Spin-induced autoionization and radiative transition rates for the $(1s 2p 2p)^4 P_J$ states in lithiumlike ions

Brian F. Davis

Department of Physics, University of North Carolina at Wilmington, Wilmington, North Carolina 28403-3297

Kwong T. Chung

Department of Physics, North Carolina State University, Raleigh, North Carolina 27695-8202

(Received 17 July 1987)

INTRODUCTION

The lifetimes of the lithiumlike 1s2p2p ${}^{4}P_{J}$ systems have been studied extensively both theoretically and experimentally. An interesting feature discovered in these studies is the differential metastability for the various Jstates. In 1978 Livingston and Berry¹ did an experiment on C IV, N v, and O VI. They found that, even for these low Z systems, the lifetimes of the $J = \frac{3}{2}$ states are much longer than those with $J = \frac{5}{2}$. In the case of O VI, the lifetime is longer by a factor of 10. In a more recent experiment, this differential metastability was observed for B III (Ref. 2) also.

Perhaps the most extensive theoretical calculations on the lifetimes of the 1s2p2p ${}^{4}P_{J}$ systems was done by Chen *et al.*³ By using Dirac-Hartree-Slater wave functions and the Moller relativistic two-electron operator, these authors computed the lifetimes for selected nuclear charges ranging from Z = 6 to Z = 30. Even though correlation effects were not included in this calculation, the agreement between theory and experiment appears to be very good. In the case of C IV, the agreement is excellent.

In the past we have calculated the energies and radiative lifetimes of lithiumlike quartet systems using a multiconfiguration interaction wave function.⁴⁻⁶ The relativistic corrections were accounted for by first-order perturbation theory in the *LSJ* coupling scheme. Although the calculated lifetimes agreed excellently with previous (low Z) experiments, differential metastability was not an element of these calculations.

In this work, we extend the LSJ coupling with intermediate coupling in order to study differential metastability. Each LSJ term is modified with the other L'S'Jterms of the same configuration as well as the adjacent continua by the coupling via the Pauli-Breit operator. The Auger width of the LSJ state is obtained by using the saddle-point complex-rotation method where the spin-dependent relativistic perturbations are explicitly included in the total Hamiltonian. We have applied this method to the lithium isoelectronic series from Z = 3 to Z = 10. Our results, while in agreement with previous theory and experiment in some cases, differ substantially with the existing results in the literature for C IV.

I. THE SPIN-INDUCED AUTOIONIZATION WIDTH

The perturbation potentials responsible for the coupling of the $1s 2p 2p {}^{4}P_{J}$ with the other *LSJ* terms are the spin-orbit, spin-other-orbit, and spin-spin interactions. In the Pauli-Breit approximation, the corresponding terms in the Hamiltonian are

$$H_{\rm s.o.} = \frac{\alpha^2}{2} Z \sum_{i=1}^{3} \frac{\mathbf{l}_i \cdot \mathbf{s}_i}{r_i^3} , \qquad (1)$$

$$H_{\text{s.o.o.}} = -\frac{\alpha^2}{2} \sum_{\substack{i,j=1\\i\neq j}}^3 \left(\frac{\mathbf{r}_{ij}}{\mathbf{r}_{ij}^3} \times \mathbf{p}_i \right) \cdot (\mathbf{s}_i + 2\mathbf{s}_j) , \qquad (2)$$

$$H_{\text{s.s.}} = \alpha^2 \sum_{\substack{i,j=1\\i< j}}^{3} \frac{1}{r_{ij}^3} \left[\mathbf{s}_i \cdot \mathbf{s}_j - \frac{3(\mathbf{s}_i \cdot \mathbf{r}_{ij})(\mathbf{s}_j \cdot \mathbf{r}_{ij})}{r_{ij}^2} \right].$$
(3)

Since the total angular momentum J and parity operator commute with these perturbations, the wave function for a $1s_2p_2p {}^4P_J$ state, to first order, can be written as

$$\Psi = \psi (1s 2p 2p {}^{4}P_{J}) + c \psi (1s 2p 2p {}^{2}L_{J}) + \psi \{ [(1s 1s)^{1}S, kL]^{2}L_{J} \} .$$
(4)

