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$(1s)^2 3s\,^2S$, $(1s)^2 3p\,^2P$, and $(1s)^2 3d\,^2D$ states of the lithium isoelectronic sequence*

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A $1/Z$-perturbation-expansion method is used to calculate the eigenvalues and eigenfunctions for the $(1s)^2 3s\,^2S$, $(1s)^2 3p\,^2P$, and $(1s)^2 3d\,^2D$ states of the lithium isoelectronic sequence. The eigenfunctions are used, together with those of the $2\,^2S$ and $2\,^2P$ states, to determine the dipole-length and dipole-velocity forms of the oscillator strengths for the $2p$-$3s$, $3s$-$3p$, $2s$-$3p$, $3p$-$3d$, and $2p$-$3d$ transitions. The results are compared with those obtained from Hartree-Fock calculations for individual values of the nuclear charge. The calculations include members of the lithium series for which accurate eigenenergies or oscillator strengths are not well known.

I. INTRODUCTION

Because of the continuing importance of the highly ionized members of the lithium isoelectronic sequence in solar and laboratory plasmas, this research utilizes the Z-expansion method[1] to provide accurate wave functions and eigenenergies for the $3\,^2S$, $3\,^2P$, and $3\,^2D$ states of the series. Variational wave functions expressed in terms of configuration interaction allow greater accuracy in representing these states than in earlier work.[2] Since the calculations are performed as a function of nuclear charge, they are easily extended to include more members of the sequence with only a negligible addition of computer time. Oscillator strengths for the lithium sequence from C IV to Si XII are determined for transitions among the $l = 3$ levels and with the $2\,^2S$ and $2\,^2P$ levels studied in a previous paper.[3]

II. THEORY

A complete theoretical discussion has been presented previously[3] and only a brief resume will be given here. We seek a solution to the Schrödinger equation where the nonrelativistic and spin-independent Hamiltonian H, in appropriate units of $Z^{-1}a_0$ for length and Z^2 a.u. for energy, is given by

$$H = H_0 + (1/Z)V \; . \tag{1}$$

H_0 is the hydrogenic Hamiltonian and the electronic repulsion term V can be treated as a stationary perturbation.

Following Dalgarno and Drake[1] we introduce a finite basis set Φ_k, which, in our case, consists of three-electron determinantal functions representing the configurations k. One of these, Φ_0, is the hydrogenic solution and zero-order solution $\psi_n^{(0)}$ to the set of Rayleigh-Schrödinger perturbation equations obtained by expanding the wave function and energy according to

$$|\psi_n\rangle = \sum_{s=0}^{\infty} Z^{-s} |\psi_n^{(s)}\rangle \, , \quad E_n = \sum_{s=0}^{\infty} Z^{-s} E_n^{(s)} \; . \tag{2}$$

The equivalent variational form for the set is

$$\delta J_n^{(s)} = 0 \; , \tag{3}$$

where the functional $J_n^{(s)}$ is given by

$$J_n^{(s)} = \langle \psi_n^{(s)} | H_0 - E_n^{(0)} | \psi_n^{(s)} \rangle + 2 \langle \psi_n^{(s)} | \, V - E_n^{(1)} | \psi_n^{(s-1)} \rangle - 2 \sum_{r=2}^{2s-1} E_n^{(r)} \sum_{q=s-r}^{r} \langle \psi_n^{(q)} | \psi_n^{(2s-r-q)} \rangle \; . \tag{4}$$

We require that

$$\langle \Phi_k | H_0 | \Phi_{k'} \rangle = \epsilon_k \delta_{kk'} \, , \quad k, k' = 1, \, 2, \, \ldots, N \, ,$$
$$\langle \Phi_k | \Phi_{k'} \rangle = \delta_{kk'} \; . \tag{5}$$

