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

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The saddle-point complex-rotation method in the intermediate *LSJ*-coupling scheme is used with the Breit-Pauli spin-dependent perturbation operators to compute the spin-induced autoionization rates of the lithiumlike $1s2s2p\,^4P^o_J$ states from $Z=3$ to 18. The radiative transition rates of the $J=\frac{1}{2}$ and $\frac{3}{2}$ levels are also calculated in the intermediate *LSJ*-coupling scheme. The combined result yields lifetimes for these levels which are compared with the existing experimental and theoretical data in the literature.

I. INTRODUCTION

Many aspects of the lithiumlike $1s2s2p$ states have been studied both theoretically and experimentally. For instance, the $1s2s2p$ configuration forms two distinct doublet terms in the *LS* coupling scheme, $[1s,(2s2p)^3P]^2P^o$ and $[1s,(2s2p)^1P]^2P^o$. These core-excited doublet states couple to the continuum through the nonrelativistic Coulomb interaction and consequently deexcite by rapid autoionization. For small Z, nonrelativistic calculations of these systems yield Auger energies and widths or lifetimes which compare well with observations in both Auger and optical spectra.[1-3] In addition to the two doublets, the $1s2s2p$ configuration also forms a quartet term in the *LS* coupling scheme, $1s2s2p\,^4P^o$, which in the nonrelativistic approximation is spin-forbidden from decaying by either dipole optical emission to the lower doublet bound states or by autoionization to the $[(1s1s)^1S,\epsilon l]^2L^o$ continuum. The fine structure of this multiplet has been observed in radiative transitions from higher quartet levels. Calculations of this fine structure via the spin-dependent relativistic perturbations with zeroth-order wave functions formed in the LSJ coupling scheme compare well with the high-precision experiments on low-Z systems.[4] These zeroth-order wave functions of well-defined total J, M_J, L, S, and parity are constructed from the pure *LS*-coupled wave functions by

$$|JM_JLS\rangle = \sum_{M_L,M_S} |LSM_LM_S\rangle\langle LSM_LM_S|JM_J\rangle \;, \tag{1}$$

where the $\langle LSM_LM_S|JM_J\rangle$ are Clebsch-Gordan coefficients. These wave functions are adequate due to the fact that the energy separation of the $(1s2s2p)^2P^o$ states from $(1s2s2p)^4P^o$ is much greater than the fine-structure splitting. The spin-independent part of the relativistic corrections may be obtained by first-order perturbation theory with the *LS*-coupled wave functions. When these contributions are added to the energy, the resulting transition wavelengths are found to be in excellent agreement with the high-precision measurements.[4]

Relativistic coupling effects, however, become essential for an understanding of the deexcitation of this metastable $(1s2s2p)^4P^o$ system. Differential metastability has been observed for the decay of the various J levels of this system, i.e., the $J=\frac{5}{2}$, $\frac{3}{2}$, and $\frac{1}{2}$ levels all have different lifetimes, with the lifetime of the $J=\frac{5}{2}$ level being the longest. In order to obtain this differential metastability theoretically, the wave function to the first order with respect to the manifold of states formed from the $1s2s2p$ configuration along with the energy degenerate continuum must be constructed. Starting from zeroth order, we first construct the *LS*-coupled wave functions representing the $(1s2s2p)^4P^o$, $[1s,(2s2p)^3P]^2P^o$, and $[1s,(2s2p)^1P]^2P^o$ states using the Rayleigh-Ritz method for the quartet state and the saddle-point method for the Coulomb autoionizing doublet states. Then we add to this three-state basis a square-integrable basis set to represent the continuum, $[(1s1s)^1S,\epsilon l]^2L^o$, and diagonalize the relativistic spin-dependent part of the Breit-Pauli interaction via the complex-rotation method. For example, the nonrelativistic Hamiltonian $H_{\rm nr}$ is

$$H_{\rm nr} = \sum_{i=1}^{3}\left[-\frac{\hbar^2}{2m}\nabla_i^2 - \frac{Ze^2}{r_i}\right] + \sum_{i<j=1}^{3}\frac{e^2}{r_{ij}} \;. \tag{2}$$

The spin-dependent part of the Breit-Pauli interaction, $H_{\rm spin}$, is given by the sum of the operators for the spin-orbit ($H_{\rm so}$), spin-other-orbit ($H_{\rm soo}$), and spin-spin ($H_{\rm ss}$) interactions, where

$$H_{\rm so} = \frac{Ze^2\hbar}{2m^2c^2}\sum_{i=1}^{3}\frac{\mathbf{l}_i\cdot\mathbf{s}_i}{r_i^3} \;, \tag{3}$$

$$H_{\rm soo} = -\frac{e^2\hbar}{2m^2c^2}\sum_{\substack{i,j=1\\ i\neq j}}^{3}\left[\frac{\mathbf{r}_{ij}}{r_{ij}^3}\times\mathbf{p}_i\right]\cdot(\mathbf{s}_i+2\mathbf{s}_j) \;, \tag{4}$$

$$H_{\rm ss} = \frac{e^2\hbar^2}{m^2c^2}\sum_{\substack{i,j=1\\ i<j}}^{3}\frac{1}{r_{ij}^3}\left[\mathbf{s}_i\cdot\mathbf{s}_j - \frac{3(\mathbf{s}_i\cdot\mathbf{r}_{ij})(\mathbf{s}_j\cdot\mathbf{r}_{ij})}{r_{ij}^2}\right] \;. \tag{5}$$

Utilizing the notation $|\psi_0(J)\rangle$, $|\psi_1(J)\rangle$, $|\psi_2(J)\rangle$, and $|\psi_c(J)\rangle$ to refer to the basis states $(1s2s2p)^4P_J^o$, $[1s,(2s2p)^3P]^2P_J^o$, $[1s,(2s2p)^1P]^2P_J^o$, and $[(1s1s)^1S,\epsilon l]^2L_J^o$, respectively, the total Hamiltonian of interest,

$$H = H_{\rm nr} + H_{\rm spin} = H_{\rm nr} + H_{\rm so} + H_{\rm soo} + H_{\rm ss} \ ,$$

has a matrix in this basis of the following form:

$$[H] = \begin{bmatrix} H_{00} & H_{01} & H_{02} & H_{0c} \\ H_{10} & H_{11} & H_{12} & H_{1c} \\ H_{20} & H_{21} & H_{22} & H_{2c} \\ H_{c0} & H_{c1} & H_{c2} & H_{cc} \end{bmatrix} . \tag{6}$$

The off-diagonal matrix elements H_{01}, H_{02}, H_{0c} are equal to $\langle 0|H_{\rm spin}|i\rangle$ $(i=1,2,c)$ since $\langle 0|H_{\rm nr}|i\rangle = 0$ due to the orthogonality of the quartet and doublet spin functions. The interaction between the two $1s2s2p\ ^2P^0$ doublet states is determined by the relativistic interactions

$$H_{12} = \langle 1|H|2\rangle = \langle 1|H_{\rm spin}|2\rangle \ ,$$

since these states are orthogonal within the nonrelativistic approximation. The diagonal elements $\langle i|H|i\rangle (i=0,1,2,c)$ are approximated by $\langle i|H_{\rm nr}|i\rangle$ due to the smallness of $H_{\rm spin}$ relative to $H_{\rm nr}$. The off-diagonal elements $\langle 1|H|c\rangle$ and $\langle 2|H|c\rangle$ are also approximated with H replaced by $H_{\rm nr}$ for the same reason.

The off-diagonal matrix elements (which correspond to the coupling strengths between the various zeroth-order states) are J dependent, and as a result the imaginary part of the complex eigenvalue which corresponds to half the autoionization width (proportional to the autoionization transition probability) is also J dependent. Hence differential metastability results from this intermediate LSJ coupling. For small Z, autoionization is the major decay mode of the $(1s2s2p)^4P_J^o$ systems; however, radiative decay to the $(1s1s2s)^2S$ ground state becomes the dominant decay mechanism for large Z. This occurs indirectly for the $J=\frac{1}{2}$ and $\frac{3}{2}$ levels as a result of the relativistic coupling to the $(1s2s2p)^2P^o$ states.

