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Energies and lifetimes of the core-excited states of the Li isoelectronic sequence

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The energies, fine structures, widths, and radiative rates of core-excited states of a Li isoelectronic sequence ($Z=4-14$) are calculated using the saddle point and saddle-point complex-rotation methods. A restricted variational method is used to extrapolate a better nonrelativistic energy. Relativistic effects are included using first-order perturbation theory. The charged effects of the Li isoelectronic sequence are discussed. These results are compared with experimental and theoretical data in the literature.

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I. INTRODUCTION

The investigation of core-excited states is an important way to understand electron correction. In these states, the presence of autoionizing states strongly affects the character of the emission spectrum of high-temperature astrophysical and laboratory plasmas. The advances of synchrotron radiation and computer technology have revived both experimental and theoretical interest in the study of inner-shell excited states. A considerable amount of experimental work has been done on core-excited states of the Li isoelectronic sequence [1–9] over the past few decades. The calculations of energies and widths of the three-electron autoionizing states are very challenging. Among the earlier theoretical works, Bhatia [10] calculated the three lowest states of ^2S, $^2P^0$, and ^2D with the quasiprojection operator technique. Jaskolska and Woznicki [11] used the saddle-point method with correlated-coordinate wave functions. Their energies are more accurate than those in earlier theoretical works. However, they did not calculate the widths, shifts, and relativistic corrections of these resonances. This makes an unambiguous comparison with precise experiments. Using the saddle-point technique, Davis and Chung [12] calculated some low core-excited states of Li, Be^+, and B^{2+}. There, the calculation of the wave functions was limited to about 100 terms. More recently, Chen and Chung [13], using large-scale computation and a restricted variation method, calculated more accurate absolute term energies of some core-excited doublet states for the lithium atom. Recently, Safronova and Shlyaptsem [14] calculated the energies and autoionizing rates of inner-shell excited states for Li-like ions by using the $1/z$ perturbation theory method. In this work, six core-excited states of a Li isoelectronic sequence [$Z=4-14$] are studied. The resonance positions, fine-structure splittings, widths, radiative rates, and Auger branch rates are calculated with the saddle point and saddle-point complex-rotation method. A restricted variation method is used for the saturated wave functions. Relativistic corrections are computed with first-order perturbation theory. With the improvement of computing resources, we can now perform much larger calculations to improve the accuracy. It is our hope to provide more reliable theoretical data to stimulate further experimental measurements, and to test the effectiveness of theoretical methods. Furthermore, we investigate whether properties such as relativistic correction, fine-structure splitting, radiative rate, and Auger rate regularly change along the Li isoelectronic sequence.

II. THEORY

In the LS coupling scheme, the nonrelativistic Hamiltonian of the three-electron system is given by (in a.u.)

$$H=\sum_{i=1}^{3}\left(-\frac{1}{2}\nabla_i^2-\frac{Z}{r}\right)+\sum_{\substack{i<j\\ i,j=1}}^{3}\frac{1}{r_{ij}}. \tag{1}$$

To further improve the energy, relativistic corrections and the mass polarization effect are included. The explicit expressions of these perturbation operators are given in Ref. [15]; they will not be repeated here.

The saddle-point wave function of core-excited three-electron system can be written as

$$\Psi_b=A\sum C_{mnk}^{l_1l_2L_{12}l_3}[1-P(r_i)] \times\phi_{mnk}(r_1,r_2,r_3)Y_{l_1l_2L_{12}}^{l_3LM}(\hat{r}_1,\hat{r}_2,\hat{r}_3)X(1,2,3). \tag{2}$$

The radial basis functions are Slater orbitals:

$$\phi_{mnk}(r_1,r_2,r_3)=r_1^m r_2^n r_3^k e^{-(\alpha_i r_1+\beta_i r_2+\gamma_i r_3)} \tag{3}$$

In Eq. (2) the projection operator is given by

$$P(r_i)=|\phi_0(r_i))(\phi_0(r_i)|. \tag{4}$$

Here the vacancy orbital is

$$\phi_0(r)=N\exp(-qr), \tag{5}$$

where q is a parameter determined in the energy maximization processes. The linear parameters C and the nonlinear parameters α_i, β_i, and γ_i in Eqs. (2) and (3) are determined in the energy optimization processes. Using the saddle-point variational method, we find the basic wave function Ψ_b and the corresponding saddle-point energy E_b.

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TABLE I. Nonrelativistic energies, relativistic correction, mass polarization, shifts, and fine structures (μ a.u.) for some core-excited states of the Li isoelectronic sequence.

