RAPID COMMUNICATIONS

PHYSICAL REVIEW A VOLUME 36, NUMBER 4 AUGUST 15, 1987

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Complex-rotation method for spin-induced autoionization

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(Received 20 March 1987)

We report the first complex-rotation calculation which incorporates spin-dependent perturbations. By using the intermediate *LSJ* coupling scheme, the lifetimes due to the spin-induced autoionization of the lithiumlike metastable $(1s2s2p)^4P_{5/2}$ state are determined along the isoelectronic series for $Z=2-10$ and $Z=16-18$. The results are compared with experimental measurements and other theoretical results.

Relativistic autoionization processes play a major role in the decay of those highly excited atomic systems which for symmetry reasons are not able to autoionize via the Coulomb interaction. The relative weakness of the relativistic interactions versus the Coulomb interaction accounts for the metastability of these highly excited atomic states. The $(1s2s2p)^4P^{\circ}_{5/2}$ state in lithiumlike atomic systems is one example which has been studied quite extensively both experimentally and theoretically.

In the past, theoretical lifetimes have been obtained by choosing an appropriate outgoing wave function for the decay channel and then computing the width of the autoionization state with a golden-rule formula. However, the width so obtained depends sensitively on the choice of the outgoing wave function. For example, the best previous calculation for the lifetime of the $He^-(1s2s2p\ ^4P_{5/2})$ state is probably that of Estberg and LaBahn,[1] who show that by using various approximations, the lifetime of this that by using various approximations, the lifetime of this state may vary from 544 to 455 μs. In the calculations where the golden-rule formula is employed, the coupling doublet and quartet configurations) is usually ignored. On the other hand, the complex-rotation method uses square-integrable basis functions only. It has the advantage that a uniform approach can be adopted independent of whether the system of interest is a neutral, positive, or negative ion. If a calculation gives good convergence, the result so obtained is usually reliable as evidenced in some recent high-resolution experiments.[2] Another advantage is that when closed- and open-channel parts of the metastable system are both present in the complex-secular equation, the coupling effect of the channels can be adequately accounted for. The complex-rotation method has been used extensively for systems which autoionize via the Coulomb potential. In this work, we extend this method to metastable systems decaying via the spin-dependent potentials.

In this work we have computed the $(1s2s2p)^4P_{5/2}$ lifetimes for the lithium isoelectronic sequence from $Z=2$ through $Z=10$ and for $Z=16$, 17, and 18. Our theoretical approach to the calculation of relativistic autoionization has been to include the magnetic spin-dependent part (spin-orbit, spin-other-orbit, and spin-spin) of the Pauli-Briet interaction in the Hamiltonian of the saddle-point complex-rotation method. The open channels accessible via these spin-dependent operators may have *LS* symmetry different from that of the particular metastable state of interest. The total angular momentum *J* and parity are therefore the good quantum numbers. This requires that the calculation be carried out in the intermediate *LSJ* coupling scheme.

The purpose of this investigation is to assess the feasibility of the complex-rotation method with regard to the weak coupling involved in relativistic autoionization processes.

The $(1s2s2p)$ configuration forms the *LS* multiplets: $(1s2s2p)^4P^{\circ}$, $[1s,(2s2p)^3P]^2P^{\circ}$, and $[1s,(2s2p)^1P]^2P^{\circ}$. The wave function for the $J=\frac{5}{2}$ level of the multiplet originating from $(1s2s2p)^4P$ does not contain a $^2P^{\circ}$ component. Therefore the only autoionizing decay channel

open to the $(1s2s2p)^4P^o_{5/2}$ state which conserves parity and total angular momentum is the $[(1s1s)^1S,kf]^2F^o_{5/2}$ continuum. This continuum couples to $(1s2s2p)^4P^o_{5/2}$ through the spin-spin Hamiltonian,

