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Variational calculations of dispersion coefficients for interactions among H, He, and Li atoms

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The dispersion coefficients C_6, C_8, and C_{10} for the interactions among H, He, and Li are calculated using variational wave functions in Hylleraas basis sets with multiple exponential scale factors. With these highly correlated wave functions, significant improvements are made upon previous calculations and our results provide definitive values for these coefficients. [S1050-2947(96)03310-0]

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I. INTRODUCTION

At large separations R, the interaction potential between two neutral atoms can be expressed in terms of inverse powers of R, with the leading term R^{-6} [1,2]. The nature of the long-range interaction can be described by the mutual perturbations of instantaneous multipoles of individual atoms. The coefficient of the R^{-6} term comes from an instantaneous dipole-dipole interaction and the coefficient of the R^{-8} term from an instantaneous dipole-quadrupole interaction.

The precise evaluation of the dispersion coefficients between atoms is computationally challenging, because it requires a summation over all intermediate states, including the continuum. In actual calculations, it is therefore essential to have an adequate representation of the whole spectrum of the Hamiltonian. For atomic systems with more than one electron the central problem is the inclusion of electron-electron correlations.

Recently, significant progress [3,4] has been made in variational calculations for the helium and lithium atoms using double and multiple basis sets in Hylleraas coordinates. The nonrelativistic energies for helium have been obtained to better than one part in 10^{16} for the entire singly excited spectrum, whereas the nonrelativistic energies for the low-lying states of lithium are accurate to a few parts in 10^{11}–10^{12} [5]. We have also performed a high precision calculation for the lithium $2\,^2S \rightarrow 2\,^2P$ oscillator strength [6], which has been a subject of controversy for many years. Although there have been many calculations for the dispersion coefficients among H, He, and Li (see, for example, [2,7–11]), the results involving Li vary over a considerable range.

Due to the recent progress of ultracold collisions in both theory and experiment [12], precise forms of long-range interaction potentials between various atoms become very important. The purpose of this paper is to present the results of variational calculations in Hylleraas basis sets using multiple nonlinear parameters. The use of our highly correlated wave functions will improve upon previous calculations and provide more definitive values for the dispersion coefficients.

The theory of long-range forces is outlined in Sec. II. The structures of the basis sets for one, two, and three electron atomic systems are presented in Sec. III. Our final results are tabulated and comparisons are made with the various previous calculations. In the Appendix, a derivation is given of the dispersion coefficients for the Li(S)–Li(P) system.

II. FORMULATION

A. Ground-state dispersion coefficients

In this section, we concentrate on interactions between atoms in their ground states. Using second-order perturbation theory, the long-range part of interaction between two atoms a and b in their ground states can be expanded in terms of a series of inverse powers of the separation R [1,2]

$$V_{\rm ab} = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} - \cdots, \tag{1}$$

where the coefficients C_6, C_8, and C_{10} are

$$C_6 = \frac{3}{\pi} G_{ab}(1,1), \tag{2}$$

$$C_8 = \frac{15}{2\pi} G_{ab}(1,2) + \frac{15}{2\pi} G_{ab}(2,1), \tag{3}$$

$$C_{10} = \frac{14}{\pi} G_{ab}(1,3) + \frac{14}{\pi} G_{ab}(3,1) + \frac{35}{\pi} G_{ab}(2,2), \tag{4}$$

where

$$G_{ab}(l_a, l_b) = \int_0^\infty \alpha_{l_a}^{a}(i\omega)\, \alpha_{l_b}^{b}(i\omega)\, d\omega. \tag{5}$$

In Eq. (5), $\alpha_{l_a}^{\rm a}(i\omega)$ is the dynamic $2^{l_{\rm a}}$ polarizability for atom a at imaginary frequency $i\omega$. The dynamic polarizability can be expressed in terms of a sum over all intermediate states, including the continuum (in atomic units throughout):

$$\alpha_l(\omega) = \sum_n \frac{f_{n0}^{(l)}}{E_{n0}^2 - \omega^2} \tag{6}$$

with the 2^l-pole oscillator strength $f_{n0}^{(l)}$ being defined by

$$f_{n0}^{(l)} = \frac{8\pi}{2l+1} E_{n0} \left| \left\langle \Psi_0 \left| \sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) \right| \Psi_n \right\rangle \right|^2, \tag{7}$$

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where $E_{n0}=E_n-E_0$, the sum i runs over all the electrons in the atom, Ψ_0 is the ground-state wave function, E_0 is the corresponding ground state energy, and Ψ_n is the nth intermediate eigenfunction with the associated eigenvalue E_n. An oscillator strength $\overline{f_{n0}^{(l)}}$, which is independent of magnetic quantum number m is obtained by averaging over the initial-state orientation degeneracy and summing over the final-state degeneracy. It is convenient to introduce reduced matrix elements through the Wigner-Eckart theorem [13]

$$\left\langle \gamma' L' M' \left| \sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) \right| \gamma L M \right\rangle = (-1)^{L'-M'} \begin{pmatrix} L' & l & L \\ -M' & m & M \end{pmatrix} \times \left\langle \gamma' L' \left\| \sum_i r_i^l Y_l(\hat{\mathbf{r}}_i) \right\| \gamma L \right\rangle . \tag{8}$$

With the aid of a sum rule for the 3-j symbols, the oscillator strength can be written

$$\overline{f_{n0}^{(l)}} = \frac{8\pi}{(2l+1)^2(2L_0+1)} E_{n0} \left| \left\langle \Psi_0 \left\| \sum_i r_i^l Y_l(\hat{\mathbf{r}}_i) \right\| \Psi_n \right\rangle \right|^2 , \tag{9}$$

where L_0 is the total angular momentum for the initial state.