	Resonances	$1s2s^2\ ^2S$	$1s2p^2\ ^2S$	$1s(2s2p^3P^0)^2P^0$	$1s(2s2p^1P^0)^2P^0$	$1s2p^2\ ^2D$	$1s2s2p\ ^4P^0$
Be^{+}	E_{nonrel}	−10 123 422.5	−9 700 672.3	−9 960 739.7	−9 879 104.2	−9 825 849.4	−10 066 595.2
	H_{rel}	−2034.5	−1719.9	−1953.2	−1892.0	−1782.5	−1971.6
	H_{mp}	−0.6	−19.0	24.0	−23.5	−36.0	−32.5
	E_{RV}	−24.3	−42.2	−15.4	−23.4	−18.8	−7.0
	E_S	65.0	250.5	367.6	50.6	154.0	
	E_{total}	−10 125 417.0	−9 702 202.9	−9 962 316.7	−9 881 093.7	−9 827 533.3	−10 068 606.3
	Ref. [12]		−9 701 112.0	−9.961 635.0	−9 880 016.0	−9 826 952.0	
	$\Delta E_J\ J=L-1/2$			−39.44	19.43	60.46	2.74
	$\Delta E_J\ J=L+1/2$			19.72	−9.72	−40.31	−25.18
	$\Delta E_J\ J=L+3/2$						15.87
	$\nu_{3/2-1/2}$			12.98	−6.40		−6.13
	$\nu_{5/2-3/2}$					22.11	9.01
B^{2+}	E_{nonrel}	−16 341 897.6	−15 743 678.9	−16 107 612.4	−16 002 316.8	−15 919 700.7	−16 267 541.8
	H_{rel}	−5286.9	−4446.0	−4944.0	−47 839.8	−4460.0	−4992.5
	H_{mp}	−2.3	−33.9	39.6	−39.1	−53.8	−51.1
	E_{RV}	−21.6	−37.5	−43.3	−33.7	−22.2	−5.8
	E_S	125.8	280.9	414.0	−56.3	214.0	
	E_{total}	−16 347 082.5	−15 747 915.4	−16 112 146.0	−16 007 229.9	−15 924 022.8	−16 272 591.2
	Ref. [12]		−15 746 105.0	−16 110 491.0	−16 005 377.0	−15 922 876.0	
	$\Delta E_J\ J=L-1/2$			−124.21	33.56	151.05	−59.46
	$\Delta E_J\ J=L+1/2$			62.11	−16.78	−100.70	−81.27
	$\Delta E_J\ J=L+3/2$						74.00
	$\nu_{3/2-1/2}$			40.89	−11.05		−4.79
	$\nu_{5/2-3/2}$					−55.25	34.08
C^{3+}	E_{nonrel}	−24 060 422.2	−23 289 090.9	−23 754 106.4	−2 362 618.8	−23 514 328.7	−23 969 488.7
	H_{rel}	−11 409.1	−9490.0	−10 537.6	−10 260.5	−9447.7	−10 628.1
	H_{mp}	−4.4	−53.8	60.6	−59.9	−78.6	−76.6
	E_{RV}	−20.8	−33.8	−44.6	−47.6	−42.3	−6.7
	E_S	169.2	325.4	442.0	−59.5	255.5	
	E_{total}	−24 071 687.3	−23 298 342.5	−23 764 186.1	−23 636 615.8	−23 523 641.9	−23 980 200.2
	Ref. [2]	−24 050 800.0		−23 760 500.0	−23 635 600.0	−23 514 200.0	−23 973 600.0
	$\Delta E_J\ J=L-1/2$			−300.81	30.65	302.27	−230.46
	$\Delta E_J\ J=L+1/2$			150.40	−15.32	−201.51	−212.02
	$\Delta E_J\ J=L+3/2$						218.17
	$\nu_{3/2-1/2}$			99.02	−10.09		4.05
	$\nu_{5/2-3/2}$					−110.56	94.41
O^{5+}	E_{nonrel}	−43 997 673.2	−42 881 845.7	−43 546 667.5	−43 374 816.9	−43 205 391.9	−43 874 686.2
	H_{rel}	−37 616.5	−30 993.6	−34 491.0	−33 800.2	−30 849.1	−34 866.5
	H_{mp}	−8.4	−88.8	95.1	−93.8	−118.9	−118.2
	E_{RV}	−51.2	−42.1	−36.5	−37.3	−48.9	−8.7
	E_S	233.8	371.3	464.4	−57.7	313.6	
	E_{total}	−44 035 115.5	−42 912 598.9	−43 580 635.5	−43 408 805.9	−43 236 095.2	−43 909 679.6
	Ref. [1]	−44 029 100.0		−43 573 500.0	−43 389 800.0	−43 206 000.0	−43 904 300.0
	$\Delta E_J\ J=L-1/2$			−1146.49	−111.31	848.79	−1289.03
	$\Delta E_J\ J=L+1/2$			573.25	55.65	−565.86	−840.89
	$\Delta E_J\ J=L+3/2$						990.27
	$\nu_{3/2-1/2}$			377.43	36.64		98.35
	$\nu_{5/2-3/2}$					310.47	401.88
Ne^{7+}	E_{nonrel}	−69 934 778.1	−68 475 941.5	−69 338 844.0	−69 123 759.8	−68 896 769.4	−69 780 640.5
	H_{rel}	−94 291.1	−77 767.7	−86 488.6	−84 999.1	−77 005.1	−87 173.5

TABLE I. (*Continued*).