In this equation if $j = \frac{3}{2}$ or $\frac{5}{2}$ then L = 2, if $J = \frac{1}{2}$ then L = 0. The $1s 2p 2p^2 L$ states may autoionize via the nonrelativistic Coulomb interaction. Since the coupling coefficient c is of the order α^2 , this process is of the same order as the direct autoionization of the $1s 2p 2p^4 P_J$ to the doublet continuum. The $1s 2p 2p^2 P_J$ states have been ignored in the above equation since autoionization through this channel would be of a higher order. The wave functions for the 2L_J states are obtained by the saddle-point technique as in Davis and Chung.⁷ The 4P_J wave function is obtained as in Chung.⁸ The linear coefficient c is obtained by the use of first-order perturbation theory with the spin-dependent perturbations given in Eqs. (1)-(3). The last term in Eq. (4) represents the open-channel component. It is given by

$$\psi\{[(1s\,1s\,)^{1}S,kL\,]^{2}L_{J}\} = A\,\psi_{g}\sum_{i}d_{i}\,U_{i}^{L}(\mathbf{r}) \ . \tag{5}$$

Here A is an antisymmetrization operator. ψ_g is the wave function of the two-electron $(1s1s)^1S$ target state. It is a three-partial-wave eight term wave function. The details of this function have been given in Ref. 9. The U_i^L represent a one-dimensional complete set for the outgoing electron. We choose

$$U_i^L(\mathbf{r}) = r^i e^{-\gamma r} Y_L(\Omega) , \qquad (6)$$

where γ is a nonlinear variational parameter. Y_L represents the appropriate angular wave function. The azimuthal quantum number is suppressed, as is the spin part. It is understood that the proper angular and spin symmetry will be built into the ${}^{2}L_{J}$ wave function.

The wave function in Eq. (4) is used to carry out the complex-rotation calculation¹⁰ with the following Hamiltonian:

$$H = H_0 + H_{s.o.} + H_{s.o.o.} + H_{s.s.} , \qquad (7)$$

where

$$H_0 = \sum_{i=1}^{3} \left[-\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right] + \sum_{\substack{i,j=1\\i< i}}^{3} \frac{1}{r_{ij}} .$$
(8)

The spin-induced autoionization width is obtained by substituting Eq. (4) into

$$\delta\langle H \rangle = \delta \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0 .$$
⁽⁹⁾

In this work the complex-rotation is achieved by scaling, $r \Longrightarrow re^{-i\theta}$, in the argument of Eq. (6). The coordinates in the Hamiltonian as well as the other parts of the wave function are not scaled.¹¹

II. THE RADIATIVE TRANSITION RATES

The 1s2p2p ⁴P state makes radiative transitions to the 1s2s2p ⁴P^o state in the nonrelativistic approximation. This is the main decay mechanism for the low Z 1s2p2p ⁴P_J systems, especially for the $J = \frac{1}{2}$ and $J = \frac{3}{2}$ states. This transition rate is given by¹²

$$W({}^{4}P_{J} \rightarrow {}^{4}P_{J'}^{\circ}) = \frac{4}{3} \frac{\alpha}{c^{2}} \omega^{3} |\langle \psi({}^{4}P_{J}) | \mathbf{r} | \Psi({}^{4}P_{J'}^{\circ}) \rangle |^{2} ,$$
(10)

where α is the fine-structure constant, c is the speed of light, and

$$\omega = E({}^{4}P_{J}) - E({}^{4}P_{J'}) . \tag{11}$$

If we sum over all possible final states, and average over the initial states, we have

$$W({}^{4}P_{J} \to {}^{4}P^{\circ}) = \frac{1}{2J+1} \sum_{J_{z}} \sum_{J'} W({}^{4}P_{J} \to {}^{4}P^{\circ}_{J'}) .$$
(12)

Since the energy differential ω is much larger than the fine-structure splitting, W does not change much for the different J's. In this work ω is approximated by the center of gravity energy difference. Therefore, $W({}^{4}P_{J} \rightarrow {}^{4}P^{\circ})$ is the same for the different J levels.

This direct dipole decay between the quartet levels, however, is not the only radiative transition that needs to be considered. The relativistic coupling makes possible radiative decays to the lower $1s 1s 2p^2 P_{J'}^{\circ}$ states via the intermediate doublet states.

Consider the wave function of the $1s 2p 2p {}^{4}P_{J}$ state neglecting the continuum,

$$\Psi_J = \psi({}^4P_J) + c_1 \psi({}^2L_J) + c_2 \psi({}^2L_J') .$$
(13)

If $J = \frac{1}{2}$, then L = 0 and L' = 1; if $J = \frac{3}{2}$, then L = 1 and L' = 2; finally if $J = \frac{5}{2}$ then the only doublet state which needs to be considered is ²D. The linear coefficients c are obtained from first-order perturbation theory. The ²L_J states all make direct radiative dipole transitions to the $1s 1s 2p \, {}^{2}P_{J'}^{\circ}$ states, the corresponding dipole matrix element for these transitions is

$$\langle \Psi_J | \mathbf{r} | \Psi({}^2P_{J'}^\circ) \rangle$$

= $\langle c_1 \psi({}^2L_J) + c_2 \psi({}^2L_J') | \mathbf{r} | \Psi(1s \, 1s \, 2p \, {}^2P_{J'}^\circ) \rangle .$ (14)