Using the identity

$$\frac{2}{\pi}\int_0^\infty \frac{d\omega}{(a^2+\omega^2)(b^2+\omega^2)} = \frac{1}{ab(a+b)}, \quad a,b>0 \tag{10}$$

we can recast Eq. (5) into the equivalent form

$$G_{ab}(l_a,l_b) = \frac{\pi}{2} \sum_{nn'} \frac{f_{n0}^{(l_a)} f_{n'0}^{(l_b)}}{E_{n0}^a E_{n'0}^b (E_{n0}^a + E_{n'0}^b)}, \tag{11}$$

where $E_{n0}^{\mathrm{i}}=E_n^{\mathrm{i}}-E_0^{\mathrm{i}}$ is the excitation energy for atom i and is always positive for the atoms in the ground state. The procedure for evaluating $G_{ab}(l_a,l_b)$ is to diagonalize the Hamiltonian in a basis set and sum over all intermediate states directly according to Eq. (11), and a convergence study can be done by increasing the size of the basis set progressively.

The long-range part of the interaction between three ground-state atoms is not exactly equal to the interaction energies taken in pairs. There is a nonadditive term which comes from the third-order perturbation. The leading terms in the expression for the dispersion energy of the three-atom system are [1,2]

$$V_{\mathrm{abc}} = -\frac{C_6^{ab}}{r_{ab}^6} - \frac{C_6^{bc}}{r_{bc}^6} - \frac{C_6^{ca}}{r_{ca}^6} - \frac{\nu_{abc}(3\cos\theta_a\cos\theta_b\cos\theta_c+1)}{(r_{\mathrm{ab}}r_{\mathrm{bc}}r_{\mathrm{ca}})^3}, \tag{12}$$

where θ_a, θ_b, and θ_c are the internal angles of the triangle formed by r_{ab}, r_{bc} and r_{ca}, and ν_{abc} is the triple-dipole constant defined by

$$\nu_{abc} = \frac{3}{\pi}\int_0^\infty \alpha_1^{\mathrm{a}}(i\omega)\alpha_1^{\mathrm{b}}(i\omega)\alpha_1^{\mathrm{c}}(i\omega)d\omega. \tag{13}$$

B. Excited-state dispersion coefficients

For two like atoms that are not both in their ground states, the perturbation theory for calculating the dispersion coefficients was given by Marinescu and Dalgarno [10]. They worked out all the details for evaluating the dispersion coefficients of alkali-metal dimers in different excited states within a one-electron model potential formalism. In this work, we examine the important case when one lithium atom is in the $2\,^2S$ ground state and the other lithium atom is in the $2\,^2P$ state. A detailed derivation for many-electron systems is given in the Appendix.

The zero-order wave function for the Li(S)-Li(P) system can be written as a symmetrized product of two individual atomic wave functions

$$\Psi^{(0)} = \frac{1}{\sqrt{2}}[\Psi_a(L_1M_1;\mathbf{r})\Psi_b(L_2M_2;\boldsymbol{\rho}) + \beta\Psi_a(L_1M_1;\boldsymbol{\rho})\Psi_b(L_2M_2;\mathbf{r})], \tag{14}$$

where $\mathbf{r}$ and $\boldsymbol{\rho}$ represent all the internal coordinates for the two atoms, respectively, L_1 and L_2 are their total orbital angular momenta, M_1 and M_2 are the associated magnetic quantum numbers, and $\beta=\pm1$ describes the symmetry due to the Pauli exclusion principle. Following [10], first-order perturbation theory yields the interaction energy

$$V^{(1)}(L_2M_2;\beta) = -\frac{C_{2L_2+1}^{M_2\beta}}{R^{2L_2+1}}, \tag{15}$$

where

$$C_{2L_2+1}^{M_2\beta} = \beta(-1)^{1+L_2+M_2}\frac{4\pi}{(2L_2+1)^2}\begin{pmatrix} 2L_2 \\ L_2+M_2 \end{pmatrix} \times \left| \left\langle \Psi_{\mathrm{a}}(0;\mathbf{r}) \left\| \sum_i r_i^{L_2} Y_{L_2}(\hat{\mathbf{r}}_i) \right\| \Psi_{\mathrm{b}}(L_2;\mathbf{r}) \right\rangle \right|^2 . \tag{16}$$

The first-order energy correction is proportional to β. Therefore, for two unlike atoms ($\beta=0$) in the asymptotic region where overlap between two atoms can be neglected, there is no first-order correction to the interaction. For two like atoms, however, there is a first-order correction to the interaction energy as long as two atoms are in different angular momentum states. For the Li(S)-Li(P) system, the interaction is proportional to R^{-3}. The interaction between two ground-state atoms is always attractive [see Eq. (1)] but the interaction between two like atoms in different angular momentum states is equally likely to be attractive and repulsive.

The leading energy correction obtained from the second-order perturbation theory for the Li(S)-Li(P) system is

$$V^{(2)} = -\frac{C_6^{M_2}}{R^6}, \tag{17}$$

where

$$C_6^{M_2} = \sum_{st} \frac{\Omega_{st}}{E_{st}^{(0)}-E^{(0)}} \tag{18}$$

TABLE I. The algebraic coefficients $G(1,1,1,\lambda,1,M_2)$.

	$\lambda=0$	$\lambda=1$	$\lambda=2$
$M_2=0$	$\frac{64}{81}\pi^2$	$\frac{16}{81}\pi^2$	$\frac{176}{405}\pi^2$
$M_2=\pm 1$	$\frac{16}{81}\pi^2$	$\frac{40}{81}\pi^2$	$\frac{152}{405}\pi^2$

TABLE II. Values of the static polarizabilities $\alpha_1(0)$, $\alpha_2(0)$, and $\alpha_3(0)$ for the ground-state H, He, and Li atoms.

System	$\alpha_1(0)$	$\alpha_2(0)$	$\alpha_3(0)$
H	4.5	15	131.25
He	1.383 192 174 40(5)	2.445 083 101(2)	10.620 328 6(2)
Li	164.111(2)	1423.266(5)	39 650.49(8)

with

$$\Omega_{st}=\left|\left\langle \Psi_{\mathrm{a}}(0;\mathbf{r})\left\| \sum_i r_i Y_1(\hat{\mathbf{r}}_i)\right\| \chi(1;\mathbf{r})\right\rangle\right|^2$$

$$\times\sum_\lambda G(1,1,1,\lambda,1,M_2)$$

$$\times\left|\left\langle \Psi_{\mathrm{b}}(1;\boldsymbol{\rho})\left\| \sum_j \rho_j Y_1(\hat{\boldsymbol{\rho}}_j)\right\| \omega(\lambda;\boldsymbol{\rho})\right\rangle\right|^2. \quad (19)$$

In Eq. (18), the summation should exclude one term that gives rise to $E_{st}^{(0)}=E^{(0)}$. Note that $C_6^{M_2}$ is independent of β. The values of G are listed in Table I.