	Resonances	$1s2s^2\ ^2S$	$1s2p^2\ ^2S$	$1s(2s2p\,^3P^0)^2P^0$	$1s(2s2p\,^1P^0)^2P^0$	$1s2p^2\ ^2D$	$1s2s2p\ ^4P^0$
	H_{mp}	−12.5	−125.3	129.6	−128.0	−160.0	−160.2
	E_{RV}	−31.7	−26.7	−41.3	−33.6	−46.0	−23.5
	E_S	271.3	409.8	474.3	−54.3	352.7	
	E_{total}	−70 028 842.1	−68 553 451.5	−69 424 770.0	−69 208 974.7	−68 973 627.8	−69 867 997.7
	E_{total} (cm^{-1})	15 369 130	15 045 340	15 236 560	15 189 200	15 137 550	15 333 840
	Ref. [14] (cm^{-1})	15 368 580	15 042 800	15 235 960	15 188 183	15 135 576	15 331 955
	ΔE_J $J=L-1/2$			−3114.64	−654.22	1822.29	−4120.57
	ΔE_J $J=L+1/2$			1557.32	327.11	−1214.86	−2333.11
	ΔE_J $J=L+3/2$						2928.93
	$\nu_{3/2-1/2}$			1025.35	215.37		392.29
	Ref. [14]			990.0	190.0		390.0
	$\nu_{5/2-3/2}$					−666.56	1154.85
	Ref. [14]					−760.0	1180.0
Mg^{9+}	E_{nonrel}	−101 872 032.6	−100 070 626.2	−101 130 853.0	−100 872 664.6	−100 588 523.8	−101 687 063.6
	H_{rel}	−199 214.5	−164 233.8	−182 424.6	−179 909.7	−162 294.3	−183 803.6
	H_{mp}	−16.6	−162.4	−164.3	−162.1	−201.7	−202.6
	E_{RV}	−23.9	−18.4	−35.8	−29.3	−47.1	−23.1
	E_S	315.0	442.4	480.9	51.4	379.8	
	E_{total}	−102 070 972.5	−100 234 598.4	−101 312 668.3	−101 052 817.1	−100 750 687.2	−101 871 092.8
	E_{total} (cm^{-1})	22 401 482	21 998 452	22 235 056	22 178 027	22 111 719	22 357 614
	Ref. [14] (cm^{-1})	22 399 440	21 994 620	22 233 076	22 175 540	22 108 538	22 354 522
	ΔE_J $J=L-1/2$			−6892.00	−1955.35	3346.13	−10 033.1
	ΔE_J $J=L+1/2$			3446.00	977.68	−2230.75	−5254.0
	ΔE_J $J=L+3/2$						6847.0
	$\nu_{3/2-1/2}$			2268.88	643.71		1048.85
	Ref. [14]			2210.0	660.0		1030.0
	$\nu_{5/2-3/2}$					−1223.96	2655.82
	Ref. [14]					−1180.0	2720.0
Si^{11+}	E_{nonrel}	−139 809 232.8	−137 665 757.5	−138 922 839.8	−138 621 627.7	−138 280 681.2	−139 593 678.2
	H_{rel}	−373 146.8	−308 297.9	−340 696.2	−355 296.5	−304 215.6	−344 713.4
	H_{mp}	−20.8	−199.9	198.8	−196.6	−243.8	−245.2
	E_{RV}	−11.2	−21.5	−40.4	−41.9	−39.3	−14.0
	E_S	330.5	451.6	485.3	−46.1	401.1	
	E_{total}	−140 182 081.1	−137 973 825.3	−139 262 892.4	−138 977 208.8	−138 584 778.9	−139 938 650.6
	E_{total} (cm^{-1})	30 765 815	30 281 169	30 564 080	30 501 379	30 415 254	30 712 387
	Ref. [14] (cm^{-1})	30 762 010	30 275 200	30 560 650	30 493 077	30 410 336	30 707 588
	ΔE_J $J=L-1/2$			−13 414.6	−4520.75	5543.06	−20 681.2
	ΔE_J $J=L+1/2$			6707.3	2260.37	−3695.37	−10 309.2
	ΔE_J $J=L+3/2$						13 766.6
	$\nu_{3/2-1/2}$			4416.15	1488.25		2276.33
	Ref. [14]			4320.0	1550.0		2180.0
	$\nu_{5/2-3/2}$					−2027.56	5283.93
	Ref. [14]					−1460.0	5470.0