Notice the importance of the interference effect between the transition amplitudes for the ${}^{2}L_{J}$ and ${}^{2}L'_{J}$ intermediate states. Since the summed and averaged transition rate to the $1s 1s 2p {}^{2}P^{\circ}$ level is given by

$$W({}^{4}P_{J} \rightarrow {}^{2}P^{\circ}) = \frac{1}{2J+1} \sum_{Jz} \sum_{J'} \frac{4}{3} \frac{\alpha}{c^{2}} \omega'^{3} \times |\langle \Psi_{J} | \mathbf{r} | \Psi({}^{2}P_{J'}^{\circ}) \rangle|^{2} ,$$
(15)

it is essential to compute the dipole transition via the intermediate states in the above order rather than as two separate noninterfering processes. Finally, the lifetime τ_J of the 4P_J level is given by

$$\frac{1}{\tau_J} = W_{\text{tot}} = W({}^4P_J \rightarrow {}^4P^\circ) + W({}^4P_J \rightarrow {}^2P^\circ) + W_{\text{Auger}} .$$
(16)

III. RESULTS AND DISCUSSION

The wave function used for the lithiumlike states in this work is a multiconfiguration wave function similar to those of Refs. 7 and 8. It is first computed nonrelativistically using the LS coupling scheme. The energy is then corrected with the relativistic effects: kinetic energy correction, Darwin term, and orbit-orbit interaction. The mass polarization effect is also evaluated. Although the contribution of this mass polarization effect to the

power of	f ten to which the nu	umber is rais	ed; for nota	tion see Refs. 8 and 9.)					
	E			(<i>H</i> 1+ <i>H</i> 2)		(H5)	E	Δ	L
/	Nonrelativistic			Relativistic kinetic	$\langle H4 \rangle$	Mass	Relativistic	Shift	Width
Z	(a.u.)	Г	N	energy + Darwin	Orbit-orbit	polarization	(a.u.)	(a.u.)	(a.u.)
3								0.000 000	1.936[-11]
	-5.245 262	11	81	5.519[4]	+ 1.83[-5]	-2.74[-5]	- 5.245 823	0.000 000	1.4[-10]
								0.000 000.0	1.8[-10]
4								0.000 000	3.876[-11]
	- 9.870 724	11	81	-1.806[-3]	+ 6.9[-5]	-6.1[-5]	-9.872 522	0.000 000	3.002[-10]
								-0.000 001	9.683[-10]
S								0.000 000	7.750[-11]
	-16.000221	Π	78	-4.540[-3]	+ 1.71[-4]	-9.8[-5]	- 16.004 688	0.000 000	5.009[-10]
								0.000 000	5.644[-9]
9								-0.000001	5.781[-11]
	-23.631 596	11	78	-9.619[-3]	+ 3.41[-4]	-1.48[-4]	-23.641 023	0.000 000	4.688[-10]
								-0.000 002	2.221[-8]
٢								-0.000 005	2.1[-13]
	-32.763917	11	78	-1.8131[-2]	+ 5.96[-4]	-1.89[-4]	- 32.781 641	-0.000 000	1.361[-10]
								-0.000 006	6.910[-8]
8								-0.000014	2.042[-10]
	-43.396 832	11	78	-3.1365[-2]	+ 9.54[-4]	-2.31[-4]	-43.427 473	-0.000001	1.216[-10]
								-0.000018	1.799[-7]
6								-0.000036	1.586[-9]
	-55.530177	11	78	-5.0803[-2]	+ 1.433[-3]	-2.58[-4]	- 55.579 805	-0.000002	2.525[-9]
								0.000 044	4.125[-7]
10								-0.000082	6.067[-9]
	-69.163729	11	78	-7.8131[-2]	+2.039[-3]	-3.14[-4]	-69.240 135	-0.000 006	1.183[-8]
								-0.000 098	8.534[-7]

TABLE I. Energy and width of the $(ls 2p 2p)^4 P_J$ states of lithiumlike ions. The shift and width results are given in the order $J = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$. (The number in square brackets is the

energy is small, it is, nevertheless, measurable as demonstrated in recent experiments.¹³ The results for the $1s 2p 2p {}^{4}P$ states are given in the first part of Table I. The results in this table are very close to those of Ref. 8.