The analysis is not so complex for the $J=\frac{5}{2}$ states. This is because the $(1s2s2p)^2P^o$ states can only couple to form $J=\frac{1}{2}$ and $\frac{3}{2}$ states, so the corresponding off-diagonal matrix elements of the Hamiltonian (H_{01} and H_{02}) are zero. The coupling to the continuum is generated by the spin-spin interaction only for the $J=\frac{5}{2}$ fine-structure level.[5] As a result the matrix element $H_{0c} = \langle 0|H_{\rm spin}|c\rangle$ becomes simply $\langle 0|H_{\rm ss}|c\rangle$. Since the $1s2s2p\ ^2P^o$ states are not coupled to the quartet for this value of J, electric dipole transitions to the ground state are not possible, and radiation to this level can only occur through the much less rapid magnetic quadrupole branch. For these reasons, the $J=\frac{5}{2}$ level is the longest lived; more experimental measurements have been made for this J level also. In a previous paper[5] we investigated the practical feasibility of incorporating spin-dependent interactions into the "saddle-point complex-rotation method" by applying it to this well-studied $J=\frac{5}{2}$ fine-structure level. It is the purpose of this paper to extend the study to the more complex $J=\frac{1}{2}$ and $\frac{3}{2}$ fine-structure levels. This work is also motivated by the lack of accurate theoretical predictions for these lifetimes for cases of small Z. The most extensive previous calculation is perhaps that of Chen *et al.*,[6] who calculated the lifetimes of all the J levels for selected values of Z in the range $13 < Z < 92$. In that work, Dirac-Hartree-Slater wave functions were used, and the autoionization transition rate was computed using perturbation theory assuming frozen orbitals. The "golden rule No. 2" was used employing the Moller operator as the transition operator.[6] A subsequent paper by Chen *et al.*[7] added results for the lighter ions with $6 < Z < 10$. In that work the authors point out the important role that low-Z, highly stripped atoms play in astrophysical and plasma environments, and that light Li-like ions are more easily produced in the laboratory than heavy ones. The latter fact coupled with more theoretical predictions may provide an incentive for additions to the exceedingly scant experimental literature on the subject. Chen *et al.*,[7] however, do not consider the ions lighter than $Z=6$ "because for these systems electron-electron correlations may become so important as to make the present treatment inadequate." The results presented here are obtained with large configuration-interaction wave functions which do not suffer from this deficiency. Also of importance is that in the present method the interactions between the closed and open channels as manifested in the Hamiltonian matrix are able to affect the resulting final form of the open-channel component $|c\rangle$ through the complex matrix diagonalization process. In methods where a golden rule formula is used, the correlations between the initial and final states cannot be included.

The remainder of this paper is divided into the following four sections. Section II discusses the computation of the spin-induced autoionization width. Section III deals with the calculation of the spin-induced radiative transition rate to the lithiumlike ground state. Section IV combines the results of the previous sections for the decay rates for electron and photon emission to yield theoretical lifetimes for the $J=\frac{1}{2}$ and $\frac{3}{2}$ fine-structure levels of $(1s2s2p)^4P_J^o$. These results are compared with the existing theoretical and experimental results in the literature. In this section we also analyze the explicit source of the various contributions to the spin-induced Auger rate in order to understand the corresponding interference effects in this transition rate. Section V is a brief conclusion.

II. SPIN-INDUCED AUTOIONIZATION WIDTH

In this section we begin by detailing the basis which is used to construct the Hamiltonian matrix for the $1s2s2p$ configuration and associated continuum. Diagonalization of this matrix as required by the variational principle's requirement of a stationary solution yields complex eigenvalues whose imaginary parts are the half-widths due to autoionization by the theory of complex rotation.[8]

The major component of the resonant wave function is the zeroth-order $(1s2s2p)^4P_J^o$ state, $|\psi_0(J)\rangle$. This state of well-defined total angular momentum J and z component M_J is formed from the pure LS-coupled state $(1s2s2p)^4P^o$ by Eq. (1). The $(1s2s2p)^4P^o$ state is a multiconfiguration-interaction wave function similar to that of Chung and Davis.[9] For the various values of nuclear charge, Z, it is composed of either 12 or 13 partial waves with a total of from 80 to 97 Slater-like orbital terms. The linear coefficients in these wave functions were determined by the standard Rayleigh-Ritz variational method. This wave function appears as a single basis state in the Hamiltonian matrix of Eq. (1). The nonrelativistic energy of this state is given in the first column of Table I. The following three columns of this Table give first-order perturbation theory results for the relativistic perturbations: relativistic correction to the kinetic energy plus Darwin term and the orbit-orbit interaction resulting from the retardation of the Coulomb potential; and the nonrelativistic mass polarization effect. The following column of this

TABLE I. Energy and spin-induced autoionization width of the $(1s2s2p)^4P_J^o$ states of lithiumlike ions (in atomic units). $\langle H_1+H_2\rangle$, $\langle H_4\rangle$, and $\langle H_5\rangle$ are the expectation values of the relativistic operators corresponding to kinetic energy correction plus Darwin term, orbit-orbit or retardation, and the nonrelativistic mass polarization effect, respectively. E total is the sum of the nonrelativistic energy plus the aforementioned corrections. The shift Δ and the width Γ result from the interaction of this inner-shell vacancy state with the degenerate $^2P_J^o$ continuum directly via the relativistic spin-dependent operators, and indirectly via the coupling to the $[(1s(2s2p)^3P]^2P_J^o$ and $[(1s(2s2p)^1P]^2P_J^o$ states by the same spin-dependent operators. (The number in square brackets is the power of 10 to which the number is raised. The shift and width results are given in this order: $J=\frac{1}{2},\frac{3}{2},\frac{5}{2}$.)

Z	E Nonrelativistic	$\langle H_2+H_2\rangle$ (10^{-4})	$\langle H_4\rangle$ (10^{-4})	$\langle H_5\rangle$ (10^{-4})	E Total	Δ Shift (10^{-4})	Γ Width
3	−5.367 870	−6.05	0.09	−0.154	−5.368 481	0.000	1.865[−10]
						0.000	9.542[−11]
						0.000	3.411[−12]
4	−10.066 480	−20.07	0.35	−0.323	−10.068 484	0.000	1.116[−9]
						−0.001	4.934[−10]
						0.000	2.285[−11]
5	−16.267 410	−50.82	0.85	−0.508	−16.272 457	−0.001	3.486[−9]
						−0.003	1.326[−9]
						0.000	8.146[−11]
6	−23.969 335	−108.15	1.69	−0.761	−23.980 057	−0.005	8.008[−9]
						−0.013	2.554[−9]
						0.000	2.122[−10]
7	−33.171 779	−204.27	2.95	−0.966	−33.192 008	−0.016	1.532[−8]
						−0.045	3.952[−9]
						0.000	4.587[−10]
8	−43.874 525	−353.58	4.72	−1.173	−43.909 529	−0.044	2.572[−8]
						−0.124	5.070[−9]
						0.000	8.741[−10]
9	−56.077 431	−573.53	7.07	−1.308	−56.134 207	−0.106	3.943[−8]
						−0.302	5.458[−9]
						0.000	1.521[−9]
10	−69.780 524	−882.64	10.10	−1.590	−69.867 937	−0.233	5.636[−8]
						−0.664	4.783[−9]
						0.000	2.475[−9]
11	−84.983 682	−1302.75	13.88	−1.721	−85.112 742	−0.471	7.582[−8]
						−1.349	2.939[−9]
						0.00	3.816[−9]
12	−101.686 905	−1857.85	18.50	−2.010	−101.871 041	−0.90	9.744[−8]
						−2.57	7.788[−10]
						0.00	5.641[−9]
13	−119.890 179	−2573.80	24.05	−2.138	−120.145 369	−1.62	1.203[−7]
						−4.56	1.468[−10]
						0.00	8.053[−9]
14	−139.593 492	−3479.58	30.60	−2.431	−139.938 633	−2.78	1.434[−7]
						−8.01	4.618[−9]
						0.00	1.117[−8]

TABLE I. (*Continued.*)

Z	E Nonrelativistic	$\langle H_2+H_2\rangle$ (10^{-4})	$\langle H_4\rangle$ (10^{-4})	$\langle H_5\rangle$ (10^{-4})	E Total	Δ Shift (10^{-4})	Γ Width
15	$-160.796\,835$	-4605.98	38.25	-2.557	$-161.253\,864$	-4.60	1.659[−7]
						-13.28	2.006[−8]
						0.00	1.510[−8]
16	$-183.500\,204$	-5985.90	47.08	-2.853	$-184.094\,371$	-7.33	1.867[−7]
						-21.30	5.552[−8]
						0.00	2.000[−8]
17	$-207.703\,592$	-7655.23	57.17	-2.977	$-208.463\,697$	-11.34	2.049[−7]
						-33.20	1.241[−7]
						0.00	2.600[−8]
18	$-233.406\,998$	-9651.43	68.60	-2.948	$-234.365\,575$	-17.05	2.201[−7]
						-50.38	2.441[−7]
						0.00	3.325[−8]

table, labeled "E Total," is the sum of the nonrelativistic energy and the preceding spin-independent perturbations. These first-order perturbation energies, which have been computed separately for each value of Z, have been tabulated here for their interest with respect to trends along the isoelectronic sequence.

The two linearly independent $(1s2s2p)^2P^o$ states, $[1s,(2s2p)^3P]^2P^o$ and $[1s,(2s2p)^1P]^2P^o$, designated $|1\rangle$ and $|2\rangle$, play a critical role in the decay of the $(1s2s2p)^4P^o_J$ states. Their first-order coupling to the $(1s2s2p)^4P^o$ through the spin-dependent interactions (H_{so}, H_{soo}, and H_{ss} are all of order α^2 where α is the fine-structure constant) allows them to act as intermediate states for the "quartet to continuum" deexcitation. The $(1s2s2p)^2P^o$ states couple directly to the continuum, $[(1s1s)^1S,\epsilon p]^2P^o$, through the Coulomb interaction (zeroth-order with respect to α) and therefore rapidly deexcite by autoionization. Consequently, autoionization by this indirect process via the intermediate states is of the same order in α as the direct autoionization of $(1s2s2p)^4P^o$ by virtue of its direct coupling to the same continuum through the spin-dependent interactions.