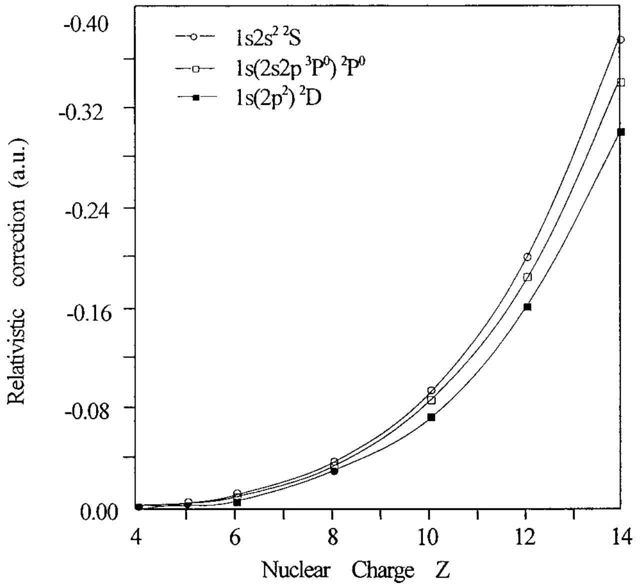

FIG. 1. Relativistic energy corrections (a.u.) of some core-excited states of the Li isoelectronic sequence.

To further improve the calculation of energy, we then expand the total wave function as

$$\Psi(1,2,3)=D_0\Psi_b(1,2,3)+\Psi_2(1,2,3), \tag{6}$$

where

$$\Psi_2(1,2,3)=A\sum_{i=1}^{t} D_i\Psi_{n(i),l(i)}(1,2,3). \tag{7}$$

Ψ_2 is a function to saturate the functional space. In practice, we will break up Ψ_2 into many parts. A secular equation will be constructed for each part. Each of the nonlinear parameters in the basis function of Ψ_2 is optimized in the restricted variational calculation [16].

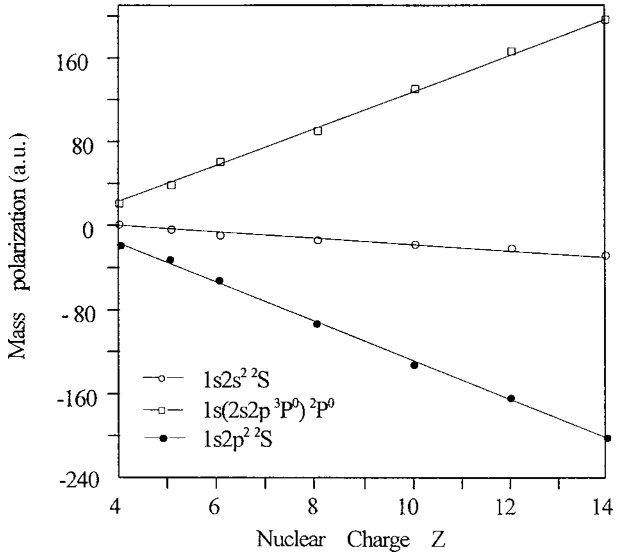

FIG. 2. Mass polarization effects (μ a.u.) of some core-excited states of the Li isoelectronic sequence.

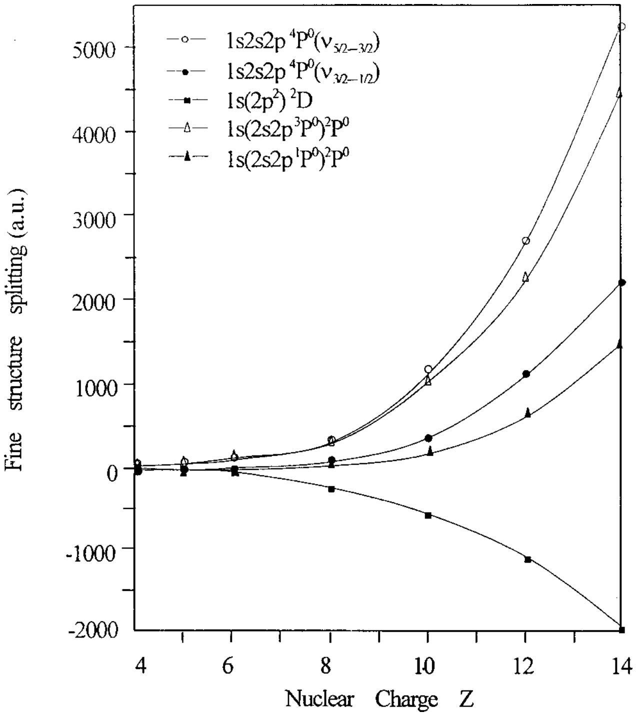

FIG. 3. Fine structure splitting (μ a.u.) for some core-excited states of the Li isoelectronic sequence.