It should be noted that the terms with $\lambda=1$ in Eq. (19), which corresponds to transitions between even parity states P^e and odd parity state P^o, are missing in one-electron model potential methods [10]. The dominant contribution comes from the radiative transition between the lowest doubly excited doublet state $1s2p2p\,^2P^e$, which is stable against autoionization [14], to the singly excited doublet state $1s^22p\,^2P^o$. The contribution of the $\lambda=1$ term to $C_6^{M_2}$ is $0.980\,82(5)$ for $M_2=\pm 1$, and $0.392\,32(2)$ for $M_2=0$.

III. CALCULATIONS AND RESULTS

For the hydrogen atom, the following Sturmian basis set [15] is used to diagonalize the Hamiltonian:

$$\{r^l e^{-\beta r/2} L_n^{(2l+2)}(\beta r)\}, \quad (20)$$

where $L_n^{(2l+2)}(\beta r)$ is the generalized Laguerre polynomial and the parameter β is chosen to be $\beta=2/(l+1)$. This basis set has proven to be numerically stable as the size of the basis set is enlarged.

For the helium atom, the basis set is constructed using Hylleraas coordinates [16]

$$\{\chi_{ijk}=r_1^i r_2^j r_{12}^k e^{-\alpha r_1-\beta r_2}\}, \quad (21)$$

and the wave functions are expanded from doubled basis sets. The explicit form for the wave function is

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\sum_{ijk}[a_{ijk}^{(1)}\chi_{ijk}(\alpha_1,\beta_1)+a_{ijk}^{(2)}\chi_{ijk}(\alpha_2,\beta_2)]$$

$$\pm\,\text{exchange}, \quad (22)$$

and $i+j+k\leqslant\Omega$. A complete optimization is then performed with respect to the two sets of nonlinear parameters α_1,β_1 and α_2,β_2. The screened hydrogenic wave function is also included explicitly in the basis set. These techniques yield much improved convergence relative to single basis set calculations.

For the lithium atom, the basis set is also constructed in Hylleraas coordinates [4]

$$\{\phi_{t,\mu_t}(\alpha_t,\beta_t,\gamma_t)=r_1^{j_1}r_2^{j_2}r_3^{j_3}r_{12}^{j_{12}}r_{23}^{j_{23}}r_{31}^{j_{31}}\,e^{-\alpha_t r_1-\beta_t r_2-\gamma_t r_3}\}, \quad (23)$$

where μ_t denotes a sextuple of integer powers j_1, j_2, j_3, j_{12}, j_{23}, and j_{31}, index t labels different sets of nonlinear parameters α_t, β_t, and γ_t. Except for some truncations, all terms are included such that

$$j_1+j_2+j_3+j_{12}+j_{23}+j_{31}\leqslant\Omega. \quad (24)$$

The wave function is expanded from the multiple basis sets

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\mathcal{A}\sum_t\sum_{\mu_t} a_{t,\mu_t}\phi_{t,\mu_t}(\alpha_t,\beta_t,\gamma_t)$$

$$\times(\text{angular function})(\text{spin function}). \quad (25)$$

A similar optimization is also performed with respect to all the nonlinear parameters.

Table II contains the values of the static polarizabilities $\alpha_1(0)$, $\alpha_2(0)$, and $\alpha_3(0)$ for H, He, and Li in their ground states. Tables III and IV present the comparison with selected previous calculations for He and Li. Using the Stur-

TABLE III. Comparison of static polarizabilities $\alpha_1(0)$, $\alpha_2(0)$, and $\alpha_3(0)$ for He$(1\,^1S)$.

Author (year)	Reference	$\alpha_1(0)$	$\alpha_2(0)$	$\alpha_3(0)$
Luyckx *et al.* (1977)	[17]	1.379	2.430	10.48
Thakkar (1981)	[18]	1.383 12	2.443 44	10.614 4
Bishop and Pipin (1993)	[7]	1.383 192	2.445 083	10.620 360
Caffarel *et al.* (1993)	[19]	1.382 7	2.406 6	10.36
Jamieson *et al.* (1995)	[9]	1.383 192		
Chen (1995)	[20]	1.383 32		
Chen and Chung (1996)	[11]	1.383 27	2.445 66	10.625 2
This work		1.383 192 174 40(5)	2.445 083 101(2)	10.620 328 6(2)

TABLE IV. Comparison of static polarizabilities $\alpha_1(0)$, $\alpha_2(0)$, and $\alpha_3(0)$ for Li$(2\,^2S)$.

Author (year)	Reference	$\alpha_1(0)$	$\alpha_2(0)$	$\alpha_3(0)$
Maeder and Kutzelnigg (1979)	[23]	164.3	1383	36 795
Muszyńska *et al.* (1982)	[24]	163.8		
Pipin and Woźnicki (1983)	[25]	163.9		
Pouchan and Bishop (1984)	[26]	164(2)		
Müller *et al.* (1984)	[27]	163.7		
Knowles and Meath (1986)	[28]	165.8	1486	36 495
Maroulis and Thakkar (1989)	[29]	164.5	1428	
Pipin and Bishop (1992)	[22]	164.1	1423	
Ponomarenko and Shestakov (1993)	[30]	165.2		
Marinescu *et al.* (1994)	[8]		1424	39 688
Wang and Chung (1994)	[31]	164.08		
Mérawa *et al.* (1994)	[32]	164.8	1430	
Kassimi and Thakkar (1994)	[33]	164.2(1)		
Laughlin (1995)	[34]	163.91		
This work		164.111(2)	1 423.266(5)	39 650.49(8)
Experiment (1974)	[35]	164.0(3.4)		