Then $\epsilon_0 = E_n^{(0)}$. Substituting the trial form

$$|\psi_n^{(s)}\rangle = \sum_{k=1}^{N} a_k^{(s)} |\Phi_k\rangle \tag{6}$$

into Eqs. (3) and (4) leads to the following expressions for the sth-order perturbed wave function and energy:

$$\langle \psi_n^{(s)} | = \sum_{k \neq 0}^{N} \frac{\langle \psi_n^{(s-1)} | V | \Phi_k \rangle \langle \Phi_k |}{\epsilon_0 - \epsilon_k} - \sum_{k \neq 0}^{N} \sum_{p=1}^{s} \frac{E_n^{(p)} \langle \psi_n^{(s-p)} | \Phi_k \rangle \langle \Phi_k |}{\epsilon_0 - \epsilon_k} \, , \tag{7}$$

$$E_n^{(s)} = \langle \psi_n^{(s-1)} | \, V | \psi_n^{(0)} \rangle - \sum_{p=1}^{s-1} E_n^{(p)} \langle \psi_n^{(s-p)} | \psi_n^{(0)} \rangle \; . \tag{8}$$

TABLE I. Configuration-interaction wave functions and screening parameters for the 3^2S, 3^2P, and $3\,^2D$ states of O VI ($Z = 8$).