The variational calculation of $(1s2s2p)^4P^o$ is straightforward since it is a bound state in the nonrelativistic approximation. On the other hand, there are an infinite number of states with lower energy but with the same angular and spin symmetry as the two $(1s2s2p)^2P^o$ states. For this reason, a variational method which attempts to accurately compute the energy and wave function of the $(1s2s2p)^2P^o$ states must be based upon a well-defined mathematical principle which allows a large multi-configuration-interaction wave function to be built up without a variational breakdown. The saddle-point technique is such a variational method.[10,11] This method generates the "correct" vacancy orbitals, and as a consequence the continuum is effectively projected out of the $^2P^o$ trial function.[2] Tables II and III give the nonrelativistic energies obtained by this saddle-point method for the $[1s,(2s2p)^3P]^2P^o$ and $[1s,(2s2p)^1P]^2P^o$ states, respectively. The corresponding wave functions all have 15 angular and spin partial waves with a total of 110 Slater-type orbital terms. These orbitals were obtained by selecting those which give the lowest energy for the case of the neon ion, $Z=10$; the nonlinear parameters in these basis functions were optimized for each particular value of Z. Details of this calculation can be found in Refs. 1 and 12. It should be mentioned that the nonrelativistic energies given in Table II for $Z=3$ and 4 and in Table III for $Z=4$ are slightly higher than results which we have previously published;[2] this is because in Ref. 2 the orbitals were chosen specifically for the ions of interest, hence the energy given in Ref. 2 is slightly better. The saddle-point method builds parametrized $1s$ vacancies directly into the trial wave function and then determines the optimal vacancy by a well-defined optimization procedure. The result of this procedure for the hydrogenic vacancies used here is the optimized value of q, which physically corresponds to the effective nuclear charge experienced by the vacancy state.[12] This q value comprises the second columns of Tables II and III. For all the ions q is approximately equal to $Z-\frac{1}{2}$ (in atomic units), indicating that the $1s$-vacancy orbital is approximately half screened by the presence of the $1s$ electron. In addition to the spin-independent relativistic perturbations considered for the $(1s2s2p)^4P^o$ state we also quote the first-order perturbation theory result for the Fermi contact term between the electrons for these doublet states in which there is a nonzero probability to find the electrons at the same spacial point. "E Total" once again represents the sum of the nonrelativistic energy plus the contributions from the spin-independent perturbations.

When the Hamiltonian matrix of the $1s2s2p$ configuration plus $1s1s\epsilon p\,^2P^o$ continuum subspace is constructed as in the Introduction, the two $(1s2s2p)^2P^o$ states each appear as single basis elements. The 110 linear coefficients predetermined by the saddle-point calculations for each doublet are held fixed in order to maintain the integrity of the zeroth-order basis, and also to keep the size of the complex matrix small for diagonalization.

Finally, the continuum $[(1s1s)^1S,\epsilon p]^2P^o$, $|\psi_c\rangle$, is constructed as follows:

TABLE II. Energy and nonrelativistic autoionization width of the $[1s(2s2p)^3P]^2P^o$ state of lithiumlike ions (in atomic units). $\langle H_1+H_2\rangle$, $\langle H_3\rangle$, $\langle H_4\rangle$, and $\langle H_5\rangle$ are the expectation values of the relativistic operators corresponding to kinetic energy correction plus Darwin term, Fermi contact, orbit-orbit or retardation, and the nonrelativistic mass polarization effect, respectively. E Total is the sum of the nonrelativistic energy plus the aforementioned corrections. The shift Δ and the width Γ result from the interaction of this inner-shell vacancy state with the degenerate $^2P^o$ continuum via the nonrelativistic Coulomb interaction.

Z	E Nonrelativistic	q	$\langle H_1+H_2\rangle$ (10^{-4})	$\langle H_3\rangle$ (10^{-4})	$\langle H_4\rangle$ (10^{-4})	$\langle H_5\rangle$ (10^{-4})	E Total	Δ Shift (10^{-4})	Γ Width (10^{-4})
3	−5.312 591	2.469	−5.88	0.06	−0.05	0.101	−5.313 168	2.76	1.38
4	−9.959 724	3.464	−19.46	0.25	−0.21	0.236	−9.961 643	3.73	1.55
5	−16.106 497	4.464	−49.38	0.61	−0.54	0.390	−16.111 389	4.17	1.54
6	−23.753 069	5.462	−105.38	1.24	−1.10	0.596	−23.763 533	4.41	1.54
7	−32.899 365	6.461	−199.59	2.20	−1.95	0.766	−32.919 222	4.57	1.54
8	−43.545 479	7.460	−346.08	3.55	−3.14	0.937	−43.579 953	4.67	1.53
9	−55.691 546	8.459	−562.05	5.36	−4.73	1.049	−55.747 583	4.73	1.52
10	−69.337 562	9.458	−865.78	7.70	−6.78	1.278	−69.423 919	4.78	1.52
11	−84.483 588	10.458	−1278.61	10.64	−9.34	1.386	−84.611 180	4.80	1.50
12	−101.129 562	11.458	−1825.06	14.25	−12.47	1.620	−101.311 727	4.82	1.49
13	−119.275 522	12.458	−2531.13	18.59	−16.23	1.725	−119.528 227	4.84	1.49
14	−138.921 467	13.457	−3671.66	23.74	−20.67	1.962	−139.263 534	4.86	1.48
15	−160.067 395	14.457	−4537.58	29.75	−25.85	2.064	−160.520 556	4.87	1.48
16	−182.713 323	15.457	−5901.44	36.71	−31.83	2.304	−183.302 749	4.88	1.47
17	−206.859 253	16.457	−7551.25	44.67	−38.67	2.404	−207.613 537	4.89	1.47
18	−232.505 173	17.457	−9528.45	53.70	−46.41	2.381	−233.457 051	4.90	1.46

$$\psi_c([(1s1s)^1S,\epsilon L]^2L_J^o)=A\psi_g\sum_k d_k U_k^L(\mathbf{r}) \,. \qquad (7)$$

Here A is an antisymmetrization operator. ψ_g is the wave function of the two-electron target state, $(1s1s)^2S$. It is a three-partial-wave eight-term wave function. The details of this function have been given in Ref. 8. The U_k^L represent a one-dimensional complete set for the outgoing electron. We choose

$$U_k^L(\mathbf{r})=r^k e^{-\gamma r}Y_L(\hat{\mathbf{r}}) \,, \qquad (8)$$

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 $^2L_J^o$ wave function. In this work for $L=1$, we use 15 U_k^L's where k runs from

TABLE III. Energy and nonrelativistic autoionization width of the $[1s(2s2p)^1P]^2P^o$ state of lithiumlike ions (in atomic units). $\langle H_1+H_2\rangle$, $\langle H_3\rangle$, $\langle H_4\rangle$, and $\langle H_5\rangle$ are the expectation values of the relativistic operators corresponding to kinetic energy correction plus Darwin term, Fermi contact, orbit-orbit or retardation, and the nonrelativistic mass polarization effect, respectively. E Total is the sum of the nonrelativistic energy plus the aforementioned corrections. The shift Δ and the width Γ result from the interaction of this inner-shell vacancy state with the degenerate $^2P^o$ continuum via the nonrelativistic Coulomb interaction.

Z	E Nonrelativistic	q	$\langle H_1+H_2\rangle$ (10^{-4})	$\langle H_3\rangle$ (10^{-4})	$\langle H_4\rangle$ (10^{-4})	$\langle H_5\rangle$ (10^{-4})	E Total	Δ Shift (10^{-4})	Γ Width (10^{-4})
3	−5.257 407	2.525	−5.82	0.04	0.07	−0.0848	−5.257 987	−0.25	3.42
4	−9.878 027	3.535	−19.35	0.15	0.26	−0.233	−9.879 945	−0.56	7.68
5	−16.001 086	4.541	−49.17	0.38	0.63	−0.388	−16.005 940	−0.65	10.9
6	−23.624 863	5.544	−104.95	0.77	1.24	−0.593	−23.635 217	−0.68	13.4
7	−32.748 945	6.546	−198.81	1.39	2.14	−0.762	−32.768 550	−0.67	15.3
8	−43.373 185	7.548	−345.14	2.26	3.38	−0.930	−43.407 228	−0.65	16.7
9	−55.497 517	8.550	−560.70	3.45	5.03	−1.041	−55.552 843	−0.62	17.9
10	−69.121 896	9.551	−864.43	4.98	7.15	−1.268	−69.207 253	−0.59	18.9
11	−84.246 328	10.552	−1278.19	6.92	9.78	−1.375	−84.372 614	−0.57	19.7
12	−100.870 781	11.552	−1825.40	9.31	12.99	−1.608	−101.051 252	−0.54	20.3
13	−118.995 253	12.554	−2532.14	12.19	16.83	−1.712	−119.245 736	−0.53	20.9
14	−138.619 738	13.554	−3427.19	15.61	21.36	−1.947	−138.958 954	−0.51	21.4
15	−159.744 231	14.554	−4539.87	19.62	26.64	−2.049	−160.193 797	−0.49	21.8
16	−182.368 735	15.554	−5904.58	24.27	32.72	−2.288	−182.953 724	−0.48	22.2
17	−206.493 246	16.556	−7556.18	29.58	39.65	−2.387	−207.242 179	−0.46	22.5
18	−232.117 760	17.556	−9532.99	35.63	47.51	−2.364	−233.062 982	−0.45	22.8