When this ${}^{4}P$ state is coupled to the continuum using Eq. (4), and the variational calculation of Eq. (9) is carried out; we obtain the shift Δ and width Γ due to the continuum from the real and imaginary parts of the complex energy eigenvalue.¹⁰ The shift and width for the three J levels are given in the last part of Table I. As might be expected, the width is small for small Z and large for large Z. For $J = \frac{5}{2}$ the width increases monotonically with Z; however, for $J = \frac{1}{2}$ and $J = \frac{3}{2}$ this width goes through an absolute minimum at $Z = \overline{7}$ and 8, respectively. This is because this spin-induced width is coming from two distinct processes, the amplitudes of which add destructively. The first autoionization process results from the direct coupling of the 1s2p2p ⁴P state with the continuum via the spin-dependent operators, while the second process results from the coupling of the $1s 2p 2p {}^{4}P$ state with the intermediate $1s 2p 2p {}^{2}L$ state which autoionizes via the nonrelativistic Coulomb interaction. These two processes add with a relative phase factor of π , i.e., the total amplitude is the difference of the two individual amplitudes (the only exceptions being the $J = \frac{3}{2}$ levels for Z = 3 and 4; in these two cases there is constructive interference, i.e., the amplitudes add). For the case of $J = \frac{5}{2}$ the second process always has the greater amplitude. For the cases of $J = \frac{1}{2}$ the first process is the largest for Z < 7, while the second process is largest for Z > 7. The two processes have approximately equal amplitudes for Z = 7; hence the minimum in the spin-induced width of this J level for Z = 7. This crossing of amplitudes occurs between Z = 7and 8 for the $J = \frac{3}{2}$ level with the second process dominating for large Z; hence, the minimum in the width for Z = 8 is not as complete for this level as it was for $J = \frac{1}{2}$. This amplitude information was obtained indirectly by setting the appropriate off-diagonal Hamiltonian matrix elements equal to zero in order to eliminate one or the other of the two processes.

For the case of Coulomb autoionization, we found

that when the width is small ($\Gamma < 10^{-6}$), the imaginary part of the energy in the complex-rotation calculation becomes somewhat unstable as the rotation angle θ and the nonlinear parameter γ in the outgoing electron's wave function are varied. Fortunately in this spininduced autoionization calculation the stability of the complex energy is very good even though the width for small Z is on the order of 10^{-10} a.u.

As discussed earlier, the wave function in Eq. (4) involves the coulombic autoionizing states $1s 2p 2p^2 D$ and $1s 2p 2p^2 S$. For Z < 6 these states were calculated and discussed in Ref. 9; for Z = 6-10, these results are calculated in this work. The results are presented in Tables II and III. These tables give the number of angular and spin partial waves used, L, the total number of linear parameters, N, the optimized value of the nonlinear parameter in the 1s-vacancy orbital, q (physically this represents the effective nuclear charge felt by the vacancy), and the first-order perturbation theory results for the relativistic corrections and the mass polarization effect. Although these saddle-point wave functions contain as many as 111 terms, in the present calculation, using the wave function given in Eq. (4), these functions are treated as single terms as is the wave function for $1s_{2p_{I}}^{2p_{I}} 2p_{I}^{4}P_{I}$. This is necessary for practical considerations when diagonalizing the Hamiltonian matrix computed with respect to the basis

 $[\psi(1s 2p 2p {}^{4}P), \psi(1s 2p 2p {}^{2}L), \psi_{g} U_{i}^{L}].$

With 15 U_i^{L} 's, this basis has 17 elements. The variation process of Eq. (9) determines the linear coefficients in the open-channel segment of the wave function, while the linear coefficients internal to the closed-channel segments are held fixed. This restriction was not used in Ref. 9, but was discussed in some detail there. The shift and width given in Tables II and III reflect this restriction of a fixed closed-channel segment.

A very important quantity in all these calculations is the coupling strength of the ${}^{4}P_{J}$ states with the various doublet states. This is represented by c in Eq. (4) and by c_{1} and c_{2} in Eq. (13). They are obtained by first-order perturbation theory,

$$c = \frac{\langle \psi(1s2p2p)^2 L_J | H_{\text{s.o.}} + H_{\text{s.o.}} + H_{\text{s.o.}} | \psi(1s2p2p)^4 P_J \rangle}{E({}^4P_J) - E({}^2L_J)}$$
 (17)

The magnitude of this coupling coefficient is the major factor for deciding upon the importance of a particular intermediate state's role in a spin-induced autoionization process or in a radiative process. The coupling coefficients are given in Table IV.