$(1s)^2 3s\ ^2S$			$(1s)^2 3p\ ^2P$			$(1s)^2 3d\ ^2D$		
ζ			ζ			ζ		
$\zeta 1s_1 = 8.38$	$\zeta 2s_7 = 4.01$		$\zeta 1s_2 = 6.33$	$\zeta 3p_4 = 2.98$		$\zeta 1s_1 = 1.01$	$\zeta 3s_5 = 2.00$	
$\zeta 1s_3 = 6.74$	$\zeta 2s_8 = 5.01$		$\zeta 1s_3 = 7.46$	$\zeta 4p_1 = 1.90$		$\zeta 1s_3 = 6.68$	$\zeta 3d_3 = 2.04$	
$\zeta 1s_5 = 8.18$	$\zeta 3s_5 = 2.40$		$\zeta 2s_3 = 6.71$	$\zeta 4p_4 = 2.20$		$\zeta 1s_4 = 5.58$	$\zeta 4d_3 = 2.14$	
$\zeta 1s_6 = 4.11$	$\zeta 3s_8 = 4.54$		$\zeta 2p_4 = 6.75$	$\zeta 3p'''' = 1.86$		$\zeta 2s_2 = 5.58$	$\zeta 3d'' = 2.00$	
$\zeta 1s_7 = 7.12$	$\zeta 4s_6 = 1.45$							
$\zeta 2s_2 = 3.27$	$\zeta 4s_7 = 1.35$							
$\zeta s''' = 1.85$								
	Configurations			Configurations			Configurations	
$(1s)^2 3s_{\text{hydrogenic}}$	$(3s')^2 3s'''$	$(5d)^2 3s'''$	$(1s)^2 3p_{\text{hydrogenic}}$	$(2s')^2 3p''''$	$(5d)^2 3p''''$	$(1s)^2 3d_{\text{hydrogenic}}$	$(2p3p)3d''$	$(5f)^2 3d''$
$(1s)^2 2s_{\text{hydrogenic}}$	$(1s2s)1s'''$	$(1s)^2 4s_7$	$(1s)^2 2p_{\text{hydrogenic}}$	$(1s3s')3p''''$	$(4f)^2 3p''''$	$(1s)^2 3d''$	$(3p)^2 3d''$	$(5g)^2 3d''$
$(1s)^2 2s''$	$(1s1s')1s'''$	$(1s')^2 4s_7$	$(1s)^2 2p''$	$(2s3s')3p''''$	$(4f5f)3p''''$	$(1s2s)3d''$	$(2p2p')3d''$	$(1s)^2 4d_3$
$(1s)^2 1s''$	$(1s2s')1s'''$	$(1s3s')4s_7$	$(1s2s)2p''$	$(1s'3s')3p''''$	$(5f)^2 3p''''$	$(2s)^2 3d''$	$(3p2p')3d''$	$(1s2s)4d_3$
$(1s_1 2s_2)^3S\,1s_3$	$(1s2s)2s'''$	$(1s2s)4s_7$	$(1s1s')2p''$	$(2s'3s')3p''''$	$(1s)^2 4p_1$	$(1s1s')3d''$	$(2p')^2 3d''$	$(1s1s')4d_3$
$(1s_1 3s_5)^3S\,1s_3$	$(1s1s')2s'''$	$(1s2s')4s_7$	$(1s2s')2p''$	$(3s')^2 3p''''$	$(1s2s)4p_1$	$(2s1s')3d''$	$(2p3p')3d''$	$(1s2s')4d_3$
$(1s)^2 3s'''$	$(1s2s')2s'''$	$(1s_5 3s_8)1s_6$	$(1s3s')2p''$	$(2p)^2 3p''''$	$(1s1s')4p_1$	$(1s')^2 3d''$	$(3p3p')3d''$	$(2p)^2 4d_3$
$(1s2s)3s'''$	$(1s3s')2s'''$	$(1s_5 1s_7)1s_6$	$(2p)^2 2p''$	$(2p3p)3p''''$	$(1s3s')4p_1$	$(1s2s')3d''$	$(2p'3p')3d''$	$(1s_1 3d_3)^1D\,1s_3$
$(2s)^2 3s'''$	$(2p)^2 3s'''$	$(2s_8 2s_7)1s_6$	$(2p3p)2p''$	$(3p)^2 3p''''$	$(2p)^2 4p_1$	$(2s2s')3d''$	$(3p')^2 3d''$	$(1s_1 3d_3)^3D\,1s_3$
$(1s1s')3s'''$	$(2p3p)3s'''$	$(1s_5 3s_8)^3S\,1s_6$	$(3p)^2 2p''$	$(2p2p')3p''''$	$(1s_3 2p_4)^1P\,1s_2$	$(1s'2s')3d''$	$(3d)^2 3d''$	$(1s_1 3d_3)^1D\,1s_4$
$(2s1s')3s'''$	$(3p)^2 3s'''$	$(1s_5 1s_7)^3S\,1s_6$	$(1s)^2 2p'''$	$(3p2p')3p''''$	$(1s_3 3p_4)^1P\,1s_2$	$(2s')^2 3d''$	$(3d4d)3d''$	$(1s_1 3d_3)^3D\,1s_4$
$(1s')^2 3s'''$	$(2p2p')3s'''$	$(1s_5 4s_6)^3S\,1s_6$	$(1s)^2 3p''''$	$(3p')^2 3p''''$	$(1s_3 4p_4)^1P\,1s_2$	$(1s3s')3d''$	$(4d)^2 3d''$	$(2s_2 3d_3)^1D\,1s_3$
$(1s2s')3s'''$	$(2p3p')3s'''$	$(2s_8 2s_7)^3S\,1s_6$	$(2s)^2 3p''''$	$(2p3p')3p''''$	$(2s3p_4)^1P\,1s_2$	$(2s3s')3d''$	$(3d5d)3d''$	$(2s_2 3d_3)^3D\,1s_3$
$(2s2s')3s'''$	$(3p3p')3s'''$	$(3p2p'')^3S\,1s$	$(1s2s)3p''''$	$(3p3p')3p''''$	$(1s_3 2p_4)^3P\,1s_2$	$(1s'3s')3d''$	$(4d5d)3d''$	$(2s_2 3d_3)^3D\,1s_4$
$(1s'2s')3s'''$	$(3p')^2 3s'''$	$(2p3p)^3S\,1s$	$(1s1s')3p''''$	$(2p'3p')3p''''$	$(1s_3 3p_4)^3P\,1s_2$	$(2s'3s')3d''$	$(5d)^2 3d''$	$(2s_2 3d_3)^3D\,1s_4$
$(2s')^2 3s'''$	$(3d)^2 3s'''$	$(1s'3s')^3S\,1s_6$	$(2s1s')3p''''$	$(3d)^2 3p''''$	$(1s_3 4p_4)^3P\,1s_2$	$(3s')^2 3d''$	$(4f)^2 3d''$	$(2p)^2 3d_3$
$(1s3s')3s'''$	$(3d4d)3s'''$	$(1s2s)^3S\,3s'''$	$(1s')^2 3p''''$	$(3d4d)3p''''$	$(2s3p_4)^3P\,1s_2$	$(2p)^2 3d''$	$(4f5f)3d''$	
$(2s3s')3s'''$	$(4d)^2 3s'''$	$(1s3s')^3S\,3s'''$	$(1s2s')3p''''$	$(4d)^2 3p''''$	$(2s_3 3p_4)^3P\,1s_2$			
$(1s'3s')3s'''$	$(3d5d)3s'''$	$(2s3s')^3S\,3s'''$	$(2s2s')3p''''$	$(3d5d)3p''''$	$(2s_3 4p_4)^3P\,1s_2$			
$(2s'3s')3s'''$	$(4d5d)3s'''$	$(1s2s)^3S\,1s_3$	$(1s'2s')3p''''$	$(4d5d)3p''''$	$(1s3p_4)^3P\,1s_2$			

TABLE II. Eigenvalues for O VI ($Z = 8$) in a.u.