$k=1$ to 15. The values of the linear parameters d_k are left as variable to be later determined by the complex-rotation computation. The Hamiltonian matrix of the $1s2s2p$ configuration plus associated continuum is therefore an 18×18 matrix in this approximation. In this work the complex-rotation is achieved by scaling, $r\rightarrow re^{-i\theta}$, in the argument of Eq. (8). The coordinates in the Hamiltonian operator as well as the other parts of the basis set are not scaled.[5] Diagonalization of the resulting complex Hamiltonian matrix where the basis states are coupled to form either $J=\frac{1}{2}$ or $\frac{3}{2}$ yields 18 eigenfunctions of this subspace which correspond to certain linear combinations of the basis states

$$|\Psi_s(J)\rangle = c_0(s)|\psi_0(J)\rangle + c_1(s)|\psi_1(J)\rangle + c_2(s)|\psi_2(J)\rangle + |\psi_c^s(J)\rangle \tag{9}$$

and satisfying

$$\delta\langle H\rangle = \delta\frac{\langle\Psi_s|H|\Psi_s\rangle}{\langle\Psi_s|\Psi_s\rangle}=0 \ . \tag{10}$$

These eigenfunctions correspond to the states with well-defined J, M_J, and parity which may be labeled $(1s2s2p)^4P_J^o$, $[1s,(2s2p)^3P]^2P_J^o$, and $[1s,(2s2p)^1P]^2P_J^o$ along with 15 other states, which include approximations to bound states, $[(1s1s)^1S,np]^2P_J^o$, and nonresonant scattering states of the form $[(1s1s)^1S,\epsilon p]^2P_J^o$ which lie along the rotated branch cut

$$E=E[(1s1s)^1S]+\epsilon e^{-2i\theta}$$

in the complex energy plane (see Refs. quoted in Ref. 13). The complex resonance eigenvalues, $E_r - i(\Gamma/2)$, yield the shifted resonant energy E_r and width Γ of the state. The J-dependent coupling shift is defined by

$$\Delta_J = E_r[1s2s2p\ ^4P_J^o]-E \ , \tag{11}$$

where $E=\langle\psi_0|H_{\rm nr}|\psi_0\rangle$ is the nonrelativistic eigenvalue. It should be stressed that Δ_J is not the full perturbation energy associated with the spin-dependent interactions; it is only due to the interaction with the continuum and the two $(1s2s2p)^2P^o$ states. If we had included the small contribution

$$\langle\psi_0(J)|H_{\rm spin}|\psi_0(J)\rangle$$

in the diagonal elements $\langle\psi_0(J)|H|\psi_0(J)\rangle$, then Δ_J would be the full fine-structure perturbation energy. Table I gives the shift and autoionization widths of the $(1s2s2p)^4P_J^o$ states. We have included the results for $J=\frac{5}{2}$ in this table for completeness and because our earlier paper dealing with this state did not consider $Z=11-15$. The width results in this table are quoted in atomic units; the autoionization transition probabilities, which are proportional to the widths by a factor of $\hbar$, can be obtained in units of sec^{-1} by multiplying by $1/(2.419\times10^{-17}$ sec).

It is worth mentioning that the J-dependent autoionization widths of the two $(1s2s2p)^2P_J^o$ states become increasingly different from the nonrelativistic results of Tables II and III with increasing Z. These nonrelativistic results were obtained by diagonalizing the Hamiltonian matrix that results when the spin-dependent terms in the Hamiltonian operator are neglected, i.e., the only elements in the Hamiltonian matrix are those pertaining to the particular $(1s2s2p)^2P^o$ resonance of interest along with the continuum. For large Z these widths appear to converge to a result independent of Z, which should be expected from an analysis based on hydrogenic orbitals and the golden rule formula which employs the transition matrix element of the Coulomb interaction between the core-excited initial state and the continuum. The relativistic width results for these $1s2s2p\ ^2P_J^o$ states along with their corresponding radiative transition rates will be reported in a future paper which will give our results for their J-dependent lifetimes.

III. RADIATIVE TRANSITION RATES

The $1s2s2p\ ^4P^o$ state is stable against dipole radiative transitions in the nonrelativistic approximation. The $1s2s2p\ ^2P^o$ states, on the other hand, do make electric dipole transitions to lower doublets, predominantly to the ground state, $(1s1s2s)^2S$. Therefore the relativistic coupling of $(1s2s2p)^4P^o$ to the two $(1s2s2p)^2P^o$ states is once again critical for an understanding of the differential metastability of the $(1s2s2p)^4P_J^o$ states.

The dipole matrix element between the first-order wave function for a particular $(1s2s2p)^4P_J^o$ state, $|\Psi_s(J)\rangle$, and the $(1s1s2s)^2S_{J=1/2}$ ground state (symbolized by $|\Psi_G\rangle$), is

$$\langle\Psi_s(J)|\mathbf{r}|\Psi_G\rangle = c_1\langle\psi_1(J)|\mathbf{r}|\Psi_G\rangle + c_2\langle\psi_2(J)|\mathbf{r}|\Psi_G\rangle \ , \tag{12}$$

where the term $\langle\psi_0(J)|\mathbf{r}|\Psi_G\rangle$ has been dropped since it is identically zero by the mutual orthogonality of the doublet and quartet spin eigenfunctions. $\langle\psi_c(J)|\mathbf{r}|\Psi_G\rangle$ has been neglected since $|\psi_c(J)\rangle$ is a small component of $|\psi_s(J)\rangle$ to begin with and also because the integral $\langle\psi_c(J)|r|\psi_G\rangle$ has a small overlap in spatial coordinates.

The ground-state wave functions used to calculate these dipole matrix elements are 13-partial-wave multiconfiguration-interaction wave functions with 110 Slater-type orbital terms. They were computed by the Rayleigh-Ritz variation method in a manner similar to that of Davis and Chung.[14] Some measure of their accuracy can be obtained by comparing the nonrelativistic energy eigenvalue for the ground state of lithium, where the correlation effects are strongest along the isoelectronic sequence, with the most precise theoretical result in the literature. King and Shoup[15] used a 352-term Hylleraas-type expansion to obtain the lowest theoretical result in the literature, $-7.478\,058$ a.u. Compared with the present configuration-interaction (CI) result of $-7.477\,16$ a.u. it is only $-0.000\,898$ a.u. lower. The nonrelativistic energy eigenvalues, relativistic corrections, mass polarization effect (for ^{7}Li), and total relativistic energy for the $1s1s2s\ ^2S$ ground state is given in Table IV for $Z=3-18$.

In this calculation we take the c_i's from first-order perturbation theory,

TABLE IV. Energy and relativistic effect of the $(1s1s2s)^2S$ state of lithiumlike ions (in atomic units). $\langle H_1+H_2\rangle$, $\langle H_3\rangle$, $\langle H_4\rangle$, and $\langle H_5\rangle$ are the expectation values of the relativistic operators corresponding to kinetic energy correction plus Darwin term, Fermi contact, orbit-orbit or retardation, and the nonrelativistic mass polarization effect, respectively. E Total is the sum of the nonrelativistic energy plus the aforementioned corrections.

Z	E Nonrelativistic	$\langle H_1+H_2\rangle$ (10^{-4})	$\langle H_3\rangle$ (10^{-4})	$\langle H_4\rangle$ (10^{-4})	$\langle H_5\rangle$ (10^{-4})	E Total
3	−7.477 160	−7.14	0.99	−0.24	0.235	−7.477 775
4	−14.323 726	−25.51	2.81	−0.49	0.273	−14.326 017
5	−23.423 481	−67.47	6.10	−0.84	0.299	−23.429 672
6	−34.774 325	−147.90	11.30	−1.28	0.344	−34.788 078
7	−48.375 668	−285.43	18.85	−1.81	0.354	−48.402 471
8	−64.227 273	−502.30	29.20	−2.44	0.362	−64.274 791
9	−82.329 039	−824.52	42.77	−3.16	0.349	−82.407 494
10	−102.680 905	−1281.71	60.02	−3.97	0.374	−102.803 433
11	−125.282 846	−1907.40	81.36	−4.88	0.362	−125.465 902
12	−150.134 837	−2738.54	107.24	−5.88	0.382	−150.398 518
13	−177.236 862	−3815.75	138.10	−6.98	0.371	−177.605 288
14	−206.588 916	−5183.85	174.38	−8.17	0.388	−207.090 642
15	−238.190 989	−6890.75	216.53	−9.45	0.377	−238.859 318
16	−272.043 081	−8988.35	264.97	−10.83	0.392	−272.916 462
17	−308.145 187	−11 531.89	336.62	−12.30	0.382	−309.267 552
18	−346.497 301	−14 581.17	382.52	−13.86	0.356	−347.918 517

$$c_i=\frac{\langle \psi_i(J)|H_{\text{spin}}|\psi_0(J)\rangle}{E_0-E_i}\ . \tag{13}$$

Due to the importance of these coupling constants with respect to the spin-induced processes we tabulate their values for the various ions in Table V. We also give the following coupling constant:

$$c_{12}=\frac{\langle \psi_2(J)|H_{\text{spin}}|\psi_1(J)\rangle}{E_1-E_2}\ , \tag{14}$$

which is related to the matrix element H_{12} in the autoionization complex-rotation computation.