With the results from Tables I–IV, we are ready to tabulate the lifetimes for the $1s 2p 2p {}^4P_J$ levels. These lifetimes are obtained by summing the transition rate to the continuum along with the radiative transition rates to the 1s2s2p ⁴P° and 1s1s2p ²P° states. The results are given in Table V. In this table we note that for ⁴P_{5/2}, the transition to the continuum grows rapidly with Z, from 7.6×10^6 /sec for Z = 3 to 3.5×10^{10} /sec for Z = 10. For Z > 5, this becomes the dominating decay mode for the $J = \frac{5}{2}$ level. The situation is quite different for the $J = \frac{1}{2}$ and $\frac{3}{2}$ levels, where the transition to the continuum is much less important. These effects are best observed by examining the Auger branching ratio defined by

TA] Refs. {	BLE II. Energy an 3 and 9.)	nd width	of the (1	$(s2p2p)^2D$	state of lithiumlike ions.	(The number in so	quare brackets is	the power of ten	to which the num	ber is raised; for	notation see
	<i>E</i> Nonrelativistic				$\langle H1+H2\rangle$ Relativistic kinetic	<pre>(H3) Fermi</pre>	$\langle H4 \rangle$	<pre>(H5) Mass</pre>	∆ Shift	E Total	L Width
Z	(a.u.)	T	N	9	energy + Darwin	contact	Orbit-orbit	polarization	(a.u.)	(a.u.)	(a.u.)
3	-5.233 703	17	110	2.52	-5.599[-4]	+ 8.1[-7]	+ 8.71[-6]	-1.95[-5]	+0.000072	-5.234 201	4.04[-4]
4	-9.825287	17	111	3.18	-1.8189[-3]	+ 4.2[-6]	+3.12[-5]	-3.60[-5]	+ 0.000158	- 9.826 949	1.01[-3]
5	-15.918753	14	103	4.40	-4.543[-3]	+ 1.24[-5]	+ 7.36[-5]	-5.43[-5]	+0.000386	- 15.922 878	1.55[-3]
9	-23.513434	16	109	4.8	-9.630[-3]	+ 2.79[-5]	+ 1.41[-4]	-7.82[-5]	+0.000273	-23.522 700	1.92[-3]
7	- 32.608 483	16	109	5.6	-1.8139[-2]	+ 5.27[-5]	+ 2.41[-4]	-9.79[-5]	+0.000315	-32.626111	2.24[-3]
80	-43.203 793	16	109	6.408	-3.1354[-2]	+ 8.94[-5]	+3.80[-4]	-1.18[-4]	+ 0.000347	-43.234450	2.49[-3]
6	- 55.299 205	14	103	7.20	-5.0751[-2]	+ 1.40[-4]	+ 5.65[-4]	-1.31[-4]	+0.000377	-55.349005	2.70[-3]
10	-68.894912	14	103	8.00	-7.8063[-2]	+ 2.07[-4]	+ 8.00[-4]	-1.59[-4]	+0.000397	-68.971730	2.87[-3]

r is raised; for notation see	
ower of ten to which the numbe	
The number in square brackets is the p	
Energy and width of the $(1s 2p 2p)^2 S$ states of lithiumlike ions. (7)	
TABLE III.	efs. 8 and 9.)

Refs.	8 and 9.)										
	E				$\langle H1+H2\rangle$	$\langle H3 \rangle$		$\langle H5 \rangle$	Δ	Е	Ĺ
	Nonrelativistic				Relativistic kinetic	Fermi	$\langle H4 \rangle$	Mass	Shift	Total	Width
Z	(a.u.)	Г	N	<i>d</i>	energy + Darwin	contact	Orbit-orbit	polarization	(a.u.)	(a.u.)	(a.u.)
4	-9.699 517	16	118	3.84	-1.8427[-3]	+ 6.3[-6]	+ 3.36[-5]	-1.87[-5]	+0.000231	-9.701 108	2.18[-4]
ŝ	-15.741 852	13	104	4.78	-4.6079[-3]	+2.18[-5]	+ 8.73[-5]	-3.38[-5]	+0.000290	- 15.746 095	2.53[-4]
9	-23.286919	13	104	5.80	-9.751[-3]	+ 5.04[-5]	+ 1.78[-4]	-5.34[-5]	+ 0.000331	-23.296 165	2.97[-4]
٢	- 32.332 891	13	104	6.81	-1.8401[-2]	+ 9.67[-5]	+3.16[-4]	-7.05[-5]	+ 0.000365	-32.350 585	3.35[-4]
×	-42.879 573	13	104	7.812	-3.1856[-2]	+ 1.65[-4]	+5.13[-4]	-8.80[-5]	+ 0.000391	-42.910449	3.65[-4]
6	- 54.926487	13	104	8.814	-5.1545[-2]	+2.60[-4]	+7.78[-4]	-1.00[-4]	+0.000408	- 54.976 687	3.92[-4]
10	-68.473 541	13	104	9.824	-7.9428[-2]	+ 3.85[-4]	+ 1.123[-3]	- 1.24[-4]	+0.000422	-68.551 163	4.16[-4]