		$-E\,(1s^2 3s\,^2S)$	$-E\,(1s^2 3p\,^2P)$	$-E\,(1s^2 3d\,^2D)$
Weiss (HF)		61.268 11	61.148 67	61.112 10
This paper	variational	61.299 33	61.190 25	61.156 69
	Z-expansion	61.299 33	61.190 25	61.156 69

After diagonalizing H, these recurrence relations can easily and rapidly be evaluated. Provided the expansions converge, the results are identical to those given by diagonalizing the total Hamiltonian H in the Φ_k basis for each value of Z.

The oscillator strength for a dipole transition from an initial state ψ_n to a final state ψ'_n is given in the length formulation by

$$f_L = \tfrac{2}{3}(E'_n - E_n)\left|\langle \Psi_n |\sum_{i=1}^{3} \vec{\mathrm{r}}_i | \psi'_n\rangle\right|^2 , \qquad (9)$$

and in the velocity formulation by

$$f_V = \tfrac{2}{3}(E'_n - E_n)^{-1}\left|\langle \psi_n |\sum_{i=1}^{3} \vec{\nabla}_i | \psi'_n\rangle\right|^2 . \qquad (10)$$

Substituting Eqs. (2) into expressions (9) and (10), we may generate expansions of oscillator strengths in powers of Z^{-1}. If the wave functions are exact solutions to Schrödinger's equation, the coefficients in the length and velocity forms are identical.

III. CALCULATIONS AND RESULTS

In the method of configuration interaction, the state function is represented as a linear combination of many electron wave functions representing various electron configurations. Each configuration consists of a sum of determinantal wave functions chosen to be eigenfunctions of $\vec{\mathrm{S}}^2$ and $\vec{\mathrm{L}}^2$; that is, they are coupled to give the desired spin and angular momentum symmetry. The determinantal wave functions are composed of single-electron wave functions (Slater-type spin orbitals) which are normalized but not orthogonal.

The Z-expansion method converges more rapidly for the higher values of nuclear charge, and the 35-term function for O VI of Weiss[2,4] was used as the K-shell starting point for all three states. Moreover, some configurations representing the $2\,^2S$ and $2\,^2P$ states were added to the $3\,^2S$ states, respectively. Variational calculations with respect to the second root of the secular determinantal equation prevented energy collapse to either the $2\,^2S$ or $2\,^2P$ state. We attempted to improve the wave functions by selectively increasing the number of configurations. The second-order energy of a three-electron system may be given in terms of second-order energies of two-electron systems[5]:

$$E^{(2)}(1s^2 nl) = E^{(2)}(1s^2\,^1S) + \tfrac{1}{2}E^{(2)}(1snl\,^1L) + \tfrac{3}{2}E^{(2)}(1snl\,^3L) + \zeta(nl) , \qquad (11)$$

where $\zeta(nl)$ is a sum of single-electron integrals. The form suggests the inclusion of configurations of $^{1,3}S$-core nature for the $3\,^2S$, $^{1,3}P$ core for the $3\,^2P$, and $^{1,3}D$-core symmetry for the $3\,^2D$ states.

In all, 25 configurations involving nine optimized screening parameters (obtained in the standard variational minimization of the total energies) were added to make a 60-term $3\,^2S$. Similarly, 27 new configurations involving eight optimized screening parameters and 20 configurations with eight improved screening parameters were added to make the 60-term $3\,^2P$ and 50-term $3\,^2D$ states, respectively. The values for the screening param-

TABLE III. Energy-expansion coefficients $E_n^{(s)}$ (a.u.).