The radiative transition rate which has been summed over all possible final states and averaged over the initial magnetic substates is given by[16]

$$W(^4P_J^o\rightarrow {}^2S)=\frac{1}{2J+1}\sum_{J_z}\frac{4\alpha}{3c^2}\omega_J^3|\langle \Psi_s(J)|\mathbf{r}|\Psi_G\rangle|^2\ , \tag{15}$$

where α is the fine-structure constant and

$$\omega_J=E(^4P_J^o)-E(^2S_{1/2})\ . \tag{16}$$

The results for these transition rates are given in Tables

TABLE V. First-order perturbation theory coupling constants for the states $(1s2s2p)^4P_J^o$, $[1s(2s2p)^3P]^2P_J^o$, and $[1s(2s2p)^1P]^2P_J^o$ of lithiumlike systems. For notation, see text Eqs. (13) and (14). (The number in square brackets is the power of 10 to which the number is raised.)

	$J=\frac{1}{2}$			$J=\frac{3}{2}$		
Z	c_1	c_2	$c_{1,2}$	c_1	c_2	$c_{1,2}$
3	−1.9681[−4]	−4.2043[−5]	+1.9923[−4]	−2.4665[−4]	+5.5145[−5]	−9.9616[−5]
4	4.5511[−4]	2.0491[−5]	7.5155[−4]	6.0937[−4]	−2.2623[−4]	−3.7578[−4]
5	−8.6968[−4]	7.1162[−5]	1.8785[−3]	−1.2094[−3]	5.4691[−4]	−9.3924[−4]
6	−1.4750[−3]	2.6262[−4]	3.7812[−3]	−2.0996[−3]	1.0662[−3]	−1.8906[−3]
7	−2.3072[−3]	5.8348[−4]	6.6713[−3]	−3.3375[−3]	1.8311[−3]	−3.3357[−3]
8	−3.4033[−3]	1.0653[−3]	1.0753[−2]	−4.9819[−3]	2.8913[−3]	−5.3767[−3]
9	−4.8006[−3]	1.7345[−3]	1.6243[−2]	−7.0904[−3]	4.2892[−3]	−8.1215[−3]
10	−6.5308[−3]	2.6226[−3]	2.3334[−2]	−9.7140[−3]	6.0741[−3]	−1.1667[−2]
11	−8.6367[−3]	3.7590[−3]	3.2247[−2]	−1.2921[−2]	8.2929[−3]	−1.6123[−2]
12	−1.1151[−2]	5.1730[−3]	4.3182[−2]	−1.6762[−2]	1.0992[−2]	−2.1591[−2]
13	−1.4109[−2]	6.8968[−3]	5.6327[−2]	−2.1293[−2]	1.4221[−2]	−2.8164[−2]
14	−1.7549[−2]	8.9575[−3]	7.1918[−2]	−2.6575[−2]	1.8025[−2]	−3.5959[−2]
15	−2.1506[−2]	1.1382[−2]	9.0158[−2]	−3.2662[−2]	2.2446[−2]	−4.5079[−2]
16	−2.6015[−2]	1.4207[−2]	1.1124[−1]	−3.9613[−2]	2.7540[−2]	−5.5621[−2]
17	−3.1119[−2]	1.7459[−2]	1.3536[−1]	−4.7491[−2]	3.3350[−2]	−6.7679[−2]
18	−3.6843[−2]	2.1166[−2]	1.6274[−1]	−5.6339[−2]	3.9922[−2]	−8.1369[−2]

VI and VII for the $J=\frac{1}{2}$ and $\frac{3}{2}$ states, respectively. In these calculation we have approximated ω_J with the nonrelativistic center of gravity energy difference, $E(^4P^o)-E(^2S)$, i.e. we have used our nonrelativistic energy eigenvalues to compute the energy difference. The error introduced in this approximation is small. For example, in the case of the argon ion, $Z=18$, where the relativistic corrections are the largest, using the relativistic corrected energies with the spin-dependent perturbations included changes the result by only about 1%. The spin-dependent perturbation energies for $Z=18$ are $+0.042\,341\,3$, $-0.030\,771\,8$, and $-0.065\,480\,3$ a.u., respectively, for the $J=\frac{5}{2}$, $\frac{3}{2}$, and $\frac{1}{2}$ levels.

Note that quantum interference effects are present in these radiative rates. This interference results from the two alternate pathways for the photon emission to proceed, i.e., via the coupling to either of the two doublet $1s2s2p\,^2P^o$ states. The transition amplitudes (dipole matrix elements) via the two doublets must first be added and then the amplitude squared is taken to obtain the transition rate. This can be seen more clearly after simplifying Eq. (15) by writing it in terms of the reduced dipole matrix elements,[17] $\langle \psi_i \| r \| \Psi_G \rangle$, between the ground state and the two doublet $1s2s2p\,^2P^o$ states:

TABLE VI. Radiative, autoionization, and total transition rates and lifetimes of the $1s2s2p\,^4P^o_{J=1/2}$ levels of lithiumlike ions. Transition rates are given in $\sec^{-1}$, and lifetimes are given in sec. (The number in square brackets is the power of 10 to which the number is raised.)

		This work				Other theory		Experiment
Z	W(rad)	W(Aug)	W(total)	Lifetime	W(rad)	W(Aug)	Lifetime	Lifetime
3	4.58[+2]	7.71[+6]	7.71[+6]	1.30[−7]			> 100.0[−7][a] 24.0[−7][c]	1.4±0.7[−7][b]
4	1.56[+4]	4.61[+7]	4.61[+7]	2.17[−8]				
5	2.05[+5]	1.44[+8]	1.44[+8]	6.94[−9]				
6	1.57[+6]	3.31[+8]	3.33[+8]	3.01[−9]	1.73[+6][d]	2.69[+8][d]	3.69[−9][d]	
7	8.49[+6]	6.33[+8]	6.42[+8]	1.56[−9]	9.30[+6][d] 5.10[+6][e]	5.21[+8][d] 2.44[+7][e]	1.89[−9][d]	
8	3.60[+7]	1.06[+9]	1.10[+9]	9.10[−10]	3.86[+7][d] 2.32[+7][e]	8.81[+8][d] 7.55[+7][e]	1.09[−9][d]	1.87±0.1[−9][f]
9	1.27[+8]	1.63[+9]	1.76[+9]	5.69[−10]	1.34[+8][d] 1.37[+8][g]	1.36[+9][d] 7.02[+8][g]	6.69[−10][d]	
10	3.87[+8]	2.33[+9]	2.72[+9]	3.68[−10]	4.07[+8][d] 2.86[+8][e] 4.10[+8][g]	1.98[+9][d] 3.64[+8][e] 1.32[+9][g]	4.19[−10][d]	4.0±1.9[−10][h]
11	1.06[+9]	3.13[+9]	4.19[+9]	2.39[−10]	1.10[+9][g]	2.34[+9][g]		
12	2.64[+9]	4.03[+9]	6.66[+9]	1.50[−10]	2.69[+9][g]	3.92[+9][g]		
13	6.09[+9]	4.97[+9]	1.11[+10]	9.04[−11]	6.33[+9][i] 6.09[+9][g]	4.22[+9][i] 6.28[+9][g]	9.52[−11][i]	
14	1.32[+10]	5.93[+9]	1.91[+10]	5.24[−11]	1.29[+10][g]	9.66[+9][g]		
15	2.69[+10]	6.86[+9]	3.38[+10]	2.96[−11]	2.58[+10][g]	1.43[+10][g]		
16	5.25[+10]	7.72[+9]	6.03[+10]	1.66[−11]	3.88[+10][e] 4.91[+10][g]	1.16[+10][e] 2.07[+10][g]		
17	9.83[+10]	8.47[+9]	1.07[+11]	9.36[−12]	8.96[+10][g]	2.90[+10][g]		
18	1.77[+11]	9.10[+9]	1.86[+11]	5.37[−12]	1.67[+11][i] 1.56[+11][g]	9.96[+9][i] 3.97[+10][g]	5.65[−12][i]	

[a] Mason, Ref. 20.

[b] Levitt *et al.*, Ref. 18.

[c] Balashov *et al.*, Ref. 19.

[d] Chen *et al.*, Ref. 7.

[e] Bhalla and Gabriel, Ref. 24.

[f] Richard *et al.*, Ref. 21; preliminary result from Charalambidis, Koulen, and Brenn is 1.6±0.4[−9] (Ref. 21).

[g] Vainshtein and Safronova, Ref. 25.

[h] Schumann *et al.*, Ref. 23.

