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Energies and oscillator strengths for lithiumlike ions

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The Hylleraas-type variational method is used to calculate the energies of the lithium $1s^2 2s\ ^2S$ and $1s^2 2p\ ^2P$ isoelectronic sequences up to $Z=20$. The oscillator strengths for the $1s^2 2s\ ^2S \rightarrow 1s^2 2p\ ^2P$ transitions are evaluated for Z up to 20, including finite nuclear mass effects, and the corresponding lifetimes are determined. The $1/Z$ expansion method is used to extend the variational results to larger values of Z. Relativistic corrections to the dipole transition moment squared are estimated by comparison with the relativistic many-body perturbation theory results of Johnson *et al.* [At. Data Nucl. Data Tables **64**, 279 (1996)]. The final lifetime for the $1s^2 2p\ ^2P$ state of lithium is in good agreement with recent high-precision measurements. [S1050-2947(98)02602-X]

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I. INTRODUCTION

In recent years, we have done several high-precision calculations for lithium atomic properties using a fully correlated Hylleraas-type variational method [1–5]. In particular, we have performed a high-precision calculation for the $2\,^2S \rightarrow 2\,^2P$ oscillator strength [3], which is in excellent agreement with the two most recent measurements [6,7], thereby resolving a long-standing discrepancy between theory and experiment.

The purpose of this paper is to extend our variational method to lithiumlike ions. We focus on the evaluation of the $2\,^2S$ and $2\,^2P$ energy sequences, as well as the $2\,^2S \rightarrow 2\,^2P$ oscillator strength sequence. For lithiumlike ions, several calculations have been reported of energies and oscillator strengths. The lithium ground-state isoelectronic sequence was investigated Perkins [8] and by Ho [9] using Hylleraas coordinates and calculations on the lithium isoelectronic sequences for some low-lying excited S states were carried out by King [10–12]. Theodosiou *et al.* [13] calculated $2\,^2P$ lifetimes in the lithium isoelectronic sequence using the semi-empirical Coulomb approximation and Chung, Zhu, and Wang [14–16] calculated isoelectronic sequences for some low-lying excited states using a full core plus correlation (FCPC) method. Recently, transition rates for lithiumlike ions were calculated by Johnson *et al.* [17] using relativistic many-body perturbation theory (RMBPT).

The variational calculations are discussed in Sec. II. The structure of the wave functions is outlined in Sec. II A and the results for both energy and oscillator strength are presented in Secs. II B and II C. The large-Z expansion method is applied in Sec. III to these calculations and a comparison is made between the two methods. Finally, in Sec. IV relativistic corrections to the dipole transition moment squared are estimated by comparison with the RMBPT calculations for moderately large values of Z and the final results for the lifetime of the $1s^2 2p\ ^2P$ state are compared with high-precision measurements [6,7]. It is shown that both relativistic and finite nuclear mass corrections must be included in order to obtain agreement. The two effects act in opposite directions and to some extent cancel one another.

II. VARIATIONAL CALCULATIONS

A. Basis sets

A main difference from our previous work [2] is that the wave functions of the two-electron $\mathrm{Li}^+(1s^2\ ^1S)$ core and the screened hydrogenic valence electron $(n\ell)$ are included explicitly in the total wave function as a zeroth-order approximation. This is because for Rydberg states, the interaction between the core and the valence electron becomes increasingly weak with increasing ℓ, making the zeroth-order approximation increasingly accurate. A similar picture has been used in the two-electron calculations [18] and has proved to be useful in accelerating the rate of convergence and in preserving the numerical stability, particularly for the more highly excited states. However, it does no harm to the ground-state calculations. In Z-scaled atomic units, where distance is measured in units of Z^{-1} a.u. and energy is measured in units of Z^2 a.u., the total Hamiltonian H is thus decomposed into two parts

$$H = H_S + V_I, \tag{1}$$

where H_S describes the core and the valence electron

$$H_S = \left(-\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{Zr_{12}}\right) + \left(-\frac{1}{2}\nabla_3^2 - \frac{Z-2}{Zr_3}\right) \tag{2}$$

and V_I is the interaction between the core and the valence electron

$$V_I = Z^{-1}\left(\frac{1}{r_{23}} + \frac{1}{r_{31}} - \frac{2}{r_3}\right). \tag{3}$$

The solutions to the zeroth-order eigenequation

$$H_S \psi_0 = E_0 \psi_0 \tag{4}$$

can be written in the form

$$\psi_0=\phi_c(1s^2\ {}^1S)\,\phi_v\left(n\ell;\frac{Z-2}{Z}\right), \tag{5}$$

where $\phi_c(1s^2\ {}^1S)$ is the wave function of the core in the ground state and $\phi_v(n\ell;Z)$ is the hydrogenic wave function for the valence electron in the $(n\ell)$ state with the nuclear charge Z. Thus, with ψ_0 included, the trial variational wave function can be expanded according to

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\mathcal{A}\left(a_0\psi_0\chi_1+\sum_{i=1}^{N}a_i\psi_i\chi_1\right), \tag{6}$$

where ψ_i is a general term in the basis set, which has the form

$$r_1^{j_1}\,r_2^{j_2}\,r_3^{j_3}\,r_{12}^{j_{12}}r_{23}^{j_{23}}r_{31}^{j_{31}}e^{-\alpha r_1-\beta r_2-\gamma r_3}\times\mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3), \tag{7}$$

where

$$\begin{aligned}\mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}&=r_1^{\ell_1}r_2^{\ell_2}r_3^{\ell_3}\sum_{m_i}\langle\ell_1m_1;\ell_2m_2|\ell_1\ell_2;\ell_{12}m_{12}\rangle\\&\quad\times\langle\ell_{12}m_{12};\ell_3m_3|\ell_{12}\ell_3;LM\rangle\\&\quad\times Y_{\ell_1m_1}(\mathbf{r}_1)Y_{\ell_2m_2}(\mathbf{r}_2)Y_{\ell_3m_3}(\mathbf{r}_3)\end{aligned} \tag{8}$$

is a vector-coupled product of spherical harmonics for the three electrons to form a state of total angular momentum L, χ_1 is a spin function with the spin angular momentum 1/2

$$\chi_1=\alpha(1)\beta(2)\alpha(3)-\beta(1)\alpha(2)\alpha(3), \tag{9}$$

and $\mathcal{A}$ is the three-particle antisymmetrizer defined by

$$\mathcal{A}=(1)-(12)-(13)-(23)+(123)+(132). \tag{10}$$

As described previously [2], all terms from Eq. (7) are nominally included such that

$$j_1+j_2+j_3+j_{12}+j_{23}+j_{31}\leqslant\Omega \tag{11}$$

and the convergence of the eigenvalues is studied as Ω is progressively increased. However, terms that may potentially cause near linear dependences are excluded. For example, if $\ell_1=\ell_2$ and $\alpha\approx\beta$, then terms with $j_1>j_2$ are omitted, as well as terms with $j_1=j_2$ when $j_{23}>j_{31}$. The presence of the near-linear dependences in the basis set can be detected by diagonalizing the positive-definite overlap matrix to see if there is any abnormally small or negative eigenvalue.