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

The spin-spin operator is the result of the contraction of two second-order tensors,

$$H_{SS}=-\frac{\alpha^2}{r_{ij}^3}\sqrt{(24\pi/5)}S^{(2)}\cdot Y^{(2)} , \quad (2)$$

where $S^{(2)}$ is the tensor product of the spin operators of the two interacting electrons, and $Y^{(2)}$ is the spherical-harmonic tensor of order two. The matrix elements which couple the closed channel to the open channel can be expressed with the aid of the Wigner-Eckart theorem and reduced matrix elements

$$\langle L'S'JM|S^{(k)}\cdot Y^{(k)}|LSJM\rangle=(-1)^{(J+S'+L)}\begin{Bmatrix}L' & k & L\\ S & J & S'\end{Bmatrix}\langle L'S'\|S^{(k)}\cdot Y^{(k)}\|LS\rangle . \quad (3)$$

This expression shows, as a result of the triangle inequalities for the 6-j symbol, why the spin-spin interaction ($k=2$) contributes to the coupling and the spin-orbit and spin-other-orbit interactions ($k=1$) do not.

The wave function for this state is therefore,

$$\Psi=a\Psi_c\{(1s2s2p)^4P^o_{5/2}\}+\Psi_0\{[(1s1s)^1S,kf]^2F^o_{5/2}\} . \quad (4)$$

This eigenfunction of total angular momentum $J=\frac{5}{2}$ and z-component M is formed from the LS states by

$$|JMLS\rangle=\sum_{M_L,M_s}|LSM_LM_s\rangle\langle LSM_LM_s|JM\rangle . \quad (5)$$

The wave function of the closed-channel component is a multiconfiguration-interaction wave function which can be represented by

$$\Psi_c=\sum_i B_i\phi_i^L(R_3,\Omega_3,\alpha,q) , \quad (6)$$

where the ϕ_i are optimized antisymmetrized basis functions which are predetermined by either a saddle-point or Rayleigh-Ritz variational calculation. R_3 and Ω_3 in Eq. (6) represent collectively the radial and angular coordinates of the three electrons. For a more complete discussion of the procedure for computing the closed-channel wave function, we refer the reader to Ref. 3. The open-channel component of the resonance wave function is given by

$$\Psi_0\{[(1s1s)^1S,kf]^2F_{5/2}\}=A\sum_j C_j\psi_g(R_2,\Omega_2)U_j^L(re^{-i\theta}) . \quad (7)$$

The C_j in this equation and a in Eq. (4) are linear variation parameters. ψ_g is the $(1s1s)^1S$ two-electron target state. For this state we use a three-partial-wave eight-term configuration-interaction wave function.[6] The U_j^L, which form a one-dimensional complete set for representing the ejected f-wave electron are given by

$$U_j^L(re^{-i\theta})=(re^{-i\theta})^j e^{-\gamma re^{-i\theta}}Y_L(\Omega) , \quad (8)$$

where γ is a nonlinear variation parameter. θ is the complex-rotation parameter. In Eq. (7), the angular and spin couplings of the target state ψ_g with the U_j^L is suppressed; these functions are coupled to form the ^2F symmetry. In our previous works (Refs. 4–6), the complex rotation is carried out by scaling the radial coordinates in the Hamiltonian, the closed-channel wave function, and the target-state wave function by $r\rightarrow re^{+i\theta}$. The only radial coordinates that were not scaled were those in the basis functions of the ejected electron, the U_j^L's. In the present work, the equivalent is achieved[7] by transforming only the radial coordinates in the ejected electron's basis functions by the inverse of the previous transformation, $r\rightarrow e^{-i\theta}$. Further details concerning the complex-rotation method can be found in Refs. 4 and 8, and the references quoted in these works.

The energy and width of the resonances described by the trial functions in Eqs. (4)–(8) are obtained by the variation

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

where H is given by

$$H=H_0+H_{SS} , \quad (10)$$

with

$$H_0=\sum_{i=1}^{3}\left[-\frac{1}{2}\nabla_i^2-\frac{Z}{r_i}\right]+\sum_{\text{pairs}}\frac{1}{r_{ij}} , \quad (11)$$

and H_{SS} is given by Eq. (1).