[i] Chen *et al.*, Ref. 6.

$$W({}^4P_J^o \to {}^2S_{1/2}) = \frac{1}{2J+1}\frac{4\alpha\omega^3}{3c^2}\left[(-1)^{J'+L+S+1}[(2J+1)(2J'+1)]^{1/2}\begin{Bmatrix} L & 1 & L' \\ J' & S & J \end{Bmatrix}(\langle\psi_1\|r\|\Psi_G\rangle c_1+\langle\psi_2\|r\|\Psi_G\rangle c_2)\right]^2 . \tag{17}$$

In this expression, the primed quantities correspond to the ground state, $J'=\frac{1}{2}$, $L'=0$; and the unprimed quantities correspond to the intermediate $1s2s2p\ {}^2P^o$ states, $L=1$, $S=\frac{1}{2}$. The factors

$$(-1)^{J'+L+S+1}[(2J+1)(2J'+1)]^{1/2}\begin{Bmatrix} L & 1 & L' \\ J' & S & J \end{Bmatrix}$$

are equal to $(-1)(2)(0.408\,248\,29)$ and $(-1)(\sqrt{8})(-0.408\,248\,29)$ for $J=\frac{1}{2}$ and $\frac{3}{2}$, respectively. The reduced dipole matrix elements are given in Table VIII and the coupling constants have already been presented in Table V. From these quantities and Eq. (17) it can be seen that the transition amplitudes via the two intermediate $1s2s2p\ {}^2P^o$ states always add together with

TABLE VII. Radiative, autoionization, and total transition rates and lifetimes of the $1s2s2p\ {}^4P^o_{J=3/2}$ levels of linthiumlike ions. Transition rates are given in $\sec^{-1}$, and lifetimes are given in sec. (The number in square brackets is the power of 10 to which the number is raised.)

	This work				Other theory			Experiment
Z	W(rad)	W(Aug)	W(total)	Lifetime	W(rad)	W(Aug)	Lifetime	Lifetime
3	8.42[+2]	3.94[+6]	3.95[+6]	2.53[−7]			3.0[−7][a] 8.5[−7][c]	4.6±1.0[−7][b]
4	3.49[+4]	2.04[+7]	2.04[+7]	4.89[−8]				
5	4.87[+5]	5.48[+7]	5.52[+7]	1.81[−8]				
6	3.83[+6]	1.06[+8]	1.09[+8]	9.14[−9]	4.30[+6][d]	7.15[+7][d]	1.32[−8][d]	
7	2.10[+7]	1.63[+8]	1.84[+8]	5.42[−9]	2.30[+7][d] 1.28[+7][e]	1.07[+8][d] 6.18[+8][e]	7.69[−9][d]	
8	8.94[+7]	2.10[+8]	2.99[+8]	3.34[−9]	9.63[+7][d] 9.70[+7][g] 5.85[+7][e]	1.31[+8][d] 2.82[+8][g] 1.93[+8][e]	4.40[−9][d]	3.48±0.08[−9][f]
9	3.16[+8]	2.26[+8]	5.42[+8]	1.84[−9]	3.38[+8][d] 3.35[+8][g]	1.27[+8][d] 6.79[+8][g]	2.15[−9][d]	2.000±0.025[−9][h]
10	9.69[+8]	1.98[+8]	1.17[+9]	8.57[−10]	1.03[+9][d] 1.01[+9][g] 7.30[+8][e]	8.89[+7][d] 1.45[+9][g] 9.51[+8][e]	8.94[−10][d]	16.0±2.4[−10][i]
11	2.65[+9]	1.21[+8]	2.77[+9]	3.60[−10]	2.74[+9][9]	2.86[+9][g]		
12	6.62[+9]	3.22[+7]	6.65[+9]	1.50[−10]	6.77[+9][g]	5.26[+9][g]		
13	1.53[+10]	6.07[+6]	1.53[+10]	6.54[−11]	1.63[+10][j] 1.55[+10][g]	1.18[+8][j] 9.13[+9][g]	6.06[−11][j]	
14	3.31[+10]	1.91[+8]	3.33[+10]	3.01[−11]	3.33[+10][g]	1.51[+10][g]		
15	6.77[+10]	8.29[+8]	6.85[+10]	1.46[−11]	6.76[+10][g]	2.41[+10][g]		
16	1.32[+11]	2.30[+9]	1.34[+11]	7.44[−12]	1.30[+11][g] 1.07[+11][e]	3.71[+10][g] 3.37[+10][e]		
17	2.47[+11]	5.13[+9]	2.52[+11]	3.96[−12]	2.42[+11][g]	5.55[+10][g]		
18	4.46[+11]	1.01[+10]	4.56[+11]	2.19[−12]	4.59[+11][j] 4.32[+11][g]	1.12[+10][j] 8.08[+10][g]	2.12[−12][j]	

[a] Mason, Ref. 20.
[b] Levitt *et al.*, Ref. 18.
[c] Balashov *et al.*, Ref. 19.
[d] Chen *et al.*, Ref. 7.
[e] Bhalla and Gabriel, Ref. 24.
[f] Moore *et al.*, quoted in Richard *et al.*, Ref. 21; preliminary result from Charalambidis, Koulen, and Brenn is 4.3±0.2[−9] (Ref. 21).
[g] Vainshtein and Safronova, Ref. 25.
[h] Richard *et al.*, Ref. 22.
[i] Schumann *et al.*, Ref. 23.
[j] Chen *et al.*, Ref. 6.

TABLE VIII. Reduced dipole matrix elements for radiative transitions from the $[1s,(2s2p)^3P]^2P^o$ and $[1s,(2s2p)^1P]^2P^o$ states to the $[(1s1s)^1S,2s]^2S$ ground state for lithiumlike ions (in atomic units; for notation, see text). (The number in square brackets is the power of 10 to which the number is raised.)

Z	$\langle\psi_1\|r\|\Psi_G\rangle$	$\langle\psi_2\|r\|\Psi_G\rangle$
3	4.3709[−1]	−7.8662[−2]
4	3.7434[−1]	−1.0369[−1]
5	3.1411[−1]	−9.4460[−2]
6	2.6834[−1]	−8.3236[−2]
7	2.3358[−1]	−7.3575[−2]
8	2.0651[−1]	−6.5773[−2]
9	1.8491[−1]	−5.9259[−2]
10	1.6733[−1]	−5.3862[−2]
11	1.5275[−1]	−4.9346[−2]
12	1.4048[−1]	−4.5468[−2]
13	1.3002[−1]	−4.2219[−2]
14	1.2100[−1]	−3.9355[−2]
15	1.1314[−1]	−3.6835[−2]
16	1.0624[−1]	−3.4639[−2]
17	1.0012[−1]	−3.2701[−2]
18	9.4661[−2]	−3.0946[−2]

the same relative phase for both J levels; hence there is overall constructive interference. A closer examination of the transition amplitudes via the individual interactions spin-orbit, spin-other-orbit, and spin-spin does reveal, however, that there is destructive interference among these different interactions for a given total J. More explicitly, if the coupling constants c_i are examined in the form

$$c_i = c_i(\mathrm{so}) + c_i(\mathrm{soo}) + c_i(\mathrm{ss}) \ ,$$

then we find the following: for $J=\frac{1}{2}$, the spin-other-orbit and spin-spin transition amplitudes via the $[1s,(2s2p)^1P]^2P^o$ state add with opposite sign as compared to all other amplitudes; for $J=\frac{3}{2}$, the spin-spin transition amplitude via the $[1s,(2s2p)^3P]^2P^o$ state and the spin-other-orbit transition amplitude via the $[1s,(2s2p)^1P]^2P^o$ state add with opposite sign as compared to all other amplitudes.

This interference, while obvious from the formulas we have written down here, is not as obvious in the case of the autoionization transition rate where it occurs also. This is because we have not taken a golden-rule-type approach to the calculation of the autoionization transition rate. Nevertheless, interference effects do result from the various ways in which the coupling to the continuum is affected; these points will be examined in Sec. IV.

IV. RESULTS AND DISCUSSION

The J-dependent lifetimes τ_J of the $(1s2s2p)^4P_J^o$ states are given by

$$1/\tau_J = W_J(\mathrm{auto}) + W_J(\mathrm{rad}) \ . \tag{18}$$

These results appear in Tables VI and VII for the $J=\frac{1}{2}$ and $\frac{3}{2}$ states, respectively. The transition rate is dominated for low Z by autoionization, while for high Z the radiative transitions dominate. The autoionization rate grows monotonically with Z for the $J=\frac{1}{2}$ state, while this rate has a dip at $Z=13$ for the $J=\frac{3}{2}$ state. More precisely, the $J=\frac{3}{2}$ rate increases with Z until $Z=9$, then it begins to decrease at $Z=10$ until it reaches a minimum at $Z=13$. This minimum occurs because there are distinct amplitudes for the different mechanisms that the initial $1s2s2p\ ^4P_J^o$ state takes to reach the same final continuum state, $[(1s1s)^1S,\epsilon p]^2P_J^o$. The relative phases for these various processes are different for the two J levels, resulting in different degrees of constructive and destructive interference for the net amplitude squared or total autoionization transition rate.

The relative contributions of autoionization and radiation to the total transition rate are most easily seen in the Auger and radiative branching ratios defined by

$$B_{\mathrm{Auger}} = 100\frac{W_{(\mathrm{auto})}}{W(\mathrm{auto})+W(\mathrm{rad})} \ , \tag{19}$$

with $B_{\mathrm{rad}} = 100 - B_{\mathrm{Auger}}$. These quantities are given in Table IX. For an accurate theoretical determination of the Auger branching ratio as a function of Z, the destructive interference mentioned above becomes very important. This is because small errors in the various amplitudes for autoionization may magnify into large errors for the combined total autoionization transition rate, as is the case for the ions with $Z\approx 13$ where the net amplitude nearly vanishes. This can be seen in Tables VI and VII where the present results for the various transition rates are compared with those of Chen *et al.*[6,7] The radiative rates are generally in good agreement; for low Z ($Z=6$), they differ by about 10%, and for high Z ($Z=18$), they differ by only 5%. This is expected since correlation effects are more important for low-Z systems. The $J=\frac{1}{2}$ autoionization rates are also in general agreement, the difference being predictably larger (about 20%) for low-Z ions as compared to high-Z ions (about 10%). Once again, the correlation effects are most likely accounting

TABLE IX. Autoionization and radiation branching ratios for the $(1s2s2p)^4P_J^o$ states of lithiumlike ions. See Eq. (19).