The basis sets $\{\psi_i, i=1,\ldots,N\}$ are constructed as follows. For a given angular momentum L, the angular coupling for the three electrons is

$$(\ell_1,\ell_2,\ell_3)=(0,0,0)_A\quad\text{for } S \text{ states},$$

$$(\ell_1,\ell_2,\ell_3)=(0,0,1)_A,(0,1,0)_B\quad\text{for } P \text{ states}.$$

The block $(0,0,L)_A$ can further be divided into five sectors [2] with different nonlinear parameters α, β, and γ. The basis sets thus contain five sectors for S states and six sectors for P states. Finally, the size of each sector is separately controlled by assigning to each an Ω_i value according to

$$\{\Omega_1,\Omega_2,\Omega_3,\Omega_4,\Omega_5\}=\{\Omega,\Omega,\Omega,(\Omega,9)_{\min},(\Omega,9)_{\min}\},\ L=0$$

$$\begin{aligned}&\{\Omega_1,\Omega_2,\Omega_3,\Omega_4,\Omega_5,\Omega_6\}\\&=\{\Omega,\Omega,(\Omega,9)_{\min},(\Omega,7)_{\min},(\Omega,7)_{\min},(\Omega-2,7)_{\min}\},\ L=1,\end{aligned}$$

where $(a,b)_{\min}$ denotes $\min(a,b)$.

B. Nonrelativistic eigenvalues

The nonlinear parameters are optimized for each sector according to the variational principle. The procedure is to calculate the derivatives analytically from

$$\frac{\partial E}{\partial\alpha}=2\left\langle\Psi\middle|H\middle|\frac{\partial\Psi}{\partial\alpha}\right\rangle-2E\left\langle\Psi\middle|\frac{\partial\Psi}{\partial\alpha}\right\rangle, \tag{12}$$

where α represents any nonlinear parameter and $\langle\Psi|\Psi\rangle=1$ is assumed, and then to locate the zeros of the derivatives by Newton's method.

Table I lists the convergence study for the nonrelativistic energies, as the size of basis set is enlarged. The ratio $R(\Omega)$ is defined by

$$R(\Omega)=\frac{E(\Omega-1)-E(\Omega-2)}{E(\Omega)-E(\Omega-1)}. \tag{13}$$

The extrapolated values for $\Omega=\infty$ are obtained by assuming the functional form [2]

$$R(\Omega)=1+\frac{a}{\Omega^b} \tag{14}$$

and determining the parameters a and b by a least-squares fit to the tabulated values. The two-electron core wave functions are represented by 135 Hylleraas-type functions, which yield, for example, the Li^+ energy of $-7.279\,913\,412$ a.u. The present results have improved our previous calculations and demonstrated the importance of including the core wave function ψ_0 in the basis set, especially for P states. Typically, the use of ψ_0 for P states improves the results by about a factor of 4 to 5 (in the sense of percentage error). The overall accuracy we have achieved for the lithium $2\ {}^2S$ and $2\ {}^2P$ states is about a few parts in 10^{12}. Table II contains the nonrelativistic energies for the $2\ {}^2S$ and $2\ {}^2P$ isoelectronic sequences up to $Z=20$. Values are given for both the infinite nuclear mass case and the finite nuclear mass case with the mass polarization term included explicitly in the Hamiltonian. The electron to nuclear mass ratios used in the latter case are as listed in Table III. Table IV shows a comparison with some published results for lithiumlike ions. Our calculation improves the accuracy of previous values by several orders of magnitude.

C. Oscillator strengths

In Ref. [3] we discussed a generalized equivalence between the length and velocity forms of the transition operator

TABLE I. Convergence of the nonrelativistic energies for the $1s^22s\ ^2S$ and $1s^22p\ ^2P$ states of lithium, in atomic units.

Ω	No. of terms	$E(\Omega)$	$E(\Omega)-E(\Omega-1)$	$R(\Omega)$
		$1s^22s\ ^2S$		
2	19	−7.477 555 720 321 8		
3	51	−7.477 995 835 140 8	−0.000 440 114 819 0	
4	121	−7.478 053 567 299 9	−0.000 057 732 159 1	7.623
5	257	−7.478 059 464 463 7	−0.000 005 897 163 8	9.790
6	503	−7.478 060 228 080 1	−0.000 000 763 616 4	7.723
7	919	−7.478 060 311 092 9	−0.000 000 083 012 9	9.199
8	1590	−7.478 060 321 724 7	−0.000 000 010 631 8	7.808
9	2626	−7.478 060 323 416 8	−0.000 000 001 692 1	6.283
10	3502	−7.478 060 323 618 9	−0.000 000 000 202 1	8.371
∞		−7.478 060 323 650 3(71)		
		$1s^22p\ ^2P$		
2	20	−7.410 088 210 427		
3	56	−7.410 146 240 952	−0.000 058 030 525	
4	139	−7.410 155 057 909	−0.000 008 816 956	6.582
5	307	−7.410 156 274 821	−0.000 001 216 912	7.245
6	623	−7.410 156 490 483	−0.000 000 215 662	5.643
7	1175	−7.410 156 524 272	−0.000 000 033 789	6.383
8	1846	−7.410 156 530 070	−0.000 000 005 798	5.828
9	2882	−7.410 156 531 534	−0.000 000 001 464	3.960
10	3463	−7.410 156 531 721	−0.000 000 000 187	7.813
∞		−7.410 156 531 763(42)		

that takes finite nuclear mass effects into full account. By introducing two effective radiative charges

$$Z_p=\frac{Zm+M}{M},\quad Z_r=\frac{Zm+M}{\Lambda m+M},\tag{15}$$

where m is the electron mass, M the nuclear mass, Z the nuclear charge, and Λ the number of electrons, the oscillator strength for a $\gamma L\to\gamma' L'$ transition, as well as the equivalence between the length and velocity forms, can be expressed according to