States Z	${}^{4}P_{1/2}$ (1s2p2p) ² S _{1/2}	${}^{4}P_{1/2}$ (1s2p2p) ² P _{1/2}	${}^{4}P_{3/2}$ (1s2p2p) ${}^{2}P_{3/2}$	${}^{4}P_{3/2}$ $(1s2p2p)^{2}D_{3/2}$	${}^{4}P_{5/2}$ $(1s2p2p)^{2}D_{5/2}$
3				3.9902[-4]	-8.3603[-4]
4	4.2997[-4]			1.7217[-4]	-1.2706[-3]
5	1.0032[-3]	-6.5067[-4]	-1.4183[-3]	-3.1292[-5]	-2.3547[-3]
6	1.9365[-3]	1.1222[-3]	2.2968[-3]	4.0002[-4]	4.0511[-3]
7	3.3088[-3]	1.7791[-3]	3.4913[-3]	9.9102[-4]	6.4584[-3]
8	5.2099[-3]	-2.6516[-3]	-5.0486[-3]	1.8566[-3]	9.6915[-3]
9	7.7183[-3]	-3.7698[-3]	-7.0160[-3]	-3.0521[-3]	-1.3878[-2]
10	1.0920[-2]	-5.1656[-3]	-9.4447[-3]	-4.6252[-3]	-1.9144[-2]

TABLE IV. The coupling constants for the $1s 2p 2p {}^{4}P$ states with the ${}^{2}S_{J}$, ${}^{2}P_{J}$, and the ${}^{2}D_{J}$ levels of lithiumlike systems [c in Eq. (4)]. (The number in square brackets is the power of ten to which the number is raised.)

TABLE V. Transition rates and lifetimes of the 1s2p2p ${}^{4}P_{J}$ states of lithiumlike systems. (Transition rates are given in 10⁹/sec, lifetimes are given in ns.) W_{1} is the transition rate to 1s2s2p ${}^{4}P^{\circ}$. W_{2} is the transition rate to 1s1s2p ${}^{2}P^{\circ}$. W_{3} is the spin-induced autoionization rate to the continuum.

						Other	theory		
Ζ	J	\boldsymbol{W}_1	<i>W</i> ₂	<i>W</i> ₃	lifetime	Ref. 3	Ref. 16	Expe	riment
3	$\frac{1}{2}$ $\frac{3}{2}$ $\frac{5}{2}$	0.1731 0.1731 0.1731	0.0000 0.0000 0.0000	0.0008 0.0059 0.0076	5.749 5.586 5.534				
4	$\frac{1}{2}$ $\frac{3}{2}$ $\frac{5}{2}$	0.3165 0.3165 0.3165	0.0000 0.0000 0.0000	0.0016 0.0124 0.0400	3.143 3.040 2.805				
5	$\frac{\frac{1}{2}}{\frac{3}{2}}$	0.4538 0.4538 0.4538	0.0003 0.0008 0.0007	0.0032 0.0207 0.2333	2.187 2.104 1.454				$2.2{\pm}0.15^{a}$ $1.45{\pm}0.15^{a}$
6	$\frac{1}{2}$ $\frac{3}{2}$ $\frac{5}{2}$	0.5872 0.5872 0.5872	0.0024 0.0055 0.0058	0.0024 0.0194 0.9182	1.689 1.634 0.662	2.551 2.577 0.889		2.5±0.3 ^b 0.9±0.1 ^b	1.66±0.13° 0.71±0.07°
7	$\frac{1}{2}$ $\frac{3}{2}$ $\frac{5}{2}$	0.7190 0.7190 0.7190	0.0139 0.0279 0.0317	0.0000 0.0056 2.8567	1.364 1.329 0.277	1.952 2.046 0.339		1.4±0.1 ^b 1.7±0.3 ^b 0.3±0.05 ^b	
8	$\frac{\frac{1}{2}}{\frac{3}{2}}$	0.8496 0.8496 0.8496	0.0618 0.1116 0.1346	0.0084 0.0050 7.4383	1.087 1.035 0.119	1.032 1.501 0.135		1±0.1 ^b 1.1±0.1 ^b 0.1±0.01 ^b	
9	$\frac{1}{2}$ $\frac{3}{2}$ $\frac{5}{2}$	0.9787 0.9787 0.9787	0.2258 0.3780 0.4760	0.0655 0.1044 17.0543	0.787 0.684 0.0540	0.754 0.909 0.0592			0.059±0.007 ^d
10	$\frac{\frac{1}{2}}{\frac{3}{2}}$	1.1077 1.1077 1.1077	0.7296 1.1520 1.4614	0.2508 0.4890 35.2808	0.479 0.364 0.0264	0.530 0.449 0.0281	0.529 0.110	0.54±0.05 ^e 0.408±0.04 ^e <0.05	$\begin{array}{c} 0.53 \! + \! 0.05^{\rm f} \\ 0.40 \! \pm \! 0.04^{\rm f} \\ < \! 0.05 \end{array}$