	$J=\frac{1}{2}$		$J=\frac{3}{2}$	
Z	Auger	Radiation	Auger	Radiation
3	99.99	0.01	99.98	0.02
4	99.97	0.03	99.83	0.17
5	99.86	0.14	99.12	0.88
6	99.53	0.47	96.50	3.50
7	98.68	1.32	88.62	11.38
8	96.73	3.27	70.09	29.91
9	92.79	7.21	41.62	58.38
10	85.75	14.25	16.94	83.06
11	74.76	25.24	4.38	95.62
12	60.45	39.55	0.48	99.52
13	44.97	55.03	0.04	99.96
14	31.05	68.95	0.57	99.43
15	20.30	79.70	1.21	98.79
16	12.81	87.19	1.71	98.29
17	7.93	92.07	2.03	97.97
18	4.88	95.12	2.21	97.79

for the low-Z difference. The $J=\frac{1}{2}$ autoionization rates are, however, in more serious disagreement. The 30% difference between the two results for $Z=6$ grows to a difference of almost two orders of magnitude for $Z=13$.

In order to understand this destructive interference more thoroughly we consider the following expression for the autoionization transition rate which is based on the concept of a golden rule formula for the net transition amplitude squared:

$$\Gamma=\left[\sum_{i=1}^{3}\left[g_{J,i}^{D}+\sum_{k=1}^{2}g_{J,i}^{I,k}\right]\right]^{2} . \tag{20}$$

In this expression the quantities g represent generalized transition amplitudes. More specifically, $g_{J,i}^{D}$ represents the J-dependent amplitude resulting from "direct" coupling to the continuum via the spin-dependent interactions $i=1$ (spin-orbit), $i=2$ (spin-other-orbit), and $i=3$ (spin-spin). With the same meaning ascribed to the index i, $g_{J,i}^{I,k}$, represents the J-dependent amplitude resulting from the "indirect" coupling to the continuum via the intermediate $[1s,(2s(2p)^3P]^2P_J^o$ $(k=1)$ and $[1s,(2s2p)^1P]^2P_J^o$ $(k=2)$ states. This expression for the autoionization rate can be generalized further by extracting out the J dependence of the amplitudes via $6j$ symbols as follows:

$$g_{J,i}^{D}=(-1)^{J+S'+L}\begin{Bmatrix} L' & K(i) & L \\ S & J & S' \end{Bmatrix} a_i^D , \tag{21a}$$

$$g_{J,i}^{I,k}=(-1)^{J+S'+L}\begin{Bmatrix} L' & K(i) & L \\ S & J & S' \end{Bmatrix} a_i^{I,k} , \tag{21b}$$

where $K(1)=K(2)=1$ and $K(3)=2$. The unprimed and primed quantities correspond to $^4P^o$ and $^2P^o$ symmetries, respectively. The a_i^D are to be interpreted as reduced direct transition amplitudes of the form $\langle \psi_c \| H_i \| \psi_0 \rangle$. In the context of first-order perturbation theory the reduced indirect amplitudes may be expressed as

$$a_i^{I,k}=\langle C_k(i)\rangle g(k) , \tag{22}$$

where $\langle C_k(i)\rangle$ is a reduced coupling constant for the ith interaction and $g(k)$ is the positive square root of the corresponding J-independent nonrelativistic $1s2s2p\ ^2P^o$ width of Tables II and III.

Equation (20) can be brought into reconciliation with our $(1s2s2p)^4P_J^o$ width from the saddle-point complex-rotation method by deducing the values of a_i^D by carrying out selected diagonalizations of the Hamiltonian matrix [Eq. (6)] with all but the interaction of interest "turned off" by artificially setting the matrix elements dealing with the other processes to zero. The spin-orbit operator is a one-electron operator; and since two-electron orbitals must be changed to directly couple the initial state $1s2s2p$ to the continuum $1s1s\epsilon p$ the value of a_1^D is zero. The values of a_2^D and a_3^D resulting from the direct coupling of the two-electron operators, spin-other-orbit and spin-spin, respectively, are obtained by setting the matrix elements involving the $(1s2s2p)^2P^o$ states equal to zero and carrying out the complex-rotation diagonalization with the matrix elements

$$H_{0c}=\langle \psi_0(J)|H_{\text{soo}}|\psi_c(J)\rangle$$

and

$$H_{0c}=\langle \psi_0(J)|H_{\text{ss}}|\psi_c(J)\rangle ,$$

respectively.

To illustrate this procedure we choose to use $Z=13$ as an example. The largest error should occur for this particular ion since the sum of the transition amplitudes nearly cancels for the $J=\frac{1}{2}$ level; however, the source of the minimum in the $J=\frac{1}{2}$ autoionization rate will be clearly illustrated. We find for the reduced direct transition amplitudes (results are given in atomic units): $a_2^D=+1.963\,17\times10^{-7}$ and $a_3^D=-3.910\,46\times10^{-9}$. The reduced coupling constants are

$$\langle C_1(1)\rangle=-7.310\,84\times10^{-2} ,$$

$$\langle C_1(2)\rangle=-8.886\,91\times10^{-3} ,$$

and

$$\langle C_1(3)\rangle=+1.853\,83\times10^{-3} ,$$

$$\langle C_2(1)\rangle=+5.958\,14\times10^{-2} ,$$

$$\langle C_2(2)\rangle=-7.712\,51\times10^{-3} ,$$

and

$$\langle C_2(3)\rangle=+6.055\,47\times10^{-3} .$$

The full J-dependent coupling constants of Table V can be obtained by

$$c_k=(-1)^{J+S'+L}\begin{Bmatrix} L' & 1 & L \\ S & J & S' \end{Bmatrix}[\langle C_k(1)\rangle+\langle C_k(2)\rangle] +(-1)^{J+S'+L}\begin{Bmatrix} L' & 2 & L \\ S & J & S' \end{Bmatrix}\langle C_k(3)\rangle . \tag{23}$$

Here the primed quantities correspond once again to the $1s2s2p\ ^2P^o$ and the unprimed quantities correspond to the $1s2s2p\ ^4P^o$. The results determined by Eq. (21) are displayed in Table X. At this point it is important to bring attention to the signs of the amplitudes given in this table. Since we have deduced these amplitudes from partial transition rates, phase information was lost when taking the square root. The amplitudes corresponding to the indirect processes, $g_{J,i}^{I,1}$ and $g_{J,i}^{I,2}$, were constructed by chosing the real positive square roots [$g(1)$ and $g(2)$] of the nonrelativistic widths of $[1s,(2s2p)^3P]^2P^o$ and $[1s,(2s2p)^1P]^2P^o$, respectively. The amplitudes corresponding to the direct processes, $g_{J,i}^{D}$ were obtained by taking a positive square root for the spin-other-orbit interaction (i.e., $a_2^D>0$) and a negative square root for the spin-spin interaction (i.e., $a_3^D<0$). These choices were necessary for a meaningful final result. The results of Table X, based on the analysis of Eq. (20), shows that the indirect spin-orbit amplitude $g_{J,1}^{I,2}$ destructively combines (negative amplitude) with the other amplitudes for both J

TABLE X. Analysis of the various autoionization transition amplitudes for Al XI $(1s2s2p)^4P^o_J$, based on the golden-rule-type formula, Eq. (20). The table shows the sources of the near complete destructive interference for the $J=\frac{3}{2}$ width which is given by the net amplitude squared. For notation and discussion see text. Results are in atomic units. (The number in square brackets is the power of 10 to which the number is raised.)