$$\begin{aligned}f(\gamma\to\gamma')&=\frac{2m\omega_{\gamma\gamma'}}{3}\left(\frac{Z_r}{Z_p}\right)\left|\left\langle\gamma\left|\sum_{i=1}^{\Lambda}\mathbf{r}_i\right|\gamma'\right\rangle\right|^2\\&=\frac{2}{3m\omega_{\gamma\gamma'}}\left(\frac{Z_p}{Z_r}\right)\left|\left\langle\gamma\left|\sum_{i=1}^{\Lambda}\mathbf{p}_i\right|\gamma'\right\rangle\right|^2,\end{aligned}\tag{16}$$

where $\omega_{\gamma\gamma'}$ is the transition energy. It can be shown that this definition of the oscillator strength satisfies the Thomas-Reiche-Kuhn sum rule $\Sigma_{\gamma'}f(\gamma\to\gamma')=\Lambda$, independent of m/M. It should be emphasized that in the calculation of wave functions for the finite nuclear mass case, the mass polarization term $M^{-1}\Sigma_{i>j}\mathbf{p}_i\cdot\mathbf{p}_j$ is included explicitly in the Hamiltonian. The transition rate is

$$A_{\gamma'\gamma}=Z_rZ_p\omega^2_{\gamma\gamma'}\frac{g_\gamma}{g_{\gamma'}}f(\gamma\to\gamma')\times 3.213\,001\,846\times10^{10}\ \mathrm{s}^{-1},\tag{17}$$

where g_γ and $g_{\gamma'}$ are the statistical weights of the initial and final states and $\omega_{\gamma\gamma'}$ is in atomic units. The lifetime for the state γ is then

$$\tau=\frac{1}{\sum_{\gamma'}A_{\gamma\gamma'}},\tag{18}$$

where the summation is over all states lower than γ.

Table V displays a convergence study for the lithium $2\,^2S\to2\,^2P$ oscillator strength in both length and velocity forms for the case of infinite nuclear mass. The corresponding sizes of basis set is denoted by (N_1,N_2) in the first column, where N_1 and N_2 are the number of terms of the lower and upper states, respectively. The length form is more rapidly convergent than the velocity form. Nevertheless, the agreement between the two forms is about 4 ppm (parts per 10^6). The present result, which has an accuracy of 13 ppb (parts per 10^9), is about a factor of 100 improvement upon the best published result of Yan and Drake [3]. The equivalence between the length and velocity forms Eq. (16) for the finite nuclear mass case has also been verified by our calculations. For example, for $Z=6$, the two forms agree with each other at the 1-ppm level. Table VI lists $2\,^2S\to2\,^2P$ oscillator strengths and $2\,^2P$ state lifetimes of lithium and lithiumlike ions for both infinite and finite nuclear mass cases. Table VII presents a comparison with selected published values.

III. LARGE-Z EXPANSION CALCULATIONS

For large Z, it is advantageous to perform a perturbation expansion in powers of Z^{-1} so that the entire lithium iso-

TABLE II. Nonrelativistic energies for the $1s^22s\ ^2S$ and $1s^22p\ ^2P$ state isoelectronic sequences. Each pair of numbers gives results for infinite nuclear mass (in units of $2R_\infty$) and finite nuclear mass (in units of $2R_M$) as indicated, using the mass ratios listed in Table III.

Z	$1s^22s\ ^2S$	$1s^22p\ ^2P$
3	−7.478 060 323 650 3(71)[a]	−7.410 156 531 763(42)
	−7.478 036 728 105 9(82)[b]	−7.410 137 246 10(18)
4	−14.324 763 176 465 4(62)	−14.179 333 292 357(43)
	−14.324 735 613 615 4(73)	−14.179 323 188 90(22)
5	−23.424 605 720 957(70)	−23.204 441 192 360(22)
	−23.424 575 528 36(24)	−23.204 445 369 92(24)
6	−34.775 511 275 626(12)	−34.482 103 179 278(33)
	−34.775 476 534 410(81)	−34.482 125 788 63(29)
7	−48.376 898 319 137(11)	−48.011 054 281 682(27)
	−48.376 862 493 054(75)	−48.011 095 942 56(29)
8	−64.228 542 082 701(50)	−63.790 739 579 263(40)
	−64.228 505 407 079(96)	−63.790 800 952 10(17)
9	−82.330 338 097 298(12)	−81.820 880 913 294(30)
	−82.330 302 742 162(89)	−81.820 958 069 35(25)
10	−102.682 231 482 398(10)	−102.101 324 295 077(30)
	−102.682 193 627 290(55)	−102.101 426 131 00(24)
11	−125.284 190 753 647 3(87)	−124.631 977 820 154(50)
	−125.284 154 128 019(47)	−124.632 094 903 58(18)
12	−150.136 196 604 459 4(71)	−149.412 783 333 673(25)
	−150.136 157 945 647(40)	−149.412 926 478 22(21)
13	−177.238 236 559 961(15)	−176.443 702 276 939(23)
	−177.238 199 034 098(58)	−176.443 860 182 00(18)
14	−206.590 302 212 278 0(87)	−205.724 708 091 496(20)
	−206.590 262 973 971(45)	−205.724 893 010 79(15)
15	−238.192 387 694 146 1(81)	−237.255 781 895 246(23)
	−238.192 349 496 810(41)	−237.255 981 166 53(16)
16	−272.044 488 790 072 5(82)	−271.036 909 900 167(22)
	−272.044 449 117 485(47)	−271.037 136 864 05(15)
17	−308.146 602 395 255 6(67)	−307.068 081 805 460(40)
	−308.146 563 681 624(36)	−307.068 322 775 56(17)
18	−346.498 726 173 671 4(78)	−345.349 289 761 848(17)
	−346.498 690 161 179(42)	−345.349 532 034 98(15)
19	−387.100 858 334 561(11)	−385.880 527 684 010(23)
	−387.100 819 210 531(59)	−385.880 810 587 66(15)
20	−429.952 997 482 762 6(67)	−428.661 790 781 805(23)
	−429.952 957 200 514(38)	−428.662 102 325 70(13)

[a] Energy for infinite nuclear mass.

[b] Energy with the mass polarization term included in the Hamiltonian.

TABLE III. Electron reduced mass to nuclear mass ratios μ/M for various atoms.