The energy and width of the $(1s2s2p)^4P^o_{5/2}$ resonance are obtained from the complex eigenvalue $E-i(\Gamma/2)$, which results from the variation in Eq. (9). These results are given in Table I for the various ions. Also given in this table are the results of first-order perturbation theory for the other relativistic corrections (relativistic correction to the kinetic energy, Darwin term, the orbit-orbit interaction, and the nonrelativistic mass polarization effect). The evaluation of these expectation values has been discussed in an earlier work.[9] The relativistic energy in Table I includes all of the perturbation energies.

The calculated autoionization widths in Table I vary smoothly as a function of Z. This variation, however, deviates from a simple power law. Judging from the golden-rule expression for the autoionization width, one

TABLE I. Nonrelativistic and relativistic energy and width Γ of the $(1s2s2p)^4P_{5/2}$ of lithiumlike ions. The number in square brackets is the power of ten. L and N are the number of partial waves and linear parameters in the closed-channel wave functions, respectively. The relativistic energy E_{rel} includes the perturbation energies from the other relativistic corrections (relativistic correction to the kinetic energy and Darwin term $\langle H_1+H_2\rangle$, the orbit-orbit interaction $\langle H_4\rangle$, and the nonrelativistic mass polarization effect $\langle H_5\rangle$).

Z	E_{nonrel} (a.u.)	L	N	$\langle H_1+H_2\rangle$	$\langle H_4\rangle$	$\langle H_5\rangle$	E_{rel} (a.u.)	Γ (a.u.)
2	−2.178017	15	92	−1.127 [−4]	+5.1 [−7]	−2.61 [−6]	−2.178132	4.870 [−14]
3	−5.367838	13	97	−6.045 [−4]	+9.2 [−6]	−1.54 [−5]	−5.368448	3.395 [−12]
4	−10.066454	13	87	−2.009 [−3]	+3.5 [−5]	−3.2 [−5]	−10.068460	2.285 [−11]
5	−16.267391	12	80	−5.086 [−3]	+8.5 [−5]	−5.1 [−5]	−16.272443	8.146 [−11]
6	−23.969335	12	80	−1.0815 [−2]	+1.69 [−4]	−7.6 [−5]	−23.980057	2.122 [−10]
7	−33.171779	12	80	−2.0427 [−2]	+2.95 [−4]	−9.7 [−5]	−33.192008	4.587 [−10]
8	−43.874525	12	80	−3.5371 [−2]	+4.73 [−4]	−1.17 [−4]	−43.909540	8.741 [−10]
9	−56.077431	12	80	−5.7353 [−2]	+7.10 [−4]	−1.31 [−4]	−56.134205	1.521 [−9]
10	−69.780524	12	80	−8.8264 [−2]	+1.009 [−3]	−1.59 [−4]	−69.867937	2.475 [−9]
16	−183.500198	13	87	−5.98369 [−1]	+4.708 [−3]	−2.85 [−4]	−184.094144	2.000 [−8]
17	−207.703586	13	87	−7.65219 [−1]	+5.717 [−3]	−2.98 [−4]	−208.463386	2.600 [−8]
18	−233.406985	13	87	−9.64819 [−1]	+6.860 [−3]	−2.95 [−4]	−234.365239	3.325 [−8]

would expect a Z^4 dependence. The results of Table I (excluding the case of the negative He ion) indicate a progressively weaker dependence on Z. For small, medium, and large Z, this dependence behaves roughly like $Z^{6.2}$, $Z^{5.3}$, and $Z^{4.3}$, respectively.