mian basis sets containing up to 70 terms yields the well-known exact results for the H atom. For He, the largest size of a basis set for the ground state is 504. For the intermediate states, the largest sizes of basis sets are 728, 733, and 792, respectively for the P, D, and F symmetries. Table III shows that our value for $\alpha_1(0)$ is in perfect agreement with the best previous results of Bishop and Pipin [7] and Jamieson, Drake and Dalgarno [9] within the first seven digits. However, our value of $\alpha_1(0)$, as well as $\alpha_2(0)$ and $\alpha_3(0)$, has converged to several more significant figures, as indicated by the extrapolation uncertainty in parentheses. For Li, with the fixed size of the basis set 919 for the ground state, Table V contains the convergence studies of $\alpha_1(0)$ in both length and velocity forms, as the number of terms for the intermediate P symmetry is progressively increased. As a further numerical check, we calculated $\alpha_1(0)$ for the Li atom by solving an inhomogeneous equation, using the Dalgarno-Lewis method [21] as follows:

$$\alpha_l(0) = -\frac{8\pi}{2l+1}\left\langle \Psi(2\,^2S)\left|\sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i)\right|\Psi_1\right\rangle, \tag{26}$$

where Ψ_1 satisfies the inhomogeneous equation

$$(H_0 - E_0)\Psi_1 + \left[\sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) - E_1\right]\Psi(2\,^2S) = 0. \tag{27}$$

In the above equation, H_0 is the unperturbed Li Hamiltonian, E_0 is the Li ground-state energy, and

$$E_1 = \left\langle \Psi(2\,^2S)\left|\sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i)\right|\Psi(2\,^2S)\right\rangle. \tag{28}$$

Equation (27) is solved variationally by expanding Ψ_1 in terms of a Hylleraas basis set. The two procedures are equivalent. Using basis sets up to 2136, $\alpha_1(0)$ converges monotonically to 164.109 8. Based on these convergence studies, our final extrapolated value of $\alpha_1(0)$ is 164.111(2). We have also done similar convergence studies for $\alpha_2(0)$ and $\alpha_3(0)$. Our results for $\alpha_1(0)$ and $\alpha_2(0)$ are in good accord with the results of Pipin and Bishop [22]. The model potential results of Marinescu, Sadeghpour, and Dalgarno [8] agree with the present calculations at the 0.05% and 0.1% levels for $\alpha_2(0)$ and $\alpha_3(0)$, respectively.

Table VI shows our values of the two-body dispersion coefficients C_6, C_8, and C_{10} for the ground state H, He, and Li atoms. For the H-H case, these coefficients can be calculated to arbitrarily high precision. Our value of C_6 is in complete agreement with the value of Margoliash and Meath [36]. Comparisons with the previous calculations for He$(1\,^1S)$-He$(1\,^1S)$ and Li$(2\,^2S)$-Li$(2\,^2S)$ are listed in Tables VII and VIII.

For the He-He case, our C_6 and C_8 are in excellent agreement with the results of Bishop and Pipin [7], but more pre-

TABLE V. Convergence of Li$(2\,^2S)$ $\alpha_1(0)$ and Li$(2\,^2S)$-Li$(2\,^2S)$ C_6 in length and velocity forms.

No. of terms	$\alpha_1(0)$ (length)	$\alpha_1(0)$ (velocity)	C_6 (length)	C_6 (velocity)
56	164.002	165.218	1389.76	1409.91
139	164.048	164.201	1391.21	1393.56
307	164.082	164.131	1392.37	1393.08
623	164.095	164.107	1392.80	1392.92
1175	164.105	164.108	1393.17	1393.17
1846	164.107	164.108	1393.23	1393.21

TABLE VI. Values of C_6, C_8, and C_{10} for two ground-state atoms.

System	C_6	C_8	C_{10}
H-H	6.499 026 705 405 839 313 13	124.399 083 583 622 343 609 59	3 285.828 414 967 421 697 872 5
He-He	1.460 977 837 68(5)	14.117 857 340(5)	183.691 070 5(7)
Li-Li	1 393.39(16)	83 425.8(4.2)	$73\,721(1)\times 10^2$
H-He	2.821 343 915 28(6)	41.836 376 162(8)	871.540 471(1)
He-Li	22.507(1)	1 083.16(5)	72 602.1(1)
Li-H	66.536(5)	3 279.99(2)	223 016.6(5)

cise by about three orders of magnitude. As for C_{10}, a small disagreement of about 1 ppm exists. The value of Jamieson Drake, and Dalgarno [9] for C_6 also agrees with our value.

For the Li-Li case, convergence studies for C_6 in both length and velocity forms are listed in Table V. The agreement between the two forms is satisfactory. From Table VIII, it can be seen that the result of Stacey and Dalgarno [41] for C_6 is in close agreement with the present calculation. The model potential results of Marinescu, Sagedhpour, and Dalgarno [8] for C_6, C_8, and C_{10} differ from our calculations at the 0.1–0.3 % level.

Table IX lists the triple-dipole constants $\nu_{\rm abc}$ for the combinations among three ground-state atoms H, He, and Li, together with the previous values of Stacey and Dalgarno [41]. The overall agreement is about 1%.

Finally, Tables X and XI list values of C_3 and C_6 and a comparison with the previous calculations for the interaction between the ground state Li$(2\,^2S)$ and the excited state Li$(2\,^2P)$. C_3, which is proportional to the square of the resonant dipole matrix element, has recently been calculated to high precision [6]. As for C_6, our values agree with the model potential calculations of Marinescu and Dalgarno [10] at about the 0.3% level.