Z	Mass No.	$\mu/M\times10^4$
3	7	0.782 081 472
4	9	0.608 857 508
5	11	0.498 411 622
6	12	0.457 275 303
7	14	0.391 864 185
8	16	0.343 065 530
9	19	0.288 825 546
10	20	0.274 468 993
11	23	0.238 681 808
12	24	0.228 780 296
13	27	0.203 370 692
14	28	0.196 134 943
15	31	0.177 161 655
16	32	0.171 630 071
17	35	0.156 921 737
18	40	0.137 310 693
19	39	0.140 828 282
20	40	0.137 310 693

electronic sequence can be covered in a single calculation. Early work of this type was done by Dalgarno and coworkers [26]. For a review, see Ref. [27].

In Z-scaled atomic units, the Schrödinger equation is

$$H\phi=\epsilon\phi, \tag{19}$$

where the Hamiltonian is

$$H=H_0+Z^{-1}V, \tag{20}$$

with H_0 being the three-electron hydrogenic Hamiltonian

$$H_0=\sum_{i=1}^{3}\left(-\frac{1}{2}\nabla_i^2-\frac{1}{r_i}\right) \tag{21}$$

and V the interaction potential among the three electrons

$$V=\frac{1}{r_{12}}+\frac{1}{r_{23}}+\frac{1}{r_{31}}. \tag{22}$$

Taking Z^{-1} as a perturbation parameter, one has

$$\epsilon=\epsilon_0+Z^{-1}\epsilon_1+Z^{-2}\epsilon_2+\cdots, \tag{23}$$

$$\phi=\phi_0+Z^{-1}\phi_1+Z^{-2}\phi_2+\cdots. \tag{24}$$

Substituting the above two expansions into Eq. (19), the Schrödinger equation becomes a set of equations

$$H_0\phi_0=\epsilon_0\phi_0, \tag{25}$$

$$(H_0-\epsilon_0)\phi_1+V\phi_0=\epsilon_1\phi_0. \tag{26}$$

In general,

$$(H_0-\epsilon_0)\phi_p+V\phi_{p-1}=\sum_{i=1}^{p}\epsilon_i\phi_{p-i}. \tag{27}$$

These equations can be solved recursively and the first few energy expansion coefficients can be written

$$\epsilon_1=\langle\phi_0|V|\phi_0\rangle, \tag{28}$$

$$\epsilon_2=\langle\phi_0|V-\epsilon_1|\phi_1\rangle=\langle\phi_1|\epsilon_0-H_0|\phi_1\rangle, \tag{29}$$

$$\epsilon_3=\langle\phi_1|V-\epsilon_1|\phi_1\rangle-2\epsilon_2\langle\phi_1|\phi_0\rangle, \tag{30}$$

with the assumption that $\langle\phi_0|\phi_0\rangle=1$. In general, knowledge of the wave-function coefficients up to nth order is sufficient

TABLE IV. Comparison of nonrelativistic energies of lithium and lithiumlike ions, in atomic units. HR denotes the Hylleraas result, CI denotes the configuration interaction, and MCHF denotes the multiconfiguration Hartree-Fock result.

Author	Method	Ref.	$1s^22s\ ^2S$	$1s^22p\ ^2P$
			$Z=3$	
King and Bergsbaken	HR	[19]	−7.478 059 53	
Chung and Zhu	FCPC	[14]	−7.478 059 7(9)	−7.410 157 8(9)
McKenzie and Drake	HR	[20]	−7.478 060 326(10)	
Pipin and Bishop	CI-HR	[21]	−7.478 060 1	−7.410 155 4
Lüchow and Kleindienst	HR	[22]	−7.478 060 25	
Tong *et al.*	MCHF	[23]	−7.478 060 9	−7.410 153 1
Yan and Drake	HR	[2]	−7.478 060 323 10(31)	−7.410 156 521 8(13)
Pestka and Woźnicki	CI-HR	[24]	−7.478 060 10	−7.410 155 91
This work			−7.478 060 323 650 3(71)	−7.410 156 531 763(42)
			$Z=4$	
Perkins	HR	[8]	−14.324 57	
Ho	HR	[9]	−14.324 696	
King	HR	[10]	−14.324 760	
Chung and Zhu	FCPC	[14]	−14.324 761 0(11)	−14.179 332 0
This work			−14.324 763 176 465 4(62)	−14.179 333 292 357(43)
			$Z=5$	
Perkins	HR	[8]	−23.424 36	
Ho	HR	[9]	−23.424 523	
King	HR	[11]	−23.424 604	
Chung and Zhu	FCPC	[14]	−23.424 603 1(13)	−23.204 443 4
This work			−23.424 605 720 957(70)	−23.204 441 192 360(22)
			$Z=6$	
Perkins	HR	[8]	−34.775 22	
Ho	HR	[9]	−34.775 418	
King	HR	[11]	−34.775 509	
Chung and Zhu	FCPC	[14]	−34.775 508 2(15)	−34.482 098 2
This work			−34.775 511 275 626(12)	−34.482 103 179 278(33)
			$Z=7$	
Perkins	HR	[8]	−48.376 57	
Ho	HR	[9]	−48.376 798	
King	HR	[11]	−48.376 896	
Chung and Zhu	FCPC	[14]	−48.376 894 9(18)	−48.011 048 0
This work			−48.376 898 319 137(11)	−48.011 054 281 682(27)
			$Z=8$	
Perkins	HR	[8]	−64.228 19	
Ho	HR	[9]	−64.228 435	
King	HR	[11]	−64.228 540	
Chung and Zhu	FCPC	[14]	−64.228 538 5(19)	−63.790 731 5
This work			−64.228 542 082 701(50)	−63.790 739 579 263(40)
			$Z=9$	
King	HR	[11]	−82.330 336	
Chung and Zhu	FCPC	[14]	−82.330 334 8(21)	−81.820 874 4
This work			−82.330 338 097 298(12)	−81.820 880 913 294(30)
			$Z=10$	
King	HR	[11]	−102.682 229	
Chung and Zhu	FCPC	[14]	−102.682 227 8(22)	−102.101 315 8
This work			−102.682 231 482 398(10)	−102.101 324 295 077(30)

to calculate the energy coefficients up to $(2n+1)$th order, as proved by Dalgarno and Stewart [28].

