

Polarizabilities of heliumlike ions in the $1s2p\ ^1P$ and $1s2p\ ^3P$ states

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The static dipole, quadrupole, and octupole polarizabilities of heliumlike ions are calculated for the $1s2p\ ^1P$ and $1s2p\ ^3P$ states with Z up to 10, using variational wave functions in Hylleraas coordinates. A general sum rule for the 2^l -pole oscillator strengths is derived.

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Recently we have evaluated polarizabilities of helium and heliumlike ions in the ground state $1s^2\ ^1S$ [1,2] and the metastable $1s2s\ ^1S$ and $1s2s\ ^3S$ states [3,4]. All these calculations were done using variational wave functions in Hylleraas coordinates. In this Brief Report, we extend our work to heliumlike ions in the $1s2p\ ^1P$ and $1s2p\ ^3P$ states. To our knowledge, there has been no precise work reported in the literature.

The static 2^l -pole polarizability for an atom is defined in terms of a sum over all intermediate states, including the continuum (in atomic units throughout):

$$\alpha_l = \sum_{n \neq 0} \frac{f_{n0}^{(l)}}{(E_n - E_0)^2}, \quad (1)$$

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

$$f_{n0}^{(l)} = f_{n0}^{(l)}(m, M_0, M_n) = \frac{8\pi}{2l+1} (E_n - E_0) \times \left| \left\langle \Psi_0 \left| \sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) \right| \Psi_n \right\rangle \right|^2, \quad (2)$$

where the sum i runs over all the electrons in the atom, Ψ_0 is the state of interest with the associated energy eigenvalue E_0 and the magnetic quantum number M_0 , and Ψ_n is one of the intermediate states with the associated energy eigenvalue E_n and the magnetic quantum number M_n . In practice, instead of $f_{n0}^{(l)}$, an averaged oscillator strength $\bar{f}_{n0}^{(l)}$, which is independent of the magnetic quantum numbers m , M_0 , and M_n , is used. The $\bar{f}_{n0}^{(l)}$ 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 [5]

$$\begin{aligned} & \left\langle \gamma' L' M' \left| \sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) \right| \gamma L M \right\rangle \\ &= (-1)^{L'-M'} \begin{pmatrix} L' & l & L \\ -M' & m & M \end{pmatrix} \\ & \times \left\langle \gamma' L' \left| \left| \sum_i r_i^l Y_l(\hat{\mathbf{r}}_i) \right| \right| \gamma L \right\rangle. \end{aligned} \quad (3)$$

With the aid of a sum rule for the $3j$ symbols, we have

$$\begin{aligned} \bar{f}_{n0}^{(l)} &= \frac{8\pi}{(2l+1)^2(2L_0+1)} (E_n - E_0) \\ & \times \left| \left\langle \Psi_0 \left| \left| \sum_i r_i^l Y_l(\hat{\mathbf{r}}_i) \right| \right| \Psi_n \right\rangle \right|^2, \end{aligned} \quad (4)$$

where L_0 is the total angular momentum for the initial state (the state of interest). The allowed possible symmetries of intermediate states can be obtained by the selection rules of the $3j$ symbol and parity. Thus, if the symmetry of the initial state is P , then the allowed symmetries are $S+P+D$, $P+D+F$, and $D+F+G$ for the dipole, quadrupole, and octupole polarizabilities, respectively. In the case of dipole polarizability, the intermediate P symmetry can be represented by the configurations $(n p n' p)^1 P^e$ and $(n p n' p)^3 P^e$ for the singlet and triplet states, respectively, where the lowest member in $(n p n' p)^3 P^e$ is $(2 p 2 p)^3 P^e$. For the quadrupole polarizability, the intermediate D symmetry can be represented by the configurations $(n p n' d)^1 D^o$ and $(n p n' d)^3 D^o$ respectively. Finally, for the octupole polarizability, the required configurations are $(n p n' f) + (n d n' d)$ to form $^1 F^e$ and $(n p n' f) + (n d n' d)$ to form $^3 F^e$, where the lowest member in $(n d n' d)^3 F^e$ is $(3 d 3 d)^3 F^e$. The rest of the intermediate symmetries can be implemented by including singly excited configurations explicitly. All the other doubly excited configurations are included implicitly through Hylleraas coordinates. It should be pointed out that one of the intermediate states of P symmetry, which overlaps with the initial state, should be excluded in the summation over n in Eq. (1).