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APPENDIX

We discuss the dispersion coefficients for the Li(S)-Li(P) system. The zero-order wave function for this system can be written as a symmetrized product of two individual atomic wave functions

$$\Psi^{(0)}=\frac{1}{\sqrt{2}}[\Psi_a(L_1M_1;\mathbf{r})\Psi_b(L_2M_2;\boldsymbol{\rho}) + \beta\Psi_a(L_1M_1;\boldsymbol{\rho})\Psi_b(L_2M_2;\mathbf{r})], \tag{A1}$$

where $\mathbf{r}$ and $\boldsymbol{\rho}$ represent all the internal coordinates for the two atoms, respectively, L_1 and L_2 are their total orbital angular momenta, M_1 and M_2 are the associated magnetic quantum numbers, and $\beta=\pm 1$ describes the symmetry due to the Pauli exclusion principle. Following [10], the interaction potential for two neutral atoms is

$$V=\sum_{l=1}^{\infty}\sum_{L=1}^{\infty}\frac{V_{lL}}{R^{l+L+1}}, \tag{A2}$$

where

$$V_{lL}=(-1)^L 4\pi(l,L)^{-1/2}\sum_{ij}\sum_{\mu}K^{\mu}_{lL}r_i^l\rho_j^L Y_{l\mu}(\hat{\mathbf{r}}_i)Y_{L-\mu}(\hat{\boldsymbol{\rho}}_j). \tag{A3}$$

In the above equation, $(l,L,\dots)=(2l+1)(2L+1)\cdots$, and

$$K^{\mu}_{lL}=\left[\binom{l+L}{l+\mu}\binom{l+L}{L+\mu}\right]^{1/2}. \tag{A4}$$

1. The first-order energy

The first-order energy is given by

$$V^{(1)}=\tfrac{1}{2}A_1+\tfrac{1}{2}A_2+\beta A_3 \tag{A5}$$

TABLE VII. Comparison of C_6, C_8, and C_{10} for the He$(1\,^1S)$-He$(1\,^1S)$ system.

Author (year)	Reference	C_6	C_8	C_{10}
Luyckx *et al.* (1977)	[17]	1.458	14.06	182.16
Glover and Weinhold (1977)	[37]	1.459 7(55)		
Margoliash and Meath (1978)	[36]	1.458		
Bartolotti (1980)	[38]	1.463 8	14.131	183.47
Thakkar (1981)	[18]	1.460 82	14.111 8	183.600
Rérat *et al.* (1993)	[39]	1.459 3	13.883	
Bishop and Pipin (1993)	[7]	1.460 977 8	14.117 855	183.691 25
Jamieson *et al.* (1995)	[9]	1.460 978		
Chen (1995)	[40]	1.461 1	14.120	183.74
Chen and Chung (1996)	[11]	1.461 06	14.120 8	183.765
This work		1.460 977 837 68(5)	14.117 857 340(5)	183.691 070 5(7)

TABLE VIII. Comparison of C_6, C_8, and C_{10} for the Li($2\,^2S$)-Li($2\,^2S$) system.

Author (year)	Reference	$10^{-3}C_6$	$10^{-4}C_8$	$10^{-6}C_{10}$
Stacey and Dalgarno (1968)	[41]	1.391		
Manakov and Ovsiannikov (1977)	[42]	1.360		
Margoliash and Meath (1978)	[36]	1.387		
Maeder and Kutzelnigg (1979)	[23]	1.389	8.089	6.901
Müller *et al.* (1984)	[27]	1.386		
Bussery and Aubert-Frécon (1985)	[43]	1.383	7.578 3	4.816 675
Marinescu *et al.* (1994)	[8]	1.388	8.324	7.365
Mérawa *et al.* (1994)	[32]	1.407 8	8.431 65	
This work		1.393 39(16)	8.342 58(42)	7.372 1(1)

with

$$A_1=\langle\Psi_a(L_1M_1;\mathbf{r})\Psi_b(L_2M_2;\boldsymbol{\rho})|\times V|\Psi_a(L_1M_1;\mathbf{r})\Psi_b(L_2M_2;\boldsymbol{\rho})\rangle, \tag{A6}$$

$$A_2=\langle\Psi_a(L_1M_1;\boldsymbol{\rho})\Psi_b(L_2M_2;\mathbf{r})|\times V|\Psi_a(L_1M_1;\boldsymbol{\rho})\Psi_b(L_2M_2;\mathbf{r})\rangle, \tag{A7}$$

$$A_3=\langle\Psi_a(L_1M_1;\mathbf{r})\Psi_b(L_2M_2;\boldsymbol{\rho})|\times V|\Psi_a(L_1M_1;\boldsymbol{\rho})\Psi_b(L_2M_2;\mathbf{r})\rangle. \tag{A8}$$

Substituting Eq. (A2) into Eq. (A6), one has

$$A_1=\sum_{lL\mu}\frac{(-1)^L4\pi}{R^{l+L+1}}(l,L)^{-1/2}K_{lL}^{\mu}\times\left\langle\Psi_a(L_1M_1;\mathbf{r})\left|\sum_i r_i^lY_{l\mu}(\hat{\mathbf{r}}_i)\right|\Psi_a(L_1M_1;\mathbf{r})\right\rangle\times\left\langle\Psi_b(L_2M_2;\boldsymbol{\rho})\left|\sum_j \rho_j^LY_{L-\mu}(\hat{\boldsymbol{\rho}}_j)\right|\Psi_b(L_2M_2;\boldsymbol{\rho})\right\rangle. \tag{A9}$$

From the Wigner-Eckart theorem Eq. (8), one has

$$\left\langle\Psi_a(L_1M_1;\mathbf{r})\left|\sum_i r_i^lY_{l\mu}(\hat{\mathbf{r}}_i)\right|\Psi_a(L_1M_1;\mathbf{r})\right\rangle=(-1)^{L_1-M_1}\begin{pmatrix}L_1 & l & L_1\\ -M_1 & \mu & M_1\end{pmatrix}\times\left\langle\Psi_a(L_1;\mathbf{r})\left\|\sum_i r_i^lY_l(\hat{\mathbf{r}}_i)\right\|\Psi_a(L_1;\mathbf{r})\right\rangle. \tag{A10}$$