Order s	$(1s)^2 3s\,^2S$	$(1s)^2 3p\,^2P$	$(1s)^2 3d\,^2D$
0	−1.055 555 56(0)	−1.055 555 56(0)	−1.055 555 56(0)
1	8.182 067 86(−1)	8.381 195 11(−1)	8.467 987 06(−1)
2	−2.888 903 85(−1)	−3.350 270 59(−1)	−3.725 900 71(−1)
3	−2.710 299 45(−2)	−4.808 533 70(−2)	−6.240 405 29(−2)
4	1.376 946 79(−1)	4.854 924 33(−2)	5.626 590 59(−1)
5	2.514 446 71(−1)	3.509 586 80(−1)	−2.208 389 01(0)
6	8.042 915 88(−1)	7.435 292 04(−1)	−5.252 026 58(0)
7	2.941 795 34(0)	−6.239 883 42(0)	4.668 582 25(1)
8	−1.053 329 40(1)	−3.551 460 56(1)	1.287 532 07(2)
9	−7.835 011 83(1)	1.792 530 08(2)	−3.821 604 22(2)
10	−7.600 777 67(1)	−8.125 576 78(2)	−1.034 704 32(3)

TABLE IV. $1/Z$-expansion eigenvalues (in a.u.) for the lithium sequence.

Z	$-E((1s)^2 3s\ ^2S)$	$-E((1s)^2 3p\ ^2P)$	$-E((1s)^2 3d\ ^2D)$
5	22.583 84	22.540 99	22.526 98
6	33.378 65	33.312 18	33.294 01
7	46.283 66	46.195 56	46.170 04
8	61.299 33	61.190 25	61.156 69
9	78.425 86	78.296 25	78.254 29
10	97.663 37	97.513 37	97.462 96
11	119.011 91	118.841 64	118.782 73
12	142.471 52	142.281 06	142.213 61
13	168.042 21	167.831 61	167.755 61
14	195.724 00	195.493 30	195.408 73

eters and the list of configurations for the three states are shown in Table I. Table II contains a comparison of the energies obtained from Hartree-Fock wave functions with the variational energies calculated here.

Using the basis sets derived from the new variational wave functions, perturbed wave functions and eigenenergies for the lithium isoelectronic sequence were generated from expressions (7) and (8). Our basis sets were found to give values of $E^{(2)}(1s^2 3s\,^2S) = -0.288\,890\,4$ a.u., $E^{(2)}(1s^2 3p\,^2P) = -0.335\,027\,1$ a.u., and $E^{(2)}(1s^2 3d\,^2D) = -0.372\,590\,1$ a.u. for the second-order perturbed energies. These may be compared with the exact values of Horak *et al.*[6] which give $E^{(2)}(1s^2 3s\,^2S) = -0.304\,231\,7$ a.u., $E^{(2)}(1s^2 3p\,^2P) = -0.344\,156\,2$ a.u., and $E^{(2)}(1s^2 3d\,^2D) = -0.378\,060\,3$ a.u. Table II shows the excellent agreement between the eigenenergies derived variationally for O VI and those obtained from the $1/Z$-expansion theory. The energy-expansion coefficients for the $3\,^2S$, $3\,^2P$, and $3\,^2D$ states of the lithium series are given through

TABLE V. Oscillator strengths for O VI ($Z = 8$).

Transition	Weiss (Hartree Fock)[a]	Configuration interaction	$1/Z$ expansion
$2p$-$3s$			
length	0.0861	0.0835	0.0835
velocity	0.0885	0.0862	0.0862
$2s$-$3p$ length	0.2617	0.2596	0.259(5)
velocity	0.2558	0.2622	0.262(0)
$2p$-$3d$ length	0.6615	0.6595	0.660(0)
velocity	0.6563	0.6642	0.664(3)
$3s$-$3p$ length	0.3345	0.3353	0.3353
velocity	0.3557	0.3232	0.31(6)
$3p$-$3d$			
length	0.0481	0.0485	0.048(5)
velocity	0.0467	0.0423	0.04(2)

[a] Reference 2.

TABLE VI. Length f_L and velocity f_V expansion coefficients.