Since H_0 consists of a sum of three hydrogen-atom Hamiltonians, the zeroth-order solutions ϕ_0 and ϵ_0 to Eq. (25) are known exactly. ϵ_1 can thus be calculated analytically. However, Eq. (26) can only be solved numerically for systems with two or more electrons. One approach is to choose a basis set $\{\theta_i, i=1,\ldots,N\}$ in Hylleraas coordinates

TABLE V. Convergence of lithium $1s^22s\ ^2S \rightarrow 1s^22p\ ^2P$ oscillator strengths in length and velocity forms for the case of infinite nuclear mass.

No. of terms	f(length)	f(velocity)
(51, 56)	0.748 504 001 2	0.752 133 1
(121, 139)	0.747 111 655 3	0.747 521 7
(257, 307)	0.746 989 731 2	0.747 172 7
(503, 623)	0.746 961 017 2	0.747 040 0
(919, 1175)	0.746 957 923 7	0.746 980 3
(1590, 1846)	0.746 957 253 8	0.746 969 1
(2626, 2882)	0.746 956 966 5	0.746 960 7
(3502, 3463)	0.746 956 949 4	0.746 960 3
extrapolation	0.746 956 939 6(98)	0.746 959 7(50)

with three nonlinear parameters α, β, and γ being hydrogenic values 1, 1, and $1/n$, respectively, and then to expand ϕ_1 according to

$$\phi_1 = \sum_{i=1}^{N} x_i \theta_i . \tag{31}$$

Then Eq. (26) is reduced to a matrix equation

$$AX = B, \tag{32}$$

where A is an $N \times N$ matrix with elements defined by

$$a_{ij} = \langle \theta_i | H_0 | \theta_j \rangle - \epsilon_0 \langle \theta_i | \theta_j \rangle \tag{33}$$

and B is an $N \times 1$ matrix with elements defined by

$$b_i = -\langle \theta_i | V | \phi_0 \rangle + \epsilon_1 \langle \theta_i | \phi_0 \rangle . \tag{34}$$

Once Eq. (32) is solved for $X = (x_1, x_2, \ldots, x_N)$, the energy coefficients can be calculated according to

TABLE VII. Comparison of nonrelativistic $1s^22s\ ^2S \rightarrow 1s^22p\ ^2P$ oscillator strengths of lithium and lithiumlike ions for the case of infinite nuclear mass. HR denotes the Hylleraas result.

Author	Method	Ref.	f
	$Z=3$		
Pipin and Bishop	CI-HR	[21]	0.747 0
Chung	FCPC	[15]	0.747 04
Yan and Drake	HR	[3]	0.746 957 2(10)
Godefroid	MCHF	[25]	0.746 955
This work	HR		0.746 956 939 6(98)
	$Z=4$		
Chung	FCPC	[15]	0.498 13
This work	HR		0.498 067 381(25)
	$Z=5$		
Chung	FCPC	[15]	0.363 29
This work	HR		0.363 243 128 5(92)
	$Z=6$		
Chung	FCPC	[15]	0.284 29
This work	HR		0.284 204 795 2(30)
	$Z=7$		
Chung	FCPC	[15]	0.232 99
This work	HR		0.232 970 178 3(15)
	$Z=8$		
Chung	FCPC	[15]	0.197 25
This work	HR		0.197 228 627 94(79)
	$Z=9$		
Chung	FCPC	[15]	0.170 94
This work	HR		0.170 928 220 91(35)
	$Z=10$		
Chung	FCPC	[15]	0.150 79
This work	HR		0.150 784 741 14(60)

TABLE VI. Nonrelativistic $1s^22s\ ^2S \rightarrow 1s^22p\ ^2P$ oscillator strengths and $1s^22p\ ^2P$ state lifetimes for lithiumlike ions.

Z	f_∞	f_M	τ_∞ (ns)	τ_M (ns)
3	0.746 956 939 6(98)	0.746 786 698(97)	27.109 821 58(36)	27.117 323 6(35)
4	0.498 067 381(25)	0.497 931 746(32)	8.863 696 22(44)	8.866 620 46(56)
5	0.363 243 128 5(92)	0.363 137 829(12)	5.302 957 83(14)	5.304 830 18(17)
6	0.284 204 795 2(30)	0.284 113 118 4(42)	3.816 231 313(41)	3.817 733 521(56)
7	0.232 970 178 3(15)	0.232 894 936 9(21)	2.994 456 336(19)	2.995 636 553(27)
8	0.197 228 627 94(79)	0.197 165 010 5(12)	2.469 925 447 5(98)	2.470 896 976(14)
9	0.170 928 220 91(35)	0.170 876 154 10(29)	2.104 656 018 6(43)	2.105 436 961 6(36)
10	0.150 784 741 14(60)	0.150 736 399 84(52)	1.835 014 013 4(73)	1.835 729 834 2(63)
11	0.134 871 576 95(16)	0.134 830 345 87(29)	1.627 462 651 3(19)	1.628 067 301 3(35)
12	0.121 987 039 487(97)	0.121 948 161 65(21)	1.462 593 520 2(12)	1.463 159 410 4(25)
13	0.111 343 880 771(37)	0.111 309 802 143(99)	1.328 368 728 56(44)	1.328 861 778 1(12)
14	0.102 405 290 73(24)	0.102 372 820 83(32)	1.216 912 322 2(29)	1.217 379 803 2(38)
15	0.094 792 869 42(16)	0.094 763 849 24(22)	1.122 847 884 5(19)	1.123 263 978 5(26)
16	0.088 232 313 73(14)	0.088 204 460 32(20)	1.042 376 212 0(17)	1.042 774 200 7(24)
17	0.082 519 982 805(24)	0.082 494 725 710(92)	0.972 734 388 85(28)	0.973 094 197 8(11)
18	0.077 501 550 373(15)	0.077 479 611 89(12)	0.911 863 827 18(18)	0.912 175 536 2(15)
19	0.073 057 947 005(52)	0.073 035 594 992(21)	0.858 198 550 71(61)	0.858 515 433 25(24)
20	0.069 095 845 451(62)	0.069 074 181 584(96)	0.810 525 722 35(73)	0.810 832 240 5(11)

$$\epsilon_2 = -\sum_{i=1}^{N} x_i b_i , \tag{35}$$

$$\epsilon_3 = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \langle \theta_i | V - \epsilon_1 | \theta_j \rangle - 2\epsilon_2 \sum_{i=1}^{N} x_i \langle \theta_i | \phi_0 \rangle . \tag{36}$$