For $L_1=0$, the 3-j symbol is zero when $l\geqslant1$. Thus, $A_1=0$. Similarly, $A_2=0$. For A_3, after using the Wigner-Eckart theorem, we obtain

$$A_3=\sum_{lL\mu}\frac{(-1)^L4\pi}{R^{l+L+1}}(l,L)^{-1/2}K_{lL}^{\mu}\times\left\langle\Psi_a(L_1;\mathbf{r})\left\|\sum_i r_i^lY_l(\hat{r}_i)\right\|\Psi_b(L_2;\mathbf{r})\right\rangle\times\left\langle\Psi_b(L_2;\boldsymbol{\rho})\left\|\sum_j \rho_j^LY_L(\hat{\boldsymbol{\rho}}_j)\right\|\Psi_a(L_1;\boldsymbol{\rho})\right\rangle g, \tag{A11}$$

where, for $L_1=0$,

$$g=(-1)^{L_1-M_1}\begin{pmatrix}L_1 & l & L_2\\ -M_1 & \mu & M_2\end{pmatrix}(-1)^{L_2-M_2}\times\begin{pmatrix}L_2 & L & L_1\\ -M_2 & -\mu & M_1\end{pmatrix}=\frac{(-1)^{L_2-M_2}}{2L_2+1}\delta_{l,L_2}\delta_{L,L_2}\delta_{\mu,-M_2}. \tag{A12}$$

TABLE IX. Values of the triple-dipole constants ν_{abc} for the three ground-state atoms H, He, and Li.

System	C_6 (This work)	C_6 (Ref. [41])
H-H-H	21.642 464 510 635 978 338 11	
He-H-H	8.102 240 874 3(2)	
He-He-H	3.268 064 896 1(1)	
He-He-He	1.479 558 606 3(1)	
Li-H-H	275.979(7)	276
Li-He-H	89.830(5)	89.6
Li-He-He	29.824(5)	29.6
Li-Li-H	6 133.5(5)	6.12×10^3
Li-Li-He	1 917.27(5)	1.91×10^3
Li-Li-Li	170 595(6)	1.69×10^5

TABLE X. Values of C_3 and C_6 for the interaction between Li($2\,^2S$) and Li($2\,^2P$).

M_2	β	C_3	C_6
0	1	11.000 226(15)	2 075.05(5)
0	–1	–11.000 226(15)	2 075.05(5)
±1	1	–5.500 113 3(74)	1 406.08(5)
±1	–1	5.500 113 3(74)	1 406.08(5)

TABLE XI. Comparison of C_6 for the Li($2\,^2S$)-Li($2\,^2P$) system.

Author (year)	Reference	$C_6(M_2=0)$	$C_6(M_2=\pm 1)$
Konowalov and Fish (1983)	[44]	2100(50)	1750(100)
Vigné-Maeder (1984)	[45]	2025	1374
Bussery and Aubert-Frécon (85)	[43]	1927	1301
Marinescu and Dalgarno (1995)	[10]	2066	1401
This work		2075.05(5)	1406.08(5)

Since [13]

$$\langle L'\|Y_l\|L\rangle=(-1)^{L'-L}\langle L\|Y_l\|L'\rangle, \tag{A13}$$

we finally have

$$V^{(1)}(L_2M_2;\beta)=-\frac{C^{M_2\beta}_{2L_2+1}}{R^{2L_2+1}}, \tag{A14}$$

where

$$C^{M_2\beta}_{2L_2+1}=\beta(-1)^{1+L_2+M_2}\frac{4\pi}{(2L_2+1)^2}\binom{2L_2}{L_2+M_2}\times\left|\left\langle \Psi_a(0;\mathbf{r})\left\|\sum_i r_i^{L_2}Y_{L_2}(\hat{\mathbf{r}}_i)\right\|\Psi_b(L_2;\mathbf{r})\right\rangle\right|^2. \tag{A15}$$

2. The second-order energy

Let the complete set of the system be

$$\{\chi(L_sM_s;\mathbf{r})\omega(L_tM_t;\boldsymbol{\rho})\} \tag{A16}$$

with the energy eigenvalue $E_{st}^{(0)}=E_s^{(0)}+E_t^{(0)}$ The energy for the unperturbed system is $E^{(0)}=E_1^{(0)}+E_2^{(0)}$. According to the second-order perturbation theory, the second-order energy is

$$V^{(2)}=-\sum_{st}\frac{|\langle\Psi^{(0)}|V|\chi(L_sM_s;\mathbf{r})\omega(L_tM_t;\boldsymbol{\rho})\rangle|^2}{E_{st}^{(0)}-E^{(0)}}=-\sum_{st}\frac{T}{E_{st}^{(0)}-E^{(0)}}, \tag{A17}$$

where T can be written as

$$T=B_1+B_2+\beta B_3 \tag{A18}$$

with

$$B_1=\frac{1}{2}\sum_{L_sM_s}\sum_{L_tM_t}\langle\Psi_a(L_1M_1;\mathbf{r})\Psi_b(L_2M_2;\boldsymbol{\rho})|\times V|\chi(L_sM_s;\mathbf{r})\omega(L_tM_t;\boldsymbol{\rho})\rangle^2, \tag{A19}$$

$$B_2=\frac{1}{2}\sum_{L_sM_s}\sum_{L_tM_t}\langle\Psi_a(L_1M_1;\boldsymbol{\rho})\Psi_b(L_2M_2;\mathbf{r})|\times V|\chi(L_sM_s;\mathbf{r})\omega(L_tM_t;\boldsymbol{\rho})\rangle^2, \tag{A20}$$

$$B_3=\sum_{L_sM_s}\sum_{L_tM_t}\langle\Psi_a(L_1M_1;\mathbf{r})\Psi_b(L_2M_2;\boldsymbol{\rho})|\times V|\chi(L_sM_s;\mathbf{r})\omega(L_tM_t;\boldsymbol{\rho})\rangle\langle\Psi_a(L_1M_1;\boldsymbol{\rho})\times\Psi_b(L_2M_2;\mathbf{r})|V|\chi(L_sM_s;\mathbf{r})\omega(L_tM_t;\boldsymbol{\rho})\rangle. \tag{A21}$$