Amplitude	$J=\frac{1}{2}$		$J=\frac{3}{2}$	
$g^P_{J,2}$	2.8023[−4]		4.4308[−4]	
$g^P_{J,3}$	1.9775[−4]		−6.2534[−5]	
Sum		4.7798[−4]		3.8054[−4]
$g^{I,1}_{J,1}$	1.4862[−4]		2.3499[−4]	
$g^{I,1}_{J,2}$	1.6948[−5]		2.6797[−5]	
$g^{I,1}_{J,3}$	6.5275[−6]		−2.0642[−6]	
Sum		1.7210[−4]		2.5972[−4]
$g^{I,2}_{J,1}$	−4.5405[−4]		−7.1792[−4]	
$g^{I,2}_{J,2}$	5.8775[−5]		9.2931[−5]	
$g^{I,2}_{J,3}$	7.9929[−5]		−2.5276[−5]	
Sum		−3.1535[−4]		−6.5026[−4]
Total sum		3.3472[−4]		−9.9956[−6]
Γ		1.1204[−7]		9.9911[−11]

levels, while all the spin-spin amplitudes (negative amplitudes for $J=\frac{3}{2}$) destructively combine with the rest only for the case of $J=\frac{3}{2}$. The source of the minimum in the autoionization width at $Z=13$ for $J=\frac{3}{2}$ is for the most part due to the growth rate with Z of the indirect spin-orbit amplitude $g^{I,2}_{J,1}$. It becomes the largest decay amplitude at $Z=9$ and remains the largest for both the $J=\frac{1}{2}$ and $\frac{3}{2}$ states through $Z=18$. For the $J=\frac{3}{2}$ level, the destructive interference effect from this amplitude along with the spin-spin amplitudes causes the net transition amplitude to pass through zero between $Z=12$ and 13, hence the minimum in the Auger rate at $Z=13$. It is interesting to note that prior to $Z=9$, the largest amplitude is due to the direct coupling to the continuum via the spin-other-orbit interaction, $g^P_{J,2}$. It is also of interest to note that the indirect amplitudes via the $[1s,(2s2p)^1P]^2P^o$ state, $g^{I,2}_{J,i}$, are all larger than those via the $[1s,(2s2p)^3P]^2P^o$ state, $g^{I,1}_{J,i}$. This is because the nonrelativistic Coulomb autoionization width of the former is larger. The relative magnitudes of these amplitudes for the case of $Z=13$ are such that there is almost complete destructive interference for the $J=\frac{3}{2}$ level. The error of the results given by Eq. (20) as compared to the rigorous results of Table I from the saddle-point complex-rotation method for this case for $Z=13$ are 6.8% and 32% for the $J=\frac{1}{2}$ and $\frac{3}{2}$ levels, respectively. The large error for the $J=\frac{3}{2}$ level might be expected due to the near cancellation of the various transition amplitudes. If we carry out the same analysis for $Z=10$ where there is a smaller degree of destructive interference these two errors are 3.0% and 3.6%, respectively. More explicitly this analysis yields an error that increases monotonically for the $J=\frac{1}{2}$ state, from 1.5% for $Z=3$ to 28% for $Z=18$; for the $J=\frac{3}{2}$ state the error is 2.9% for $Z=3$, reaches a maximum at $Z=13$, and decreases to 14% for $Z=18$. The larger errors that occur for high Z are for the most part due to second-order wave-function effects. If the analysis of the indirect amplitudes $a^I_{k,i}$ is considered in the context of second-order perturbation theory, then the errors for $Z=18$ are reduced to about 5% for both the $J=\frac{1}{2}$ and $\frac{3}{2}$ states.

The near cancellation of the net autoionization transition amplitude for the case of the $J=\frac{3}{2}$ level for $Z=13$ raises the question of the stability of the width coming from the saddle-point complex-rotation method. We investigate this question by examining the stability of this width with respect to changes in the open-channel basis functions. These functions depend on the nonlinear parameter γ as shown in Eq. (8), and they are "rotated" by the angle θ as explained earlier. In Table XI the width is given as a function of these parameters for both the $J=\frac{1}{2}$ and $\frac{3}{2}$ states. This table clearly shows that for the case of the $J=\frac{1}{2}$ level, where there is a small degree of destructive interference, the width is extremely stable; the variation is at the fifth or sixth digit for a range of θ from 0.3 to 0.7 and for γ from 7.25 to 12.25. On the other hand, while the $J=\frac{3}{2}$ width is not as stable it still appears to be stationary with a variation of about 20% over this same range of parameters.

The lifetimes from this work are compared to other

TABLE XI. Stability of the autoionization width (in atomic units) of Al XI $(1s2s2p)^4P_J^o$ as a function of rotation angle θ (in radians), and nonlinear parameter γ using the saddle-point complex-rotation method. (The $J=\frac{3}{2}$ and $\frac{1}{2}$ widths are the first and second entries, respectively.) (The number in square brackets is the power of 10 to which the number is raised.)

			θ		
γ	0.30	0.40	0.50	0.60	0.70
7.250			1.699 59[−10] 1.202 72[−7]		
8.1250			1.541 27[−10] 1.202 61[−7]		
9.000		1.481 85[−10] 1.202 61[−7]	1.462 10[−10] 1.202 60[−7]	1.388 31[−10] 1.202 58[−7]	
9.7500	1.477 74[−10] 1.202 63[−7]	1.478 54[−10] 1.202 61[−7]	1.467 69[−10] 1.202 60[−7]	1.483 59[−10] 1.202 61[−7]	1.646 72[−10] 1.202 65[−7]
10.5000		1.475 12[−10] 1.202 61[−7]	1.476 18[−10] 1.202 60[−7]	1.487 36[−10] 1.202 61[−7]	
11.3750			1.474 59[−10] 1.202 61[−7]		
12.2500			1.476 29[−10] 1.202 62[−7]		

theoretical calculations and experimental measurements in Tables VI and VII. Experimental results which see differential metastability, to our knowledge, exist for only $Z=3$, 8, 9, and 10. Levitt *et al.*[18] have measured the lifetimes for the lithium atom. The experimental determination of these lifetimes was complicated by the mixing of the fine-structure levels by the nuclear hyperfine interaction.[18] Their result for the $J=\frac{1}{2}$ level, 0.14 ± 0.07 μs, agrees with the result of this work, 0.13 μs, whereas the other theoretical results are considerably longer, 2.40 μs (Ref. 19) and 10.0 μs.[20] The measured lifetime of the $J=\frac{3}{2}$ level, 0.46 ± 0.10 μs, is longer than the present result of 0.25 μs and the 0.30 μs result of Manson.[20] Richard *et al.*[21] have measured a short-lived level in the oxygen ion, 1.87 ± 0.1 ns, and Moore *et al.*[21] have observed a longer-lived level for this system, 3.48 ± 0.08 ns. The 3.48 ± 0.08 ns result is very close to our result for the $J=\frac{3}{2}$ level, 3.34 ns. If we assume that the 1.87 ± 0.1 ns result corresponds to the $J=\frac{1}{2}$ level, then this measurement is longer than the result of this work, 0.910 ns, and the result of Chen *et al.*[7] 1.09 ns. Richard *et al.*[22] have observed a level with a lifetime of 2.000 ± 0.025 ns in the fluorine ion. The theoretical results indicate that this measurement corresponds to the $J=\frac{3}{2}$ level. The present result of 1.84 ns is shorter, while the result of Chen *et al.*,[7] 2.15 ns, is longer by the same amount. Schumann *et al.*[23] have measured the lifetimes of the neon ion. Their measured lifetime of 0.40 ± 0.19 ns agrees with the present result of 0.368 ns for the $J=\frac{1}{2}$ level and the result of Chen *et al.*,[7] 0.419 ns. The measured lifetime 1.60 ± 0.24 ns is considerably longer than this calculation for the $J=\frac{3}{2}$ level, 0.857 ns; however, our theoretical result agrees with the calculation of Chen *et al.*[7] for this level, 0.894 ns. We also quote the theoretical results for the radiative and autoionization transition rates of Bhalla and Gabriel,[24] and Vainshtein and Safronova,[25] in Tables VI and VII for comparison. Bhalla and Gabriel[24] did nonrelativistic Hartree-Slater calculations in intermediate coupling with only spin-orbit mixing. Their radiative and autoionization rates are both quite different from this calculation and that of Chen *et al.*[6,7] This confirms the importance of including all the spin-dependent perturbations when computing the coupling to the $(1s2s2p)^2P^o$ states and the $^2P^o$ continuum. Vainshtein and Safronova[25] used Z-dependent perturbation theory, with a closed-channel basis consisting of hydrogenlike functions and an open channel constructed from Coulomb wave functions without screening. While their radiative rates agree with this work and that of Chen *et al.*,[6,7] their autoionization rates are quite different, which may indicate the inadequacy of their open-channel wave function.

A general trend is revealed when comparing the transition rates of Chen *et al.*[6,7] with those of this work. The radiative rates of this work are smaller (the only exception is for $Z=18$), while the autoionization rates are larger (the only exceptions are for $Z=13$ and 18). The difference in the autoionization rates, however, is much larger than the corresponding differences in radiative rates on a percentage basis. These discrepancies of opposite sign have a canceling effect when the net transition rate and resulting lifetime are computed; however, these same discrepancies will magnify the difference between the calculated branching ratios.

V. CONCLUSION

In this work we have determined the lifetimes of the lithiumlike $1s2s2p\ ^4P_J^o$ levels for $J=\frac{1}{2}$ and $\frac{3}{2}$ from $Z=3$ to 18. Both the autoionization and the radiative transition rates are computed in order to determine these lifetimes. The autoionization widths were computed with the saddle-point complex-rotation method by including the full spin-dependent part of the relativistic Breit-Pauli Hamiltonian. The radiative transition rates were computed with first-order perturbation theory. All of these calculations were carried out in the intermediate LSJ-coupling scheme due to the essential role played by the $1s2s2p\ {}^2P_J^o$ states in the deexitation of the metastable $1s2s2p\ {}^4P_J^o$ systems. Comparison of the present results with the few available experimental measurements reveals discrepancies in about half of the cases; however, in the cases where discrepancies with experiment occur, the results of this work appear to agree with other theoretical calculations. More high-precision measurements for lifetimes along with measurements to reveal the branching ratios are needed to make a more critical comparison of the different theoretical methods.

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