Another procedure, as developed by Dalgarno and Drake [29], is to diagonalize H_0 in a basis set $\{\theta_i , i=1,\ldots,N\}$ such that

$$\langle \psi_i | H_0 | \psi_j \rangle = \omega_i \delta_{ij} , \tag{37}$$

$$\langle \psi_i | \psi_j \rangle = \delta_{ij} . \tag{38}$$

Then one of the ψ_i, say ψ_1, is ϕ_0 with $\omega_1 = \epsilon_0$. Thus the Green's function of Eq. (27) can be written in the form

$$(H_0 - \epsilon_0)^{-1} = \sum_{i=2}^{N} \frac{|\psi_i\rangle\langle\psi_i|}{\omega_i - \epsilon_0} . \tag{39}$$

Therefore, the solutions to Eq. (27) may be written in terms of ψ_i

$$\phi_p = \sum_{i=2}^{N} c_i^{(p)} \psi_i \tag{40}$$

and the energy coefficients ϵ_i and $c_i^{(p)}$ solved recursively [29]

$$\epsilon_1 = \langle \phi_0 | V | \phi_0 \rangle , \tag{41}$$

$$c_i^{(1)} = -\frac{\langle \psi_i | V | \phi_0 \rangle}{\omega_i - \epsilon_0} , \tag{42}$$

$$\epsilon_p = \sum_{i=2}^{N} c_i^{(p-1)} \langle \phi_0 | V | \psi_i \rangle , \quad p \geqslant 2 \tag{43}$$

$$c_i^{(p)} = \frac{1}{\omega_i - \epsilon_0} \sum_{j=1}^{p-1} \epsilon_j c_i^{(p-j)} - \frac{1}{\omega_i - \epsilon_0} \sum_{j=2}^{N} c_j^{(p-1)} \langle \psi_i | V | \psi_j \rangle , \quad p \geqslant 2. \tag{44}$$

One important property for the second-order energy ϵ_2 is that it can be written as a weighted sum of the second-order energies of possible two-electron pairs, as well as some single-electron energies [26]. Thus ϵ_2 may be expressed in the form

$$\epsilon_2(1s^2 2\ell\, {}^2L) = \epsilon_2(1s^2\, {}^1S) + \frac{1}{2}\epsilon_2(1s2\ell\, {}^1L) + \frac{3}{2}\epsilon_2(1s2\ell\, {}^3L) + \xi(2\ell) , \tag{45}$$

where $\ell = s$ or p depending on the state being evaluated. In the above expression, $\xi(2\ell)$ is a sum of single-electron integrals, which are evaluated exactly by Chisholm and Dalgarno for the S state and by Chisholm, Dalgarno, and Innes for the P state [26]. The numerical values are

$$\xi(2s) = -0.122\,130\,711\,445\,149\,712,$$

$$\xi(2p) = -0.182\,899\,631\,995\,039\,751.$$

The three-electron problem for ϵ_2 can now be reduced to a two-electron problem that can be solved with high precision, using the variational method of Drake [30]. Our results for the two-electron pair energies are

$$\epsilon_2(1s^2\, {}^1S) = -0.157\,666\,429\,469\,3(4),$$

$$\epsilon_2(1s2s\, {}^1S) = -0.114\,510\,136\,167\,2(4),$$

$$\epsilon_2(1s2s\, {}^3S) = -0.047\,409\,304\,175\,4(6),$$

$$\epsilon_2(1s2p\, {}^1P) = -0.157\,028\,662\,934\,7(2),$$

$$\epsilon_2(1s2p\, {}^3P) = -0.072\,998\,983\,472\,6(8).$$

Comparing the first value $\epsilon_2(1s^2\, {}^1S)$ with the value of Baker *et al.* [31] $-0.157\,666\,429\,469\,14$, one can see that they agree with each other within the uncertainty quoted in the result obtained here. The above results for the electron-pair energies are much more accurate than the results obtained by Chisholm and Dalgarno and by Horak *et al.* [26], which are accurate to 6 or 7 significant figures.

Our final results for the $2\,{}^2S$ and $2\,{}^2P$ energy sequences are

$$E(1s^2 2s\, {}^2S) = -\frac{9}{8}Z^2 + \frac{5965}{5832}Z - 0.408\,166\,165\,261\,15(8) - 0.016\,548\,9(20)Z^{-1} - 0.040\,604(7)Z^{-2} - 0.049\,13(5)Z^{-3} - 0.062\,39(5)Z^{-4} , \tag{46}$$

$$E(1s^2 2p\, {}^2P) = -\frac{9}{8}Z^2 + \frac{57397}{52488}Z - 0.528\,578\,868\,140\,59(11) - 0.069\,827(20)Z^{-1} - 0.092\,50(5)Z^{-2} - 0.083(4)Z^{-3} - 0.066\,9(5)Z^{-4} . \tag{47}$$

The final result for the $2\,{}^2S \rightarrow 2\,{}^2P$ oscillator strength sequence is

$$f(2\,{}^2S \rightarrow 2\,{}^2P) = \tfrac{928}{729}Z^{-1} + 2.024\,734\,556\,116\,2(36)Z^{-2} + 2.919\,51(18)Z^{-3} + 3.197\,5(23)Z^{-4} + 1.25(22)Z^{-5} - 6.65(57)Z^{-6} - 29.4(1.0)Z^{-7} . \tag{48}$$

Table VIII lists the results for $Z = 15$–50 predicted by expressions (46)–(48). Comparing with the variational results of Tables II and VI, one can see that, for $Z = 15$, the nonrelativistic energies obtained from the large-Z expansions are accurate to about 9 and 8 significant figures for the $2\,{}^2S$ and $2\,{}^2P$ states; the oscillator strength obtained from the large-Z expansion is accurate to about 5 significant figures. The accuracy increases with increasing Z.

TABLE VIII. Nonrelativistic energies (in atomic units) and oscillator strengths for the lithiumlike ions predicted by the large-Z expansion formulas.

