Excitation of ions of the lithium isoelectronic sequence in the relativistic Coulomb-Born approximation

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Cross sections for the electron-impact excitation of the $2p_{1/2}$ and $2p_{3/2}$ states of the lithiumlike ions C^{3+}, Fe^{23+}, Mo^{39+}, and W^{71+} are calculated in the relativistic Coulomb-Born approximation. A range of incident electron energies from the $2p_{1/2}$ threshold to (approximately) ten times the $2p_{3/2}$ threshold is considered. The most significant relativistic effects result from the spin-orbit splitting of the $2p$ states. An interpolation formula is presented which permits the estimation of these cross sections for similar ions of intermediate charges.

I. INTRODUCTION

The excitation of ions of the lithium isoelectronic sequence may be an important process in both controlled thermonuclear and astrophysical plasmas. There have been previous studies of excitation of these ions. Recent work includes that of Gau and Henry,[1] van Wyngaarden and Henry,[2,3] Hayes *et al.*,[4] and Callaway *et al.*[5] References to papers published prior to 1975 can be found in reviews by Bely and van Regemorter[6] and by Seaton.[7]

It is possible that in fusion reactors impurity ions of large nuclear charge will be present in highly stripped states. Relativistic effects may become important in the description of the excitation process in such ions, even though the energy of the incident electrons is not high enough for relativistic kinematics to become significant. We shall address here the question of what changes are produced by relativistic effects in the excitation of the $2s$-$2p$ transition in lithiumlike ions. Our study is based on relativistic Coulomb-Born calculation (RCBI—no exchange or unitarization) for the ions C^{3+}, Fe^{23+}, Mo^{39+}, and W^{71+}.

Relativistic effects are rather insignificant in the light ion C^{3+}, which has been the subject of extensive calculations by a variety of nonrelativistic methods. We have considered this case here in order to check our calculational procedures and establish firm results in the nonrelativistic limit as a basis for comparison. Relativistic corrections begin to be appreciable in the case of iron (Fe^{23+}) where the $2p_{1/2}$ and $2p_{3/2}$ thresholds are separated by 1.2 Ry and are quite substantial for Mo^{39+}; for which the spin-orbit splitting is 6.3 Ry. In the case of W^{71+}, spin-orbit coupling (splitting 112 Ry) leads to a description of excitation which has some aspects which are radically different from the nonrelativistic situation.

Relativistic effects in atomic scattering theory have been the subject of only a few studies. The work of Carse and Walker[8] and of Walker[9] on the relativistic calculation of the excitation of hydrogenic ions using wave functions which are solutions of the Dirac equations is closely related to this investigation. Other authors have considered heliumlike ions in an approximation in which the body relativistic effects in the target atom (spin-orbit, mass velocity, and Darwin terms) are included by perturbation theory.[10,11]

It is convenient to consider two classes of relativistic effects: (i) the modification of the states of the target atom, and (ii) the use of a relativistic description of the wave functions of the incident electron. Both are included in our calculation, however, the former is generally believed to be the more important, and we shall present more evidence supporting this point of view below. A third contribution, the relativistic modification of the interaction between the electron and the target (the Breit interaction), is not considered here.

The (one-electron) energies of the ions considered are given in Table I. The energy required to excite the $2p_{1/2}$ state increases from 0.59 Ry in C^{3+} to 14.4 Ry in W^{71+}, roughly in proportion to the charge, $Z+1$ of the heliumlike ion core. The energies of the $2s$ and $2p$ states from a nonrelativistic Hartree-Fock calculation are presented for comparison. The separation of the $2p_{1/2}$ and $2p_{3/2}$ levels, which is produced by spin-orbit coupling, increases much more dramatically; from 0.001 Ry in C^{3+} to 112 Ry in W^{71+}, roughly proportional to $(Z+1)^4$. Even with this large splitting, the $n=2$ states of W^{71+} remain well separated from the $n=3$ levels which are approximately 700 Ry above the $2s$. It should also be noted that the excitation energy of the $2p$ states in a nonrelativistic limit is always smaller than the relativistic excitation energy for the $2p_{1/2}$ state. This effect is, presumably, a result of the relativistic contrac-

TABLE I. Orbital energies of $n=2$ states of lithiumlike ions (Ry). The first three entries for each ion are from a numerical Dirac-Fock calculation. The last two are nonrelativistic (NR) results.

State	Ion			
	C^{3+}	Fe^{23+}	Mo^{39+}	W^{71+}
$2s$	−4.732 22	−150.424 4	−420.272 4	−1449.544
$2p_{1/2}$	−4.139 67	−146.845 4	−413.923 0	−1435.146
$2p_{3/2}$	−4.138 50	−145.631 6	−404.476 9	−1323.254
$2s$(NR)	−4.730 00	−148.805 12	−408.074 14	−1310.713 76
$2p$(NR)	−4.138 42	−145.363 96	−402.369 10	−1300.378 28

tion of the $1s$ wave functions.

The increasing splitting of the $2p$ levels is the major relativistic effect with which scattering calculations must contend. The cross section for the excitation of the $2p_{1/2}$ state from the $2s$, which we will denote σ_1, is in C^{3+} almost exactly $\frac{1}{2}$ of that for the excitation of the $2p_{3/2}$ state σ_3, and the curves are essentially superimposed on each other. As the ionic charge increases, the curves separate and the cross sections decrease in magnitude. The Z dependence will be discussed in detail below. However, the ratio σ_1/σ_3, when evaluated for the same value of the ratio of the incident kinetic energy to the excitation energy, increases steadily from the initial value of $\frac{1}{2}$ to a value between approximately 6.0 and 4.5, decreasing slowly with energy. If this ratio is multiplied by the ratio of the excitation energies, we find

$$[\Delta E_1 \sigma(x_1)/\Delta E_3 \sigma_3(x_3)]_{x_1=x_3} \sim 0.5 \qquad (1)$$

(where ΔE_1 is the excitation energy for the $2p_{1/2}$ state and $x_1 = E/\Delta E_1$, E being the kinetic energy of the incident electron, etc.). This suggests that the individual cross sections are not greatly altered from the nonrelativistic case apart from the shift of thresholds.

II. PROCEDURE

The energies and wave functions of the four ions considered were obtained from a Dirac-Fock calculation using a computer program developed by Desclaux.[12] The $1s^2 2s_{1/2}$, $1s^2 2p_{1/2}$, and $1s^2 2p_{3/2}$ configurations were considered. The $1s$ wave functions differ slightly in these states, but this difference was ignored in our further calculations. It is consistent with this procedure to use the one-electron energy parameters, given in Table I, to determine the excitation energies. The error introduced by these approximations seems to be quite negligible except possibly for the $2p_