To obtain the widths using the saddle-point complex-rotation method [17], we write the total wave function as

$$\Psi(1,2,3)=\Psi_b(1,2,3)+\sum_i A\phi_i(1,2)U_i(3), \tag{8}$$

where

$$U_i=\sum_n d_{i,n}r^n\exp(-\alpha_i r). \tag{9}$$

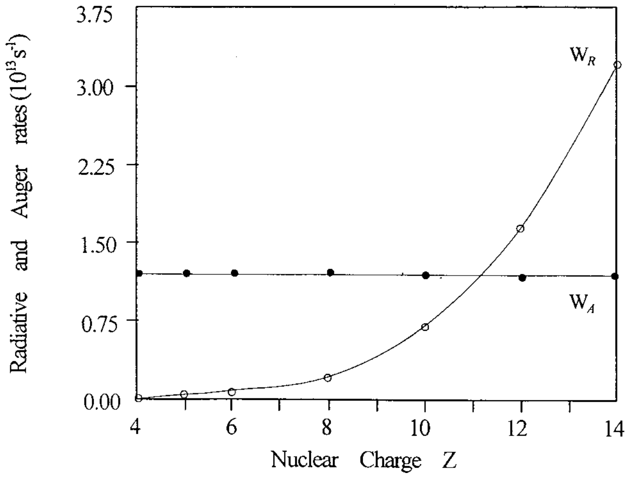

FIG. 4. Auger transition rates (W_A,$10^{13}\,\mathrm{s}^{-1}$) and radiative transiion rates (W_R,$10^{13}\,\mathrm{s}^{-1}$) for the $1s(2s2p\,^3P^0)^2P^0$ state of the Li isoelectronic sequence.

TABLE II. Oscillator strength (f_l, f_v, f_a), transition rate ($10^{11}\ \mathrm{s}^{-1}$), and transition wavelength (Å) of some core-excited states of the Li isoelectronic sequence.

Transition	f_l	f_ν	f_a	A_l	A_ν	A_a	λ
$Z=4$							
$1s^22p\ ^2P^0\rightarrow$							
$1s2s^2\ ^2S$	0.0038	0.0027	0.0026	0.060	0.043	0.041	112.44
				0.092^{a}	0.017^{a}		112.38^{a}
$1s2p^2\ ^2S$	0.0178	0.0168	0.0165	0.343	0.325	0.319	101.82
				0.54^{a}	0.42^{a}		101.46^{a}
$1s2p^2\ ^2D$	0.1068	0.1022	0.1025	0.390	0.373	0.374	104.75
				0.52^{a}	0.47^{a}		104.63^{a}
$1s^22s\ ^2S^e\rightarrow$							
$1s(2s2p^3P^0)^2P^0$	0.4041	0.3851	0.3819	0.824	0.785	0.779	104.42
				0.91^{a}	0.81^{a}		104.30^{a}
$1s(2s2p^1P^0)^2P^0$	0.0325	0.0356	0.0366	0.069	0.075	0.077	102.51
$Z=5$							
$1s^22p\ ^2P^0\rightarrow$							
$1s2s^2\ ^2S$	0.0040	0.0032	0.0031	0.182	0.147	0.142	66.41
$1s2p^2\ ^2S$	0.0230	0.0220	0.0218	1.233	1.179	1.169	61.08
$1s2p^2\ ^2D$	0.1351	0.1315	0.1319	1.381	1.345	1.349	62.56
$1s^22s\ ^2S^e\rightarrow$							
$1s(2s2p^3P^0)^2P^0$	0.4834	0.4638	0.4591	2.772	2.659	2.632	62.28
$1s(2s2p\ ^1P^0)^2P^0$	0.0448	0.0477	0.0497	0.265	0.281	0.293	61.39
$Z=6$							
$1s^22p\ ^2P^0\rightarrow$							
$1s2s^2\ ^2S$	0.0041	0.0035	0.0034	0.432	0.368	0.359	43.72
				0.48^{a}	0.22^{a}		43.74^{a}
$1s2p^2\ ^2S$	0.02627	0.02549	0.02523	3.173	3.078	3.047	40.71
				4.24^{a}	3.5^{a}		40.67^{a}
$1s2p^2\ ^2D$	0.1534	0.1504	0.1509	3.557	3.487	3.500	41.55
				4.2^{a}	3.9^{a}		41.54^{a}
$1s^22s\ ^2S^e\rightarrow$							
$1s(2s2p^3P^0)^2P^0$	0.5283	0.5151	0.5100	6.873	6.701	6.635	41.34
				7.9^{a}	7.9^{a}		41.26^{a}
$1s(2s2p^1P^0)^2P^0$	0.0519	0.0548	0.0563	0.691	0.730	0.750	40.87
$Z=8$							
$1s^22p\ ^2P^0\rightarrow$							
$1s2s^2\ ^2S$	0.0042	0.0038	0.0037	1.589	1.445	1.411	23.02
				1.6^{a}	0.98^{a}		23.03^{a}
$1s2p^2\ ^2S$	0.0304	0.0298	0.0296	12.797	12.538	12.490	21.79
				16.0^{a}	14.0^{a}		21.78^{a}
$1s2p^2\ ^2D$	0.1750	0.1730	0.1738	14.297	14.132	14.200	22.13
				16.0^{a}	15.0^{a}		22.13^{a}
$1s^22s\ ^2S^e\rightarrow$							
$1s(2s2p^3P^0)^2P^0$	0.5878	0.5775	0.5730	26.928	26.453	26.247	22.03
				28.0^{a}	27.0^{a}		22.02^{a}
$1s(2s2p^1P^0)^2P^0$	0.0603	0.0629	0.0643	2.808	2.928	2.993	21.85
$Z=10$							
$1s^22p\ ^2P\rightarrow$							
$1s2s^2\ ^2S$	0.0042	0.0040	0.0039	4.230	3.979	3.915	14.17
				4.2^{a}	2.9^{a}		14.17^{a}
							14.190^{b}
$1s2p^2\ ^2S$	0.0327	0.0323	0.0319	35.659	35.171	34.796	13.55
				42.0^{a}	37.0^{a}		13.55^{a}
							13.525^{b}