Z	$E(1s^2 2s\ ^2S)$	$E(1s^2 2p\ ^2P)$	$f(2\ ^2S \rightarrow 2\ ^2P)$
15	−238.192 387 48(14)	−237.255 778 9(18)	0.094 793 02(30)
16	−272.044 488 62(13)	−271.036 907 4(16)	0.088 232 40(22)
17	−308.146 602 26(12)	−307.068 079 7(14)	0.082 520 04(16)
18	−346.498 726 06(11)	−345.349 288 0(13)	0.077 501 58(12)
19	−387.100 858 23(11)	−385.880 526 1(12)	0.073 057 968(95)
20	−429.952 997 40(10)	−428.661 789 4(11)	0.069 095 857(74)
21	−475.055 142 441(97)	−473.693 074 0(11)	0.065 541 073(59)
22	−522.407 292 483(92)	−520.974 376 95(99)	0.062 333 917(47)
23	−572.009 446 809(88)	−570.505 695 53(93)	0.059 425 807(38)
24	−623.861 604 834(84)	−622.287 027 77(89)	0.056 776 803(32)
25	−677.963 766 076(81)	−676.318 371 94(84)	0.054 353 772(26)
26	−734.315 930 130(78)	−732.599 726 60(81)	0.052 128 995(22)
27	−792.918 096 658(75)	−791.131 090 52(77)	0.050 079 108(18)
28	−853.770 265 374(72)	−851.912 462 66(74)	0.048 184 276(16)
29	−916.872 436 034(70)	−914.943 842 14(71)	0.046 427 554(14)
30	−982.224 608 428(67)	−980.225 228 19(69)	0.044 794 379(12)
31	−1049.826 782 378(65)	−1047.756 620 14(66)	0.043 272 164(10)
32	−1119.678 957 725(63)	−1117.538 017 43(64)	0.041 849 977 1(88)
33	−1191.781 134 335(61)	−1189.569 419 54(62)	0.040 518 273 3(78)
34	−1266.133 312 089(59)	−1263.850 826 04(60)	0.039 268 686 7(69)
35	−1342.735 490 882(57)	−1340.382 236 54(58)	0.038 093 850 9(61)
36	−1421.587 670 623(56)	−1419.163 650 68(56)	0.036 987 254 7(55)
37	−1502.689 851 228(54)	−1500.195 068 17(55)	0.035 943 121 8(49)
38	−1586.042 032 627(53)	−1583.476 488 72(53)	0.034 956 309 7(44)
39	−1671.644 214 754(52)	−1669.007 912 11(52)	0.034 022 225 1(40)
40	−1759.496 397 552(50)	−1756.789 338 10(50)	0.033 136 752 9(37)
41	−1849.598 580 969(49)	−1846.820 766 50(49)	0.032 296 194 9(33)
42	−1941.950 764 958(48)	−1939.102 197 14(48)	0.031 497 219 1(30)
43	−2036.552 949 476(47)	−2033.633 629 85(47)	0.030 736 814 6(28)
44	−2133.405 134 487(46)	−2130.415 064 48(46)	0.030 012 254 8(26)
45	−2232.507 319 956(45)	−2229.446 500 91(45)	0.029 321 063 8(24)
46	−2333.859 505 851(44)	−2330.727 939 02(44)	0.028 660 988 6(22)
47	−2437.461 692 143(43)	−2434.259 378 68(43)	0.028 029 974 6(20)
48	−2543.313 878 807(42)	−2540.040 819 82(42)	0.027 426 144 1(19)
49	−2651.416 065 819(41)	−2648.072 262 32(41)	0.026 847 777 9(18)
50	−2761.768 253 156(40)	−2758.353 706 11(40)	0.026 293 298 6(16)

IV. RELATIVISTIC CORRECTIONS AND COMPARISON WITH EXPERIMENT

The high-precision lifetime measurements of Volz and Schmoranzer [6] and McAlexander *et al.* [7] for lithium are sufficiently accurate to be sensitive to relativistic corrections. Johnson *et al.* [17] have tabulated results for lithium and Li-like ions using RMBPT, but their calculations are not sufficiently accurate for low Z because of their incomplete treatment of correlation effects. The present results fully include correlation, but not relativistic effects. However, a comparison of the two calculations for intermediate values of Z allows the relativistic effects to be extracted and applied to the present results as a correction.

Since the decay rate $A_{i,f}$ is proportional to $\omega^3|\mathbf{r}_{i,f}|^2$, where ω is the transition frequency and $|\mathbf{r}_{i,f}|^2$ is the dipole transition moment squared, it is convenient to write the decay rate in terms of the correction factors

$$\begin{aligned} A_{i,f} &= A_{i,f}^{\mathrm{NR}}(1+\alpha^2 c_\omega)^3(1+\alpha^2 c_{\mathbf{r}})^2 \\ &\simeq A_{i,f}^{\mathrm{NR}}(1+3\alpha^2 c_\omega + 2\alpha^2 c_{\mathbf{r}}), \end{aligned} \tag{49}$$

where $A_{i,f}^{\mathrm{NR}}$ is the nonrelativistic decay rate and $\alpha^2 c_\omega$ and $\alpha^2 c_{\mathbf{r}}$ are the fractional relativistic corrections to the transition frequency and transition matrix element, respectively. The dominant contribution from the $3\alpha^2 c_\omega$ term can be accurately calculated from the difference between the measured transition frequency and the calculated nonrelativistic transition frequency. Using the high-precision measurements of Sansonetti *et al.* [32], the results for lithium are

$$3\alpha^2 c_\omega(2\ ^2P_{1/2} - 2\ ^2S_{1/2}) = 5.23\times 10^{-4},$$

$$3\alpha^2 c_\omega(2\ ^2P_{3/2} - 2\ ^2S_{1/2}) = 5.90\times 10^{-4}. \tag{50}$$

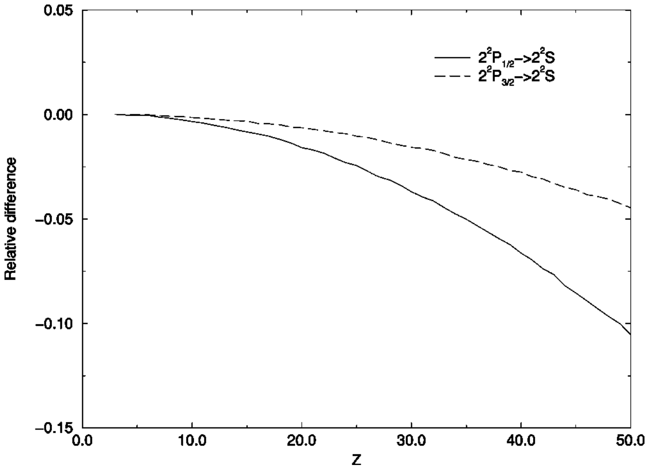

FIG. 1. Relative difference $\mathcal{R}-1$ versus Z, where $\mathcal{R}$ is defined by Eq. (51) and Z is the nuclear charge.