For a two-electron atomic system, the basis set is constructed using Hylleraas coordinates

$$\{\chi_{ijk} = r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2} \mathcal{Y}_{l_1 l_2}^{LM}(\mathbf{r}_1, \mathbf{r}_2)\}, \quad (5)$$

where $\mathcal{Y}_{l_1 l_2}^{LM}(\mathbf{r}_1, \mathbf{r}_2)$ is the vector-coupled product of solid spherical harmonics for the two electrons forming an eigenstate of total angular momentum L defined by

$$\mathcal{Y}_{l_1 l_2}^{LM}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{m_1 m_2} \langle l_1 l_2 m_1 m_2 | LM \rangle Y_{l_1 m_1}(\mathbf{r}_1) Y_{l_2 m_2}(\mathbf{r}_2), \quad (6)$$

TABLE I. Convergence of the contributions to α_1 for helium in the 2^1P state from the S , P , and D symmetries, with respect to the sizes of basis sets N_P , N_S , N_{PP} , and N_D , where N_P is for 2^1P , and N_S , N_{PP} , and N_D are for the three intermediate symmetries. Units are a.u.

N_P	N_S	N_{PP}	N_D	$\alpha_1(^1S)$	$\alpha_1((pp')^1P)$	$\alpha_1(^1D)$
440	300	372	425	-241.620 033 89	0.080 111 65	181.511 395 95
572	372	444	565	-241.620 032 17	0.080 111 74	181.511 402 18
728	454	525	733	-241.620 031 49	0.080 111 79	181.511 404 86
910	546	615	931	-241.620 031 40	0.080 111 81	181.511 405 38

and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ is the distance between electron 1 and 2. The wave functions are expanded from doubled basis sets. The explicit form for the wave function is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{ijk} [a_{ijk}^{(1)} \chi_{ijk}(\alpha_1, \beta_1) + a_{ijk}^{(2)} \chi_{ijk}(\alpha_2, \beta_2)] \pm \text{exchange}, \quad (7)$$

and $i + j + k \leq \Omega$. A complete optimization is then performed with respect to the two sets of nonlinear parameters α_1 , β_1 , and α_2 , β_2 by first calculating the derivatives analytically in

$$\frac{\partial E}{\partial \gamma} = 2 \left\langle \Psi \left| H \left| \frac{\partial \Psi}{\partial \gamma} \right. \right\rangle - 2E \left\langle \Psi \left| \frac{\partial \Psi}{\partial \gamma} \right. \right\rangle, \quad (8)$$

where γ represents any nonlinear parameter, E is the trial energy, H is the Hamiltonian, and $\langle \Psi | \Psi \rangle = 1$ is assumed, and then locating the zeros of the derivatives by Newton's method. For intermediate states of given symmetry, we diagonalize the Hamiltonian directly in a basis set where the nonlinear parameters are optimized such that the energy eigenvalue

closest to the energy of initial state E_0 is minimized. The basic integrals that appear in our variational calculations are of the form

$$I(a, b, c; \alpha, \beta) = \int d\mathbf{r}_1 d\mathbf{r}_2 \mathcal{Y}_{l_1' l_2'}^{L' M'}(\mathbf{r}_1, \mathbf{r}_2)^* \times \mathcal{Y}_{l_1 l_2}^{LM}(\mathbf{r}_1, \mathbf{r}_2) r_1^a r_2^b r_{12}^c e^{-\alpha r_1 - \beta r_2}. \quad (9)$$

The complete evaluation of these integrals can be found in Ref. [6].