	$2p$-$3s$		$3s$-$3p$		$2s$-$3p$		$3p$-$3d$		$2p$-$3d$	
s	$f_L^{(s)}$	$f_V^{(s)}$	$f_V^{(s)}$	$f_V^{(s)}$	$f_L^{(s)}$	$f_V^{(s)}$	$f_L^{(s)}$	$f_V^{(s)}$	$f_L^{(s)}$	$f_V^{(s)}$
0	−4.0769(−2)	−4.0769(−2)	0.0000(0)	0.0000(0)	4.3487(−1)	4.3487(−1)	0.0000(0)	0.0000(0)	6.9578(−1)	6.9578(−1)
1	−2.3627(−1)	−2.3781(−1)	2.1506(0)	2.0976(0)	−1.2323(0)	−1.1601(0)	3.9056(−1)	4.1645(−1)	−3.2627(−1)	−2.3683(−1)
2	−7.9039(−1)	−7.0172(−1)	2.7722(0)	4.2887(0)	−1.2683(0)	−1.9140(0)	8.0888(−2)	9.4355(−1)	1.5768(−1)	−8.3899(−1)
3	−1.1070(0)	−1.4510(0)	1.7476(0)	8.2265(0)	−2.0669(0)	−7.6548(−1)	−2.7713(0)	−1.9624(1)	5.8837(0)	1.1637(−1)
4	3.7500(0)	−4.2073(0)	−1.8383(1)	−9.2146(−1)	1.0189(1)	1.1022(1)	9.9701(0)	6.2950(1)	−4.5105(1)	−3.7472(1)
5	1.2192(1)	−1.2348(1)	−9.0739(1)	8.1198(1)	3.8036(1)	7.3808(1)	−1.5038(1)	8.2645(2)	−1.8729(2)	−2.7219(2)
6	−6.6562(1)	−1.9857(1)	−2.4397(2)	7.2720(2)	−2.5780(2)	−4.0543(2)	−5.2356(2)	−2.9655(3)	1.0100(3)	9.7892(2)
7	−4.1808(2)	−5.1307(0)	−9.5963(2)	1.2600(4)	−5.6264(1)	2.2468(3)	−1.0917(3)	−2.6878(4)	6.1048(3)	7.2097(3)
8	−1.6689(2)	8.6652(1)	−3.9931(3)	−8.3846(4)	−7.8630(3)	−3.8779(4)	9.4868(3)	2.7426(4)	4.8414(2)	1.1943(3)
9	6.9056(3)	6.4092(2)	−6.2343(3)	8.9628(5)	1.3907(5)	5.0461(5)	3.1898(4)	4.9329(5)	−4.0732(4)	−3.7446(4)
10	3.3593(4)	1.9486(3)	7.6961(2)	−1.2514(7)	−1.3775(6)	−5.8113(6)	−2.0110(4)	−7.3408(5)	−3.3714(4)	6.5035(4)
11	4.7218(4)	−3.4729(3)	4.9507(5)	1.4840(8)	1.7025(7)	7.1209(7)	−6.5834(5)	−1.6182(7)	−8.6301(5)	−7.2609(5)
12	−2.2938(5)	−4.5803(4)	−1.9269(6)	−1.7965(9)	−2.1052(8)	−8.6921(8)	8.8924(6)	7.9028(6)	−7.0226(6)	−8.9115(6)

TABLE VII. Zero- and first-order length expansion coefficients.

Transition	$f_L^{(0)}$	$f_L^{(1)}$
$2s$-$3p$		
Laughlin (Ref. 9)	0.4349	−1.2353
this work ($1/Z$)	0.4349	−1.2323
$2p$-$3s$		
Laughlin (Ref. 9)	0.0408	0.2388
this work ($1/Z$)	0.0408	0.2363
$2p$-$3d$		
Laughlin (Ref. 9)	0.6958	−0.3492
this work ($1/Z$)	0.6958	−0.3263
$3s$-$3p$		
Laughlin (Ref. 9)	0.0	2.1506
this work ($1/Z$)	0.0	2.1506
$3p$-$3d$		
Laughlin (Ref. 9)	0.0	0.3906
this work ($1/Z$)	0.0	0.3906

tenth order in Table III. Table IV lists the $1/Z$-expansion eigenvalues for the lithium isoelectronic sequence from B III to Si XII.

