and $C_6(\pm,\pm)$, respectively. The mainly negative contributions are from the pair of transitions 2 ^3S–2 ^3P and 2^1P–1 ^1S whose values −6.150732811 and −1.537683203 for $C_6(0,\pm)$ and $C_6(\pm,\pm)$, respectively, are much smaller than those from the corresponding positive dominant transitions.

Table IV lists $C_3(M,\pm)$, $C_6(M,\pm)$, $C_8(M,\pm)$, $C_9(M,\pm)$, and $C_{10}(M,\pm)$ for the He($n\,^{\lambda}S$)–He($n'\,^{\lambda'}P$) systems except for the He(2 ^3S)–He(2 ^3P) system [1]. For $C_3(M,\pm)$, our results agree with Drake's values [7]. To our knowledge, there are no other published calculations on the dispersion coefficients for the He($n\,^{\lambda}S$)–He($n'\,^{\lambda'}P$) system.

TABLE II. $C_6(0,\pm)$, $C_8(0,\pm)$, and $C_{10}(0,\pm)$, in atomic units, for He(1 ^1S)–He(2 ^1S).

C_n	$^{\infty}$He-$^{\infty}$He	^{4}He-^{4}He	^{3}He-^{3}He
$C_6(0,+)$	44.750434(3)	44.783606(3)	44.794465(4)
$C_6(0,-)$	38.932199(1)	38.961030(3)	38.970467(1)
$C_8(0,+)$	3406.535(3)	3408.196(2)	3408.739(1)
$C_8(0,-)$	3214.354(3)	3215.913(2)	3216.425(3)
$C_{10}(0,+)$	353414.63(3)	353584.78(1)	353640.47(1)
$C_{10}(0,-)$	345572.365(3)	345738.985(3)	345793.517(3)

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TABLE III. Contributions to $C_6(M,\pm)$, in atomic units, for $^{\infty}$He($n\,^{\lambda}S$)–$^{\infty}$He($n'\,^{\lambda}P$) from different symmetries of intermediate states.

$^{\infty}$He(1 ^1S)–$^{\infty}$He(2 ^1P)	$C_6(0,\pm)$	$C_6(\pm,\pm)$
$(^1P,^1S)$	29.80734050(1)	7.451835124(4)
$(^1P,(pp)^1P)$	0.054285059(2)	0.135712646(2)
$(^1P,^1D)$	29.011666(2)	25.055529(1)
$^{\infty}$He(2 ^1S)–$^{\infty}$He(2 ^1P)	$C_6(0,\pm)$	$C_6(\pm,\pm)$
$(^1P,^1S)$	1296.69(1)	324.176(3)
$(^1P,(pp)^1P)$	1.237417(2)	3.093539(1)
$(^1P,^1D)$	4331.449(1)	3740.798(1)
$^{\infty}$He(2 ^1S)–$^{\infty}$He(2 ^3P)	$C_6(0,\pm)$	$C_6(\pm,\pm)$
$(^1P,^3S)$	−9439.93818(1)	−2359.98454(2)
$(^1P,(pp)^3P)$	1.8805763(3)	4.7014403(3)
$(^1P,^3D)$	3199.1416(2)	2762.89489(1)
$^{\infty}$He(2 ^3S)–$^{\infty}$He(2 ^1P)	$C_6(0,\pm)$	$C_6(\pm,\pm)$
$(^3P,^1S)$	11520.93(2)	2880.22(1)
$(^3P,(pp)^1P)$	0.8674943(1)	2.1687357(2)
$(^3P,^1D)$	2602.9197(1)	2247.9762(2)

TABLE IV. $C_3(M,\pm)$, $C_6(M,\pm)$, $C_8(M,\pm)$, $C_9(M,\pm)$, and $C_{10}(M,\pm)$, in atomic units, for He($n\,^{\lambda}S$)–He($n'\,^{\lambda'}P$).