Table I contains a typical convergence pattern for the contributions to the dipole polarizability of helium in the 2^1P state from the three intermediate 1S , $(n p n' p)^1P$, and 1D symmetries, as the sizes of basis sets increase progressively. Table II lists the values of the polarizabilities α_1 , α_2 , and α_3 of heliumlike ions in the $1s2p^1P$ and $1s2p^3P$ states, with the nuclear charge Z up to 10. It is interesting to see that all the dipole polarizabilities α_1 for heliumlike ions are negative except for the $1s2p^3P$ helium which is positive. This is because the only negative contribution to α_1 is

TABLE II. Values of the static polarizabilities α_1 , α_2 , and α_3 of heliumlike ions in the 2^1P and 2^3P states. Numbers in parentheses represent the estimated error in the last digit of the listed values. Z is the nuclear charge. Units are a.u.

Z	α_1	α_2	α_3
2 singlet	-60.028 514 0(2)	5 482.670 95(5)	473 456.35(2)
2 triplet	46.707 748 2(3)	3 622.790 34(2)	272 212.58(2)
3 singlet	-19.280 648 5(2)	87.541 556 0(5)	1 900.986 5(5)
3 triplet	-5.790 965 718(2)	59.809 929(2)	1 145.598 2(2)
4 singlet	-6.659 933 85(5)	7.649 312 9(2)	73.651 79(1)
4 triplet	-2.899 849 915(2)	5.575 919 8(4)	48.421 32(2)
5 singlet	-2.980 463 65(3)	1.350 815 55(3)	7.293 930(2)
5 triplet	-1.492 679 740(2)	1.035 957 35(4)	5.131 571(1)
6 singlet	-1.572 734 264(2)	0.351 583 018(2)	1.211 781(2)
6 triplet	-0.852 184 682 7(2)	0.280 084 726(2)	0.896 794 0(2)
7 singlet	-0.926 678 093 0(4)	0.117 039 515(4)	0.279 525 5(2)
7 triplet	-0.528 700 907 61(5)	0.095 979 305(4)	0.214 985 0(3)
8 singlet	-0.590 519 083 2(4)	0.046 184 420(4)	0.080 894 5(2)
8 triplet	-0.349 511 782 2(2)	0.038 740 979 0(1)	0.064 113 6(2)
9 singlet	-0.398 916 829 1(5)	0.020 642 083 7(3)	0.027 641 09(1)
9 triplet	-0.242 709 047 25(3)	0.017 631 555 0(3)	0.022 439 38(2)
10 singlet	-0.281 907 798 0(2)	0.010 147 003 8(4)	0.010 722 68(2)
10 triplet	-0.175 247 853 120(1)	0.008 796 158 8(4)	0.008 876 95(2)

TABLE III. Oscillator strength sum rules for the heliumlike ion B^{3+} ($Z=5$) in the initial state of 2^1P .

$S_S^{(1)}$	-0.0565606	$S_P^{(2)}$	0.6645502	$S_D^{(3)}$	5.501445
$S_D^{(1)}$	1.8080750	$S_F^{(2)}$	3.3415984	$S_G^{(3)}$	15.210450
$3S_S^{(1)} + \frac{6}{5}S_D^{(1)}$	2.0000082	$2S_P^{(2)} + \frac{9}{7}S_F^{(2)}$	5.6254412	$\frac{9}{5}S_D^{(3)} + \frac{4}{3}S_G^{(3)}$	30.183201
		$M_{20}(0)$	2.0439853	$M_{42}(0)$	2.751726
		$M_{22}(0)$	0.7688053	$M_{40}(0)$	6.916432
		$2M_{20}(0) + 2M_{22}(0)$	5.6255812	$\frac{24}{7}M_{42}(0) + 3M_{40}(0)$	30.183785

from the $2s-2p$ transition, which is coincidentally canceled by a large contribution from the $3d-2p$ transition, that is,

$$\frac{\bar{f}_{2s2p}^{(1)}}{(E_{2s} - E_{2p})^2} = -101.552, \quad (10)$$

$$\frac{\bar{f}_{3d2p}^{(1)}}{(E_{3d} - E_{2p})^2} = 101.525. \quad (11)$$

The 2^l -pole polarizabilities follow the large- Z scaling $\alpha_l \sim 1/(Z - a_l)^{2l+2}$, where a_1 is -3 , and a_2 and a_3 are 1.