TABLE II. (*Continued*).

Transition	f_l	f_ν	f_a	A_l	A_ν	A_a	λ
$1s2p^2\ ^2D$	0.1872	0.1859	0.1866	39.788	39.507	39.657	13.72
				44.0[a]	42.0[a]		13.72[a]
							13.703[b]
$1s^22s\ ^2S^e\rightarrow$							
$1s(2s2p^3P^0)^2P^0$	0.6232	0.6138	0.6109	74.197	73.085	72.736	13.67
				77.0[a]	74.0[a]		13.66[a]
							13.651[b]
$1s(2s2p^1P^0)^2P^0$	0.0649	0.0672	0.0686	7.827	8.107	8.277	13.58
							13.564[b]
$Z=12$							
$1s^22p\ ^2P^0\rightarrow$							
$1s2s^2\ ^2S$	0.0044	0.0041	0.0040	9.645	8.898	8.774	9.58
$1s2p^2\ ^2S$	0.0343	0.0339	0.0337	80.483	79.612	78.990	9.23
$1s2p^2\ ^2D$	0.1952	0.1941	0.1948	89.698	89.200	89.532	9.33
$1s^22s\ ^2S^e\rightarrow$							
$1s(2s2p^3P^0)^2P^0$	0.6445	0.6379	0.6354	165.761	164.057	163.413	9.30
$1s(2s2p\ ^1P^0)^2P^0$	0.0681	0.0701	0.0714	17.708	18.223	18.548	9.25
$Z=14$							
$1s^22p\ ^2P^0\rightarrow$							
$1s2s^2\ ^2S$	0.0043	0.0042	0.0041	18.080	17.417	17.196	6.91
$1s2p^2\ ^2S$	0.0354	0.0351	0.0349	157.980	156.637	155.926	6.69
$1s2p^2\ ^2D$	0.2007	0.1999	0.2005	175.956	175.260	175.808	6.76
$1s^22s\ ^2S^e\rightarrow$							
$1s(2s2p^3P^0)^2P^0$	0.6606	0.6544	0.6526	323.948	320.931	320.036	6.73
$1s(2s2p^1P^0)^2P^0$	0.0701	0.0718	0.0728	34.706	35.545	36.036	6.70

[a] Reference [18].

[b] Reference [19].

$\phi_i(1,2)$'s are the target states of the open channels. U_i represents the wave function of the outgoing electron; in U_i r is complex scaled. The proper angular and spin coupling between ϕ_i and U_i to obtain the correct total L and M is implicitly assumed in the above equation. In the calculation, the nonlinear parameters obtained from the saddle-point calculation in $\Psi_b(1,2,3)$ are retained, but the linear parameters are recalculated to allow for full interaction between the closed- and open-channel wave functions. The complex energy obtained from $\Psi(1,2,3)$, $E-i\Gamma/2$, gives the position and width of the resonance. The difference $E_s=E-E_b$ represents the shift from the saddle-point energy to the resonance energy.