The variational wave functions derived for O VI were used with the $2\,^2S$ and $2\,^2P$ wave functions developed previously[2] to calculate both the dipole-length and dipole-velocity forms of the oscillator strengths for the $2p$-$3s$, $3s$-$3p$, $2s$-$3p$, $3p$-$3d$, and $2p$-$3d$ transitions. Table V compares the oscillator-strength values obtained for O VI using variational wave functions with those determined by Weiss[2] employing Hartree-Fock wave functions. We have used experimental energy differences[7,8] to compute ΔE so that the inaccuracies in the calculation arise solely from the transition integral.

The oscillator strength may also be expanded in powers of Z^{-1}. Table VI gives the length (f_L) and velocity (f_V) expansion coefficients through 12th order for the five transitions. For each transition, the correct value for the leading term in each series is the hydrogenic value. Table VII is a comparison between the zero- and first-order length expansion coefficients derived here with those determined by Laughlin *et al.*[9] Table V displays the excellent agreement between the oscillator strengths obtained variationally for O VI with those derived from the $1/Z$-expansion theory. Table VIII is a collection of the dipole-length and dipole-velocity oscillator strengths for C IV through Si XII. It is to be noted that the series expansions for the oscillator strengths exhibited poor convergence for the low values of Z.

Table VIII also shows that for high-Z values the length formulation is more accurate for predicting the values of the oscillator strength. Dalgarno and Lewis[10] demonstrated that, in general,

TABLE VIII. Oscillator strengths for the lithium isoelectronic sequence.

Z	6	7	8	9	10	11	12	13	14
$2s$-$3p$									
length (HF)[a]	0.2004	0.2354	0.2617	0.2819	0.2979				
velocity (HF)[a]	0.1923	0.2286	0.2558	0.2768	0.2934				
length ($1/Z$)	0.19	0.23	0.259(5)	0.2813	0.2981	0.3121	0.3234	0.3329	0.3399[b]
velocity ($1/Z$)	0.19	0.23	0.262(0)	0.2834	0.3003	0.3135	0.3245	0.3336	0.3423[b]
$2p$-$3s$									
length (HF)[a]	0.1127	0.0965	0.0861	0.0789	0.0736				
velocity (HF)[a]	0.1159	0.0993	0.0885	0.0810	0.0755				
length ($1/Z$)	0.104	0.0921	0.0835	0.0775	0.0728	0.0692	0.0663	0.0639	0.0620
velocity ($1/Z$)	0.113(3)	0.0966	0.0862	0.0789	0.0738	0.0698	0.0667	0.0642	0.0620
$2p$-$3d$									
length (HF)[a]	0.6542	0.6580	0.6615	0.6646	0.6671				
velocity (HF)[a]	0.6455	0.6514	0.6563	0.6603	0.6639				
length ($1/Z$)	0.65(8)	0.655(4)	0.660(0)	0.6636	0.6662	0.6694	0.6717	0.6736	0.6753
velocity ($1/Z$)	0.66(5)	0.662(1)	0.664(3)	0.6671	0.6703	0.6718	0.6736	0.6751	0.6763
$3s$-$3p$									
length (HF)[a]	0.4812	0.3949	0.3345	0.2902	0.2561				
velocity (HF)[a]	0.5107	0.4195	0.3557	0.3084	0.2722				
length ($1/Z$)		0.45(5)	0.3353	0.2919	0.2563	0.2326	0.2121	0.1945	0.1677[b]
velocity ($1/Z$)		0.4(5)	0.31(6)	0.27(7)	0.24(8)	0.218(8)	0.196(4)	0.1783	0.1750[b]
$3p$-$3d$									
length (HF)[a]	0.0623	0.0544	0.0481	0.0432	0.0382				
velocity (HF)[a]	0.0568	0.0516	0.0467	0.0420	0.0389				
length ($1/Z$)		0.05(4)	0.048(5)	0.0438	0.0383	0.0365	0.0337	0.0314	0.0266[b]
velocity ($1/Z$)		0.04(1)	0.04(2)	0.04(0)	0.038(3)	0.034(1)	0.0314	0.0291	0.0300[b]

[a] Reference 2.

[b] Theoretical nonrelativistic energy differences.

for transitions occurring between closely spaced energy levels, the dipole-length form is to be preferred; whereas, for widely spaced levels, the dipole-velocity form is to be preferred.

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