The use of the observed transition frequencies instead of the theoretical ones to calculate the relativistic corrections does not introduce a material difference since the calculated center of gravity for the two transitions [2] and the fine-structure splitting of the $2\,^2P$ state [33] are both in good agreement with experiment to the required accuracy. However, it does introduce a small ($\sim 10\%$) decrease in the corrections due to Lamb shift terms of order α^3. A similar calculation of the c_ω term was performed separately for each of the Li-like ions.

An estimate of the $2\alpha^2 c_{\mathbf{r}}$ term can be obtained by first dividing out the respective factors of ω^3 from the RMBPT decay rates and from the nonrelativistic decay rates to obtain $|\mathbf{r}_{i,f}|^2$ for the two cases and then taking the ratio of these quantities. Provided Z is neither too low (where correlation effects are important) nor too high (where higher-order relativistic effects are important), the ratio $\mathcal{R}$ can be expanded in the form

$$\mathcal{R}=\frac{[|\mathbf{r}_{i,f}|^2]_{\mathrm{RMBPT}}}{[|\mathbf{r}_{i,f}|^2]_{\mathrm{NR}}}=1+2\alpha^2 Z^2[c_{\mathbf{r}}^{(0)}+c_{\mathbf{r}}^{(1)}Z^{-1}+O(Z^{-2})]. \tag{51}$$

The numerical values of $\mathcal{R}-1$ are plotted in Fig. 1. The leading term $c_{\mathbf{r}}^{(0)}$ on the right-hand side can be calculated exactly from hydrogenic Dirac wave functions. The next term can be obtained by a least-squares fit to the data in the range $7 \leqslant Z \leqslant 36$, but the accuracy of the RMBPT values is not sufficient to go beyond this. The final results are thus

$$2c_{\mathbf{r}}(2\,^2P_{1/2}-2\,^2S_{1/2})=-Z^2[\tfrac{5}{6}-2.18(7)Z^{-1}+O(Z^{-2})], \tag{52}$$

$$2c_{\mathbf{r}}(2\,^2P_{3/2}-2\,^2S_{1/2})=-Z^2[\tfrac{1}{3}-0.58(7)Z^{-1}+O(Z^{-2})]. \tag{53}$$

To within the accuracy of the RMBPT calculations, these equations reproduce the relativistic corrections to the dipole transition matrix element squared over the entire range of Z up to about 40. For lithium, the numerical values are $2\alpha^2 c_{\mathbf{r}}=-0.51\times 10^{-4}$, and -0.67×10^{-4}, respectively, for $j=\frac{1}{2}$ and $\frac{3}{2}$. Since the uncertainty due to the next term of $O(Z^{-2})$ is largest in this case, we take the entire amount of the correction due to $c_{\mathbf{r}}$ to be the uncertainty. However, this still yields results of useful accuracy for the total relativistic correction because the $2|c_{\mathbf{r}}|$ term is only about 10% of the $3c_\omega$ term.

TABLE IX. Summary of contributions to the lifetimes of the ^{7}Li $2\,^2P$ states (in units of ns) and comparison with experiment. τ_∞ is the nonrelativistic lifetime for infinite nuclear mass and the finite mass correction scales linearly with μ/M.

Contribution	$^2P_{1/2}$	$^2P_{3/2}$
τ_∞	27.109 821 58(36)	27.109 821 58(36)
finite mass correction	0.007 502 02	0.007 502 02
relativistic correction	−0.012 8(14)	−0.014 2(18)
total	27.104 5(14)	27.103 1(18)
RMBPT [a]	27.10	27.10
Experiment	27.102(7)[b] 27.11(6)[c]	

[a] Reference [17].
[b] Reference [7].
[c] Reference [6].

The various contributions to the lifetimes for lithium are summarized in Table IX and compared with experiment. It is clear that both finite mass and relativistic corrections must be included to obtain agreement with the measured values. The RMBPT result quoted in the table is not sufficiently accurate and it does not include a complete treatment of finite mass effects. Table X lists the calculated decay rates for other low-Z ions and compares them with the RMBPT values. The differences are due mainly to the finite mass terms.

Results for other isotopes such as ^{6}Li can be easily obtained just by rescaling the finite mass correction in Table IX in proportion to the value of μ/M, where μ is the reduced electron mass and M is the nuclear mass. For example, for ^{6}Li with $\mu/M=0.912\,251\times 10^{-4}$, the finite mass correction

TABLE X. Decay rates for the $2\,^2P$ states of Li-like ions, including relativistic and finite mass corrections, and comparison with the RMBPT calculations of Johnson *et al.* [17]. Units are 1/ns.

	$^2P_{1/2}$		$^2P_{3/2}$	
Z	This work	RMBPT	This work	RMBPT
3	0.036894(2)	0.03690	0.036896(2)	0.03690
4	0.11289(1)	0.1129	0.11297(1)	0.1130
5	0.18886(1)	0.1889	0.18932(1)	0.1894
6	0.26281(1)	0.2630	0.26425(1)	0.2644
7	0.33556(2)	0.3357	0.33905(2)	0.3392
8	0.40764(2)	0.4078	0.41487(2)	0.4150
9	0.47949(3)	0.4796	0.49279(3)	0.4930
10	0.55269(3)	0.5528	0.57534(3)	0.5755
11	0.62330(3)	0.6235	0.65984(4)	0.6600
12	0.69507(4)	0.6952	0.75131(4)	0.7515
13	0.76779(4)	0.7679	0.85084(5)	0.8510
14	0.84071(4)	0.8408	0.95975(5)	0.9601
15	0.91663(5)	0.9168	1.07826(6)	1.079

changes to 0.008 750 65 ns and the lifetime of the $2\,^2P_{1/2}$ state changes to 27.1057(14) ns.

V. SUMMARY

We have presented in this paper definitive values for the nonrelativistic energies and oscillator strengths for the resonance transitions of lithium and the Li-like ions. Finite mass corrections have also been calculated and the relativistic corrections estimated by comparison with the RMBPT results of Johnson *et al.* [17]. The results are in good agreement with recent high-precision measurements, but additional work is required to improve the accuracy of the relativistic corrections, especially for lithium where the $1/Z$ expansion is poorly convergent. The term $c_{\mathbf{r}}^{(1)}$ can in principle be calculated analytically because the dipole transition operator is a one-electron operator and the next term can be obtained by use of perturbation theory with hydrogenic variational basis sets. These topics will be discussed in future papers.

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