It is interesting to check the completeness of our dipole oscillator-strength spectra using the Thomas-Reiche-Kuhn (TRK) sum rule for the oscillator strengths [7]:

$$\sum_n f_{n0}^{(1)}(0, M_0, M_n) = N_e, \quad (12)$$

where $f_{n0}^{(1)}$ is defined by Eq. (2) and N_e is the total number of electrons, which is two in this work. In terms of the averaged oscillator strength $\bar{f}_{n0}^{(l)}$ defined by Eq. (4), which is independent of magnetic quantum numbers, the TRK sum rule for P states reads, after letting $M_0=0$ in Eq. (12),

$$3S_S^{(1)} + \frac{6}{5}S_D^{(1)} = N_e, \quad (13)$$

where

$$S_L^{(l)} = \sum_n \bar{f}_{n0}^{(l)}(L), \quad (14)$$

and L indicates the intermediate symmetry.

For the quadrupole and octupole oscillator strengths, the corresponding expressions can be derived from the following general sum rule:

$$\sum_n (E_n - E_k) |F_{nk}|^2 = \frac{1}{2} \langle k | [F, [H, F]] | k \rangle, \quad (15)$$

where $F(\mathbf{r}, \mathbf{p})$ is an arbitrary Hermitian operator. Denoting

$$M_{mn}(M_0) = \left\langle \Psi_0 \left| \sum_{i=1}^{N_e} r_i^m P_n(\cos \theta_i) \right| \Psi_0 \right\rangle, \quad (16)$$

where $P_n(\cos \theta_i)$ is the Legendre polynomial, we have for P states

$$2S_P^{(2)} + \frac{9}{7}S_F^{(2)} = 2M_{20}(0) + 2M_{22}(0) \quad (17)$$

for the quadrupole and

$$\frac{9}{5}S_D^{(3)} + \frac{4}{3}S_G^{(3)} = \frac{24}{7}M_{42}(0) + 3M_{40}(0) \quad (18)$$

for the octupole oscillator strengths. A lengthy but straightforward calculation yields the following general expression:

$$\begin{aligned} & 2 \sum_n (E_n - E_0) \left| \left\langle \Psi_n \left| \sum_{i=1}^{N_e} r_i^l P_l(\cos \theta_i) \right| \Psi_0 \right\rangle \right|^2 \\ &= l^2 \left\langle \Psi_0 \left| \sum_{i=1}^{N_e} r_i^{2l-2} \csc^2 \theta_i [P_l^2(\cos \theta_i) + P_{l-1}^2(\cos \theta_i) \right. \right. \\ &\quad \left. \left. - 2 \cos \theta_i P_l(\cos \theta_i) P_{l-1}(\cos \theta_i)] \right| \Psi_0 \right\rangle. \end{aligned} \quad (19)$$

Table III presents a detailed list of quantities appearing in the above sum rules. We can see that these sum rules are well satisfied. The residual discrepancies are due to the fact that the results in Table III for the oscillator strengths were obtained using small basis sets (around 400 terms). However, the sum in the calculation of polarizability in Eq. (1) should be much more rapidly converged than $S_L^{(l)}$. The sum rules involving doubly excited intermediate states can also be obtained by setting $M_0 = \pm 1$ in Eq. (19). Thus, for P states, we have

$$\frac{9}{10}S_D^{(1)} + \frac{3}{2}S_P^{(1)} = N_e, \quad (20)$$

$$\frac{6}{7}S_F^{(2)} + \frac{3}{2}S_D^{(2)} + \frac{1}{2}S_P^{(2)} = 2M_{20}(1) + 2M_{22}(1), \quad (21)$$

$$\frac{3}{5}S_D^{(3)} + \frac{3}{2}S_F^{(3)} + \frac{5}{6}S_G^{(3)} = \frac{24}{7}M_{42}(1) + 3M_{40}(1). \quad (22)$$

These sum rules were also checked numerically to be held to a similar degree of accuracy.

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