After using the Wigner-Eckart theorem, we obtain

$$\begin{aligned}B_1={}&\frac{1}{2}\sum_{lL\mu}\sum_{l'L'\mu'}\sum_{L_sL_t}\sum_{M_sM_t}\frac{(4\pi)^2}{R^{l+L+l'+L'+2}}(-1)^{L+L'}(l,L,l',L')^{-1/2}K^{\mu}_{lL}K^{\mu'}_{l'L'}\left\langle\Psi_{\mathrm{a}}(L_1;\mathbf{r})\left\|\sum_i r_i^lY_l(\hat{\mathbf{r}}_i)\right\|\chi(L_s;\mathbf{r})\right\rangle\\&\times\left\langle\Psi_b(L_2;\boldsymbol{\rho})\left\|\sum_j \rho_j^LY_L(\hat{\boldsymbol{\rho}}_j)\right\|\omega(L_t;\boldsymbol{\rho})\right\rangle\left\langle\Psi_a(L_1;\mathbf{r})\left\|\sum_i r_i^{l'}Y_{l'}(\hat{\mathbf{r}}_i)\right\|\chi(L_s;\mathbf{r})\right\rangle\\&\times\left\langle\Psi_b(L_2;\boldsymbol{\rho})\left\|\sum_j \rho_j^{L'}Y_{L'}(\hat{\boldsymbol{\rho}}_j)\right\|\omega(L_t;\boldsymbol{\rho})\right\rangle\begin{pmatrix}L_1 & l & L_s\\ -M_1 & \mu & M_s\end{pmatrix}\begin{pmatrix}L_2 & L & L_t\\ -M_2 & -\mu & M_t\end{pmatrix}\\&\times\begin{pmatrix}L_1 & l' & L_s\\ -M_1 & \mu' & M_s\end{pmatrix}\begin{pmatrix}L_2 & L' & L_t\\ -M_2 & -\mu' & M_t\end{pmatrix}.\end{aligned} \tag{A22}$$

For $L_1=0$, the product of four 3-j symbols becomes

$$\delta_{l,L_s}\delta_{l',L_s}\delta_{\mu,-M_s}\delta_{\mu',-M_s}\frac{1}{2L_s+1}\begin{pmatrix} L_2 & L & L_t \\ -M_2 & M_s & M_t \end{pmatrix}\times\begin{pmatrix} L_2 & L' & L_t \\ -M_2 & M_s & M_t \end{pmatrix}. \tag{A23}$$

Defining G_1 by

$$G_1(L,L',L_s,L_t,L_2,M_2)=(-1)^{L+L'}\frac{(4\pi)^2}{2(2L_s+1)^2}\times(L,L')^{-1/2}\sum_{M_sM_t}K_{L_sL}^{-M_s}K_{L_sL'}^{-M_s}\times\begin{pmatrix} L_2 & L & L_t \\ -M_2 & M_s & M_t \end{pmatrix}\times\begin{pmatrix} L_2 & L' & L_t \\ -M_2 & M_s & M_t \end{pmatrix}, \tag{A24}$$

we have

$$B_1=\sum_{LL'L_sL_t}\frac{1}{R^{2L_s+L+L'+2}}G_1(L,L',L_s,L_t,L_2,M_2)\times\left|\left\langle\Psi_a(0;\mathbf{r})\left\|\sum_i r_i^{L_s}Y_{L_s}(\hat{\mathbf{r}}_i)\right\|\chi(L_s;\mathbf{r})\right\rangle\right|^2\times\left\langle\Psi_b(L_2;\boldsymbol{\rho})\left\|\sum_j \rho_j^{L}Y_{L}(\hat{\boldsymbol{\rho}}_j)\right\|\omega(L_t;\boldsymbol{\rho})\right\rangle\times\left\langle\Psi_b(L_2;\boldsymbol{\rho})\left\|\sum_j \rho_j^{L'}Y_{L'}(\hat{\boldsymbol{\rho}}_j)\right\|\omega(L_t;\boldsymbol{\rho})\right\rangle. \tag{A25}$$

Consider the leading term of R^{-6}. The only choice is $L_s=1$, $L=1$, and $L'=1$. If another atom is in the $L_2=1$ state, then $L_t=0$, 1, and 2. For this case,

$$B_1=\frac{1}{R^6}\left|\left\langle\Psi_a(0;\mathbf{r})\left\|\sum_i r_iY_1(\hat{\mathbf{r}}_i)\right\|\chi(1;\mathbf{r})\right\rangle\right|^2\times\sum_\lambda G_1(1,1,1,\lambda,1,M_2)\times\left|\left\langle\Psi_b(1;\boldsymbol{\rho})\left\|\sum_j \rho_jY_1(\hat{\boldsymbol{\rho}}_j)\right\|\omega(\lambda;\boldsymbol{\rho})\right\rangle\right|^2. \tag{A26}$$

Similarly, for B_2 with $L_1=0$, we have

$$B_2=\sum_{ll'L_sL_t}\frac{1}{R^{2L_t+l+l'+2}}G_2(l,l',L_t,L_s,L_2,M_2)\times\left|\left\langle\Psi_a(0;\boldsymbol{\rho})\left\|\sum_j \rho_j^{L_t}Y_{L_t}(\hat{\boldsymbol{\rho}}_j)\right\|\omega(L_t;\boldsymbol{\rho})\right\rangle\right|^2\times\left\langle\Psi_b(L_2;\mathbf{r})\left\|\sum_i r_i^{l}Y_{l}(\hat{\mathbf{r}}_i)\right\|\chi(L_s;\mathbf{r})\right\rangle\times\left\langle\Psi_b(L_2;\mathbf{r})\left\|\sum_i r_i^{l'}Y_{l'}(\hat{\mathbf{r}}_i)\right\|\chi(L_s;\mathbf{r})\right\rangle \tag{A27}$$

with

$$G_2(l,l',L_t,L_s,L_2,M_2)=\frac{(4\pi)^2}{2(2L_t+1)^2}(l,l')^{-1/2}\times\sum_{M_sM_t}K_{lL_t}^{M_t}K_{l'L_t}^{M_t}\begin{pmatrix} L_2 & l & L_s \\ -M_2 & M_t & M_s \end{pmatrix}\times\begin{pmatrix} L_2 & l' & L_s \\ -M_2 & M_t & M_s \end{pmatrix}. \tag{A28}$$