III. RESULT AND DISCUSSION

The six core-excited states of the Li isoelectronic sequence $(Z=4-14)$ we studied are the lowest two ^2S, the lowest two $^2P^0$, and the lowest ^2D and $^4P^0$ resonances. The nonrelativistic energies of these states are given in Table I. The autoionizing states of the core-excited atomic system are degenerate with the continuum. If the continuum is not carefully removed from the variational wave function, in some cases this could lead to a variational breakdown. In this work, $1s^2+kl$ is an open channel, and needs to be removed from the saddle-point wave functions. By the Pauli antisymmetry principle, there is no q value quoted for the $(1s2s2p)^4P^0$ state. In the present work, the number of linear parameters in the basic wave functions is much larger than those of Ref. [12], and more angular-spin components are used. The number of linear parameters ranges from 390 to 772, and the number of angular-spin components in the wave functions ranges from 16 to 36. As a consequence, the improvement of E_b over that of Ref. [12] ranges from -0.0002 to -0.0012 a.u. These energies are further improved by the restricted variation method with ΔE_{RV}; the total improvement ΔE_{RV} ranges from 5.8 to 51.2 μa.u.

The saddle-point energy is calculated from the closed-channel part of the wave function. It differs from the resonance position by a shift, which comes from the interaction of the closed- and open-channel wave functions. The energy levels of doubly excited states of Li-like ions lying below the $(1s2s)\ ^3S$ threshold can autoionize through only one decay channel,

$$(1s2l2l')^2L\rightarrow(1s^2)^1S+kl, \tag{10}$$

where kl represents the Auger electron with angular momentum l. In this case, we note that because of the Pauli exclusion principle, $(1s^2)^1S+kl$ is not an open channel for $(1s2s2p)^4P^0$ state. The convergence of the resonance width

TABLE III. Width (Γ_A), radiative rate (W_R), Auger transition rate (W_A), Auger branching radio (η_A), and lifetime (τ) of some coreexcited states of the Li isoelectronic sequence.

Resonances	Γ_A (meV)	W_R ($10^{13}\,\mathrm{s}^{-1}$)	W_A ($10^{13}\,\mathrm{s}^{-1}$)	η_A (%)	τ (10^{-15} s)
$Z=4$					
$1s2s^2\,{}^2S$	52.2	0.001	15.85	100.0	6.3
$1s2p^2\,{}^2S$	5.6	0.003	1.71	99.8	58.4
$1s2p^2\,{}^2D$	27.4	0.004	8.33	100.0	12.0
$1s(2s2p\,{}^3P^0)\,{}^2P^0$	3.9	0.008	1.20	99.3	82.8
$1s(2s2p\,{}^1P^0)\,{}^2P^0$	20.9	0.001	6.36	100.0	15.7
$Z=5$					
$1s2s^2\,{}^2S$	61.6	0.002	18.72	100.0	5.3
$1s2p^2\,{}^2S$	6.7	0.012	2.02	99.4	49.2
$1s2p^2\,{}^2D$	41.6	0.014	12.64	99.9	7.9
$1s(2s2p\,{}^3P^0)\,{}^2P^0$	4.0	0.028	1.21	97.8	80.8
$1s(2s2p\,{}^1P^0)\,{}^2P^0$	29.8	0.003	9.04	100.0	11.1
$Z=6$					
$1s2s^2\,{}^2S$	68.1	0.004	20.70	100.0	4.8
$1s2p^2\,{}^2S$	8.0	0.032	2.43	98.7	40.6
$1s2p^2\,{}^2D$	52.5	0.036	15.95	99.8	6.3
$1s(2s2p\,{}^3P^0)\,{}^2P^0$	4.1	0.069	1.24	94.8	79.4
$1s(2s2p\,{}^1P^0)\,{}^2P^0$	36.4	0.007	11.07	99.9	9.0
$Z=8$					
$1s2s^2\,{}^2S$	76.4	0.016	23.22	99.9	4.3
$1s2p^2\,{}^2S$	10.0	0.128	3.03	96.0	31.7
$1s2p^2\,{}^2D$	67.9	0.143	20.64	99.3	4.8
$1s(2s2p\,{}^3P^0)\,{}^2P^0$	4.1	0.269	1.24	82.2	66.3
$1s(2s2p\,{}^1P^0)\,{}^2P^0$	45.5	0.028	13.81	99.8	7.2
$Z=10$					
$1s2s^2\,{}^2S$	81.2	0.042	24.67	99.8	4.0
$1s2p^2\,{}^2S$	11.4	0.357	3.47	90.7	26.1
$1s2p^2\,{}^2D$	77.8	0.398	23.65	98.4	4.2
$1s(2s2p\,{}^3P^0)\,{}^2P^0$	4.0	0.742	1.21	62.0	51.2
$1s(2s2p\,{}^1P^0)\,{}^2P^0$	51.3	0.078	15.59	99.5	6.4
$Z=12$					
$1s2s^2\,{}^2S$	84.4	0.096	25.65	99.6	3.9
$1s2p^2\,{}^2S$	12.4	0.805	3.76	82.4	21.9
$1s2p^2\,{}^2D$	84.9	0.897	25.80	96.6	3.7
$1s(2s2p\,{}^3P^0)\,{}^2P^0$	3.9	1.658	1.19	41.8	35.1
$1s(2s2p\,{}^1P^0)\,{}^2P^0$	55.3	0.177	16.80	99.0	5.9
$Z=14$					
$1s2s^2\,{}^2S$	86.8	0.181	26.37	99.3	3.8
$1s2p^2\,{}^2S$	13.1	1.580	3.98	71.6	18.0
$1s2p^2\,{}^2D$	90.0	1.760	27.34	94.0	3.4
$1s(2s2p\,{}^3P^0)\,{}^2P^0$	4.0	3.240	1.21	27.2	22.5
$1s(2s2p\,{}^1P^0)\,{}^2P^0$	58.2	0.347	17.68	98.1	5.5

and shift is excellent for all of the states investigated. This convergence is checked with respect to the angle of complex scaling (0.3–0.6 rad), and the variation of parameter α_i. Many of the widths are stable to five digits. The number of terms used in each U_i ranges from 14 to 16. The total nonrelativistic term energy is obtained by adding ΔE_{RV}, the shift ΔE_s, and the energy upper bound E_b.

In addition to the shift E_s and E_{RV}, the energy of these resonances is further corrected by the mass polarization and relativistic perturbation. The relativistic perturbation operators considered in this work are the correction to the kinetic energy (P^4), the Darwin term, the electron-electron contact term, and the orbit-orbit interaction. The relativistic corrections are calculated using first-order perturbation theory. The mass polarization perturbation operator is accurate to all orders. These results are given in Table I. The absolute energies of the core-excited states of the Li isoelectronic sequence in this work are lower than the energies in Refs. [1], [2], [12] and Ref. [6], in which the absolute energies were calculated by using the $1/Z$ perturbation theory method. Comparisons are given in Table I. Table I and Fig. 1 give the rapidly increasing importance of relativistic corrections with increasing nuclear charge number Z. The relativistic correction of the $1s2l'nl''(n\geqslant 2)$ state is mainly determined by that of the $1s2l'$ configuration. In this case, $1s2s2s^2S$ has the largest relativistic correction, and $1s2p2p^2D$ has the smallest correction. Figure 2 shows that the mass polarization corrections of the core-excited states in this work increase linearly with increasing nuclear charge numbers Z. Although the *ab initio* calculations stop at $Z=14$, an extrapolation to higher stages of ionization can be carried out straightforwardly.

The relativistic energies in Table I are the center-of-gravity energies. If we include the effects of the spin-orbit, spin-other-orbit, and spin-spin interactions, we obtain the energies of the fine-structure-resolved J levels. The shifts of the various J levels from the center-of-gravity energy and the fine-structure splittings are given in Table I. A comparition with the measurements of Ref. [14] is also given. Figure 3 shows that fine-structure splittings of the core-excited states increase rapidly with increasing nuclear charge numbers Z.

Table II gives computed oscillator strengths, optical transition rates from the dipole length (R_l), dipole velocity (R_ν), and dipole acceleration (R_a) formulas, and the transition wave length. For radiative transitions of relatively large rates, the dipole-length, dipole-velocity, and dipole-acceleration formula results agree reasonably well. However, for those rates which are small, the three results do not agree closely. They are also compared with the results of Piangos and Nicolaides [18]. The results for these core-excited resonances are not expected to be highly accurate, because these oscillator strengths are calculated with ψ_b only, and the open-channel part of the wave function is not included. Nevertheless, the transition rates and the transition wavelengths in this work are in reasonable agreement with the data of Refs. [18] and [19]. The widths, radiative rates, Auger transition rates, and lifetimes of core-excited states of the Li isoelectron sequence are given in Table III. Knowledge of the radiative and Auger rates of the core-excited systems is important in understanding the stabilization of the core-excited states formed in collisions between multiply charged ions with atoms, molecules, and surfaces. Figure 4 shows, for the $1s(2s2p\,{}^3P^0)\,{}^2P^0$ state, that the Auger transition rates change smoothly along the Li isoelectron sequence, and that the radiative rates increase rapidly with increasing value *Z*, such that Auger rates are larger than radiative rates for the low-*Z* systems, and the lifetimes of these resonances are essentially determined by their widths due to autoionization; otherwise Auger rates are smaller than radiative rates for the high-*Z* systems. At $Z=11$ the Auger rate and radiative rate are about the same. The lifetimes of the core-excited states for the Li isoelectron sequence considered in this work are about 10^{-14}–10^{-15} s. In this work, more reliable theoretical data should be useful for studying the observed spectra in future experiments.

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