Table II compares our computed lifetimes with those of experiment and other theoretical methods. Our result for the helium ion 497 μs is in good agreement with the theoretical result 455 μs of Estberg and LaBahn[1] and the measurement of Novick and Weinflash,[10,11] 500 ± 200 μs. Manson's result[12] 1000 μs is twice our result for He^-; however, his result[12] for Li, 5.88 μs is in agreement with the measurement of Levitt, Novick, and Feldman[13] 5.8 ± 1.2 μs. Our result for the lifetime of the lithium system 7.13 μs lies near the higher end of the experimental uncertainty, but agrees with the other theoretical results in Table II. The present results agree with the measurements on the other lithiumlike ions to within the experimental uncertainties quoted. It should be mentioned that the forbidden magnetic quadrupole radiative branch $(1s2s2p)^4P^o_{5/2}\rightarrow(1s1s2s)^2S_{1/2}$ becomes important for large Z. Pegg *et al.*[17] have given estimates of the autoionization branching ratio for O VI, F VII, S XIV, Cl XV, and Ar XVI; and quoted 1.00, 0.99, 0.86, 0.80, and 0.76 for these states, respectively. Chen[19] has computed both Auger and radiative decay rates in the intermediate-

TABLE II. Comparison of lifetimes of lithiumlike $(1s2s2p)^4P_{5/2}$ (results are quoted in either microseconds μs or in nanoseconds ns). The results from this work do not include the forbidden magnetic quadrupole radiative branch $(1s2s2p)^4P_{5/2}\rightarrow(1s1s2s)^2S_{1/2}$ which becomes important for large Z (see text).

Z	This work	Other theory			Experiment
2	497 μs	1000 μs[a]		455 μs[b]	345 ± 90 μs[c]
					500 ± 200 μs[d]
3	7.13 μs	5.88 μs[a]	7.20 μs[e]	7.60 μs[f]	5.800 ± 1.20 μs[g]
4	1.06 μs				
5	0.297 μs				
8	27.67 ns	31 ns[h]		75 ns[i]	25 ± 3 ns[j]
9	15.899 ns				15 ± 1 ns[j]
10	9.774 ns				
16	1.209 ns				1.1 ± 0.1 ns[j]
17	0.9303 ns				0.91 ± 0.04 ns[j]
18	0.7275 ns	0.563 ns[k]			0.66 ± 0.04 ns[j]
	0.591 ns[l]	0.592 ns[m]			0.594 ± 0.016 ns[n]

[a]Reference 12.
[b]Reference 1.
[c]Reference 11.
[d]Reference 10.
[e]Reference 14.
[f]Reference 15.
[g]Reference 13.
[h]Reference 16.
[i]Reference 14.
[j]Reference 17.
[k]Reference 18.
[l]Includes Chen's (Ref. 19) radiative transition rate (7.65×10^{-9} a.u.).
[m]Reference 19.
[n]Reference 20.

coupling scheme using Dirac-Hartree-Slater wave functions. His calculations give 0.81 for the Ar branching ratio. Chen's width due to autoionization for Ar, 3.32×10^{-8} a.u., is in excellent agreement with our result and that of Cheng *et al.*[18] In Table II we have added Chen's magnetic quadrupole transition rate to our autoionization rate, the resulting lifetime, 0.591 ns is in agreement with the measurement of Dohmann and Mann,[20] 0.594 ± 0.016 ns.

In conclusion, we have used the complex-rotation method in the intermediate *LSJ* coupling scheme with the spin-dependent perturbation to compute the lithiumlike $(1s2s2p)^4P^{\circ}_{5/2}$ widths for $Z=2-10$ and $Z=16-18$. The results are in good agreement with the experiment. These calculations indicate that the weak relativistic coupling can be accurately incorporated into the complex-rotation method.

Width calculations are presently underway for the other J levels of $(1s2s2p)^4P^{\circ}$, and for the $(1s2p2p)^4P_J$ states. We are also investigating the lifetimes of the metastable lithium quartet states lying above the Li^+ $(1s2s)^3S$ threshold. These lifetimes have recently been measured by Mannervik, Cederquist, and Kisielinski,[21] and are found to be much shorter than the existing theoretical lifetimes. We hope by using a saddle-point complex-rotation method to account for the relativistic perturbations, these discrepancies can be resolved.

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

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