For R^{-6}, $L_t=1$, $l=1$, $l'=1$. Thus, for the case of $L_2=1$, B_2 becomes

$$B_2=\frac{1}{R^6}\left|\left\langle\Psi_a(0;\boldsymbol{\rho})\left\|\sum_j \rho_jY_1(\hat{\boldsymbol{\rho}}_j)\right\|\omega(1;\boldsymbol{\rho})\right\rangle\right|^2\times\sum_\lambda G_2(1,1,1,\lambda,1,M_2)\times\left|\left\langle\Psi_b(1;\mathbf{r})\left\|\sum_i r_iY_1(\hat{\mathbf{r}}_i)\right\|\chi(\lambda;\mathbf{r})\right\rangle\right|^2. \tag{A29}$$

Finally, for B_3 with $L_1=0$, we have

$$B_3=\sum_{Ll'L_sL_t}\frac{1}{R^{L_s+L_t+L+l'+2}}G_3(L,l',L_s,L_t,L_2,M_2)\times\left\langle\Psi_a(0;\mathbf{r})\left\|\sum_i r_i^{L_s}Y_{L_s}(\hat{\mathbf{r}}_i)\right\|\chi(L_s;\mathbf{r})\right\rangle\times\left\langle\Psi_a(0;\boldsymbol{\rho})\left\|\sum_j \rho_j^{L_t}Y_{L_t}(\hat{\boldsymbol{\rho}}_j)\right\|\omega(L_t;\boldsymbol{\rho})\right\rangle\times\left\langle\Psi_b(L_2;\boldsymbol{\rho})\left\|\sum_j \rho_j^{L}Y_{L}(\hat{\boldsymbol{\rho}}_j)\right\|\omega(L_t;\boldsymbol{\rho})\right\rangle\times\left\langle\Psi_b(L_2;\mathbf{r})\left\|\sum_i r_i^{l'}Y_{l'}(\hat{\mathbf{r}}_i)\right\|\chi(L_s;\mathbf{r})\right\rangle, \tag{A30}$$

with

$$
\begin{aligned}
G_3(L,l',L_s,L_t,L_2,M_2)={}&(-1)^{L+Ls}\frac{(4\pi)^2}{(2L_s+1)(2L_t+1)}\\
&\times(L,l')^{-1/2}\\
&\times\sum_{M_sM_t}(-1)^{M_s+M_t}K^{-M_s}_{L_sL}K^{M_t}_{l'L_t}\\
&\times\begin{pmatrix} L_2 & L & L_t\\ -M_2 & M_s & M_t\end{pmatrix}\\
&\times\begin{pmatrix} L_2 & l' & L_s\\ -M_2 & M_t & M_s\end{pmatrix}.
\end{aligned}
\tag{A31}
$$

The only term which contributes R^{-6} is the one with $L_s=1$, $L_t=1$, $l'=1$, and $L=1$. For the case of $L_2=1$, one obtains

$$
\begin{aligned}
B_3={}&\frac{1}{R^6}G_3(1,1,1,1,1,M_2)\left\langle \Psi_a(0;\mathbf{r})\left\| \sum_i r_iY_1(\hat{\mathbf{r}}_i)\right\|\chi(1;\mathbf{r})\right\rangle\\
&\times\left\langle \Psi_a(0;\boldsymbol{\rho})\left\| \sum_j \rho_jY_1(\hat{\boldsymbol{\rho}}_j)\right\|\omega(1;\boldsymbol{\rho})\right\rangle\\
&\times\left\langle \Psi_b(1;\boldsymbol{\rho})\left\| \sum_j \rho_jY_1(\hat{\boldsymbol{\rho}}_j)\right\|\omega(1;\boldsymbol{\rho})\right\rangle\\
&\times\left\langle \Psi_b(1;\mathbf{r})\left\| \sum_i r_iY_1(\hat{\mathbf{r}}_i)\right\|\chi(1;\mathbf{r})\right\rangle.
\end{aligned}
\tag{A32}
$$

For the S state $\Psi_a(0;\mathbf{r})$, the parity is $+1$, and for the P state $\Psi_b(1;\mathbf{r})$, the parity is -1. Since these two states cannot be connected simultaneously to a third parity eigenstate by a dipole operator, B_3 is therefore zero.

For two like atoms the spectra $\{\chi(LM;\mathbf{r})\}$ and $\{\omega(LM;\boldsymbol{\rho})\}$ are identical and B_1 and B_2 can be combined. The final expression for the second-order energy correction to the Li(S)-Li(P) system is

$$
V^{(2)}=-\frac{C_6^{M_2}}{R^6},
\tag{A33}
$$

where

$$
C_6^{M_2}=\sum_{st}\frac{\Omega_{st}}{E_{st}^{(0)}-E^{(0)}}
\tag{A34}
$$

with

$$
\begin{aligned}
\Omega_{st}={}&\left|\left\langle \Psi_a(0;\mathbf{r})\left\| \sum_i r_iY_1(\hat{\mathbf{r}}_i)\right\|\chi(1;\mathbf{r})\right\rangle\right|^2\\
&\times\sum_{\lambda}G(1,1,1,\lambda,1,M_2)\\
&\times\left|\left\langle \Psi_b(1;\boldsymbol{\rho})\left\| \sum_j \rho_jY_1(\hat{\boldsymbol{\rho}}_j)\right\|\omega(\lambda;\boldsymbol{\rho})\right\rangle\right|^2.
\end{aligned}
\tag{A35}
$$

In Eq. (A35), G is defined by

$$
G(1,1,1,\lambda,1,M_2)=G_1(1,1,1,\lambda,1,M_2)+G_2(1,1,1,\lambda,1,M_2).
\tag{A36}
$$

It is easy to see that

$$
G_1(1,1,1,\lambda,1,M_2)=G_2(1,1,1,\lambda,1,M_2).
\tag{A37}
$$

The algebraic coefficients $G(1,1,1,\lambda,1,M_2)$ are listed in Table I.

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