^aReference 15.

^bReference 1.

^cReference 14.

^dI. Martinson et al., Phys. Scr. 27, 201 (1983).

^eReference 17.

^fReference 18.

	S	BAuger			Brad	n an an Anna Anna an Anna Anna Anna Ann
Z	$J = \frac{1}{2}$	$J = \frac{3}{2}$	$J = \frac{5}{2}$	$J = \frac{1}{2}$	$J = \frac{3}{2}$	$J=\tfrac{5}{2}$
3	0.460	3.296	4.206	0.000	0.000	0.000
4	0.503	3.770	11.220	0.000	0.000	0.000
5	0.700	4.355	33.920	0.066	0.176	0.154
6	0.405	3.169	60.760	0.407	0.928	0.978
7	0.000	0.744	79.190	1.897	3.735	4.223
8	0.913	0.518	88.315	6.781	11.610	13.676
9	5.158	7.145	92.141	18.746	27.862	32.722
10	12.011	17.790	93.212	39.710	50.980	56.884

TABLE VI. Auger and radiative branching ratios (for notation see text).

$$\mathcal{B}_{Auger} = 100 \frac{W_{Auger}}{W_{tot}} \% .$$
 (18)

This quantity is given in Table VI. The minimum in the transition rate to the continuum as a function of Z for the $J = \frac{1}{2}$ and $\frac{3}{2}$ levels is easily seen in Table VI.

For the radiative transitions, we define the radiative branching ratio to the $1s 1s 2p^2 P^\circ$ states from the transition rates $W_1 = W({}^4P_J \rightarrow {}^4P^\circ)$ and $W_2 = W({}^4P_J \rightarrow {}^2P^\circ)$,

$$\mathcal{B}_{\rm rad} = 100 \frac{W_2}{W_{\rm rad}} \% , \qquad (19)$$

where $W_{rad} = W_1 + W_2$. This quantity is also given in Table VI. This table shows that the $1s 2p 2p {}^{4}P$ \rightarrow 1s 2s 2p ⁴P° transition dominates for Z < 9 as expected. This transition rate increases linearly with Z. On the other hand, the $1s 2p 2p {}^4P \rightarrow 1s 1s 2p {}^2P^\circ$ transition is negligible for Z < 7. However, this latter rate grows very rapidly with Z. For the $J = \frac{5}{2}$ and $\frac{3}{2}$ levels of Ne VIII, this transition rate is already larger than the corresponding rate to the $1s 2s 2p {}^{4}P^{\circ}$ levels. This is because of the Z^4 dependence of the relativistic spin-orbit matrix elements, and the Z^2 dependence of the energy difference $E({}^{4}P) - E({}^{2}P^{\circ})$. For Z > 9, it becomes the most important radiation decay mode. The transition rate to $1s 1s 2p^{2}P$, W_{2} , can be analyzed and computed from the coupling coefficients of Table IV and the reduced dipole matrix elements, $\langle \psi(^{2}L) || \mathbf{r} || \Psi(^{2}P^{\circ}) \rangle$, which are given in Table VII. In terms of these quantities the matrix element appearing in Eq. (14) becomes

TABLE VII. The reduced matrix elements $|\langle \psi(1s 2p 2p)^2 L ||\mathbf{r}|| \Psi(1s 1s 2p)^2 P^{\circ} \rangle|.$