C_n	$^{\infty}$He($1\,^1S$)–$^{\infty}$He($2\,^1P$)	^{4}He($1\,^1S$)–^{4}He($2\,^1P$)	^{3}He($1\,^1S$)–^{3}He($2\,^1P$)
$C_3(0,\pm)$	±0.3541112056(4)	±0.3541530610(1)	±0.3541667599(1)
$C_3(\pm,\pm)$	∓0.1770556028(2)	∓0.1770765307(3)	∓0.17708337999(6)
$C_6(0,\pm)$	58.873293(3)	58.923259(2)	58.939615(1)
$C_6(\pm,\pm)$	32.643077(1)	32.670985(3)	32.680118(1)
$C_8(0,+)$	9693.3127(2)	9700.5496(3)	9702.9182(3)
$C_8(0,-)$	10048.0818(1)	10055.4826(3)	10057.9047(2)
$C_8(\pm,+)$	396.5492(2)	396.4958(2)	396.4782(2)
$C_8(\pm,-)$	357.4777(2)	357.4055(3)	357.3817(2)
$C_9(0,\pm)$	∓271.24449(2)	∓271.55655(3)	∓271.65869(1)
$C_9(\pm,\pm)$	±76.76195(2)	±76.85062(2)	±76.87965(2)
$C_{10}(0,+)$	1235282.3(3)	1236209.5(3)	1236512.8(1)
$C_{10}(0,-)$	1252541.6(3)	1253475.7(2)	1253781.5(2)
$C_{10}(\pm,+)$	20803.39(2)	20815.53(3)	20819.48(1)
$C_{10}(\pm,-)$	19268.36(2)	19279.86(3)	19283.62(2)
	$^{\infty}$He($1\,^1S$)–$^{\infty}$He($2\,^3P$)	^{4}He($1\,^1S$)–^{4}He($2\,^3P$)	^{3}He($1\,^1S$)–^{3}He($2\,^3P$)
$C_6(0,\pm)$	47.72588676(2)	47.75234975(3)	47.76101019(2)
$C_6(\pm,\pm)$	26.70867089(1)	26.72351542(2)	26.72837355(2)
$C_8(0,\pm)$	7129.97(1)	7131.59(1)	7132.13(2)
$C_8(\pm,\pm)$	281.55(2)	281.38(1)	281.33(2)
$C_{10}(0,\pm)$	801678.7(1)	801717.2(3)	801729.6(2)
$C_{10}(\pm,\pm)$	13105.8(1)	13104.6(2)	13103.9(1)
	$^{\infty}$He($2\,^1S$)–$^{\infty}$He($2\,^1P$)	^{4}He($2\,^1S$)–^{4}He($2\,^1P$)	^{3}He($2\,^1S$)–^{3}He($2\,^1P$)
$C_3(0,\pm)$	±17.0096686055(3)	±17.0157415780(8)	±17.0177287170(5)
$C_3(\pm,\pm)$	∓8.5048343028(2)	∓8.5078707890(4)	∓8.5088643585(3)
$C_6(0,\pm)$	5629.39(1)	5634.35(5)	5635.95(4)
$C_6(\pm,\pm)$	4068.07(1)	4071.68(1)	4072.87(2)
$C_8(0,+)$	679008(3)	679615(3)	679815(4)
$C_8(0,-)$	4600179(4)	4603085(5)	4604034(3)
$C_8(\pm,+)$	492965(4)	493226(3)	493312(3)
$C_8(\pm,-)$	419817(3)	419939(1)	419985(4)
$C_9(0,\pm)$	±1719978(5)	±1722188(5)	±1722914(3)
$C_9(\pm,\pm)$	∓366261.1(5)	∓366698.1(2)	∓366841.3(4)
$C_{10}(0,+)$	$6.27699(1)\times10^7$	$6.28316(2)\times10^7$	$6.28518(2)\times10^7$
$C_{10}(0,-)$	$6.031831(1)\times10^8$	$6.035509(1)\times10^8$	$6.036714(2)\times10^8$
$C_{10}(\pm,+)$	$5.791649(1)\times10^7$	$5.794589(3)\times10^7$	$5.795549(2)\times10^7$
$C_{10}(\pm,-)$	$1.119933(3)\times10^7$	$1.120226(3)\times10^7$	$1.120319(1)\times10^7$
	$^{\infty}$He($2\,^1S$)–$^{\infty}$He($2\,^3P$)	^{4}He($2\,^1S$)–^{4}He($2\,^3P$)	^{3}He($2\,^1S$)–^{3}He($2\,^3P$)
$C_6(0,\pm)$	−6238.9163(2)	−6253.30080(2)	−6258.01373(1)
$C_6(\pm,\pm)$	407.611780(1)	404.83595(2)	403.92612(2)
$C_8(0,\pm)$	1962689(1)	1962880(1)	1962943(1)
$C_8(\pm,\pm)$	389203.6(2)	389217.5(3)	389221.9(1)
$C_{10}(0,\pm)$	$2.2430065(3)\times10^8$	$2.2429754(5)\times10^8$	$2.2429647(2)\times10^8$
$C_{10}(\pm,\pm)$	$2.828207(2)\times10^7$	$2.828419(1)\times10^7$	$2.828489(2)\times10^7$
	$^{\infty}$He($2\,^3S$)–$^{\infty}$He($2\,^1P$)	^{4}He($2\,^3S$)–^{4}He($2\,^1P$)	^{3}He($2\,^3S$)–^{3}He($2\,^1P$)
$C_6(0,\pm)$	14124.71(2)	14143.81(1)	14150.06(2)
$C_6(\pm,\pm)$	5130.37(1)	5136.64(2)	5138.71(1)
$C_8(0,\pm)$	1288203(1)	1289227(1)	1289563(1)
$C_8(\pm,\pm)$	162321(1)	162400(1)	162424(2)
$C_{10}(0,\pm)$	$1.640216(1)\times10^8$	$1.6413357(2)\times10^8$	$1.6417021(2)\times10^8$
$C_{10}(\pm,\pm)$	$1.161798(1)\times10^7$	$1.162275(2)\times10^7$	$1.162431(2)\times10^7$

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