Z	$(1s2p2p)^2S$	$(1s2p2p)^2P$	$(1s2p2p)^2D$
5	0.117 68	0.393 78	0.277 07
6	0.102 83	-0.33921	-0.250 84
7	-0.090 908	0.296 74	0.220 51
8	-0.080 952	-0.263 07	0.195 80
9	-0.072 866	-0.235 98	-0.175 87
10	-0.066 261	-0.213 89	-0.159 46

$$\langle \psi({}^{2}L_{J}) | \mathbf{r} | \Psi(1s \, 1s \, 2p \, {}^{2}P_{J'}^{\circ}) \rangle$$

$$= (-1)^{J'+L+1.5} \sqrt{(2J+1)(2J'+1)}$$

$$\times \begin{cases} L & 1 & 1 \\ J' & 1/2 & J \end{cases} \langle \psi({}^{2}L) ||\mathbf{r}|| \Psi({}^{2}P^{\circ}) \rangle , \qquad (20)$$

where the curly-bracketed quantity is a 6-j symbol.

In general, the lifetimes calculated in this work agree well with the existing experimental data. C IV is an obvious exception. For this system, the experimental result of Livingston and Berry¹ agrees excellently with the calculation of Chen *et al.*³ However, this result differs substantially from ours. We have been informed by Mannervik¹⁴ that new measurements on the C IV ⁴P_J lifetimes have been made and these new results are in excellent agreement with those of this calculation. For the B III lifetimes, our results also agree excellently with those of Mannervik *et al.*¹⁵ For Ne VIII, the lifetimes of the $J = \frac{1}{2}$ and $\frac{3}{2}$ levels seem to lie at the lower end of the experimental uncertainty. Here the standard deviation is about 10% in both experiments. We hope that this uncertainty can be reduced in future experiments so that a more definitive conclusion can be drawn concerning the theoretical results in the literature.

CONCLUSION

In this work, we have computed the lifetimes of the lithiumlike $1s2p2p {}^{4}P_{J}$ levels for Z=3 to Z=10. It is found that the saddle-point complex-rotation method can be adequately implemented with the Pauli-Breit relativistic perturbation operators. Most of our results agree with the existing experimental data. For those systems where the agreement is not very close, there is a need to look closely into the theoretical results as well as the experimental data. We hope that more theoretical and experimental investigations can be undertaken on these systems.

Note added in proof. In a very recent paper by Träbert,¹⁹ the lifetimes of the $(1s 2p 2p)^4 P_J$ states have been analyzed and a new improved prediction is suggested. His results appear to agree with this work.

ACKNOWLEDGMENTS

This research was supported by a grant from Research Corporation (B.F.D.); and by the National Science Foundation under Grant No. PHY-84-05649.

- ¹A. E. Livingston and H. G. Berry, Phys. Rev. A 17, 1966 (1978).
- ²E. Träbert, S. Mannervik, and H. Cederquist, Phys. Scr. **34**, 46 (1986).
- ³M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A 26, 1441 (1982).
- ⁴K. T. Chung, R. Bruch, E. Träbert, and P. H. Heckmann, Phys. Scr. **29**, 108 (1984).
- ⁵M. Agentoft, T. Anderson, K. T. Chung, and B. F. Davis, Phys. Scr. 31, 74 (1985).
- ⁶K. T. Chung and B. F. Davis, Phys. Rev. A 29, 1871 (1984).
- ⁷B. F. Davis and K. T. Chung, J. Phys. B 15, 3113 (1982).
- ⁸K. T. Chung, Phys. Rev. A 29, 682 (1984).
- ⁹B. F. Davis and K. T. Chung, Phys. Rev. A **31**, 3017 (1985).
- ¹⁰B. F. Davis and K. T. Chung, Phys. Rev. A 29, 1878 (1984).

- ¹¹B. F. Davis and K. T. Chung, Phys. Rev. A 36, 1948 (1987).
- ¹²M. Weissbluth, Atoms and Molecules (Academic, New York, 1978), p. 507.
- ¹³S. Mannervik, J. Phys. B 17, L851 (1984).
- ¹⁴L. Engstrom, R. Hutton, N. Reistad, I. Martinson, S. Huldt, S. Mannervik, and E. Träbert, Phys. Scr. 36, 250 (1987).
- ¹⁵S. Mannervik, H. Cederquist, and I. Martinson, Phys. Rev. A 34, 23 (1986).
- ¹⁶T. W. Tunnell and C. L. Bhalla, Phys. Lett. A 67, 119 (1978).
- ¹⁷A. E. Livingston, J. E. Hardis, L. J. Curtis, R. L. Brooks, and H. G. Berry, Phys. Rev. A **30**, 2089 (1984).
- ¹⁸E. J. Knystautus and M. Druetta, Phys. Rev. A **31**, 2279 (1985).
- ¹⁹E. Träbert, Nucl. Instrum. Methods B 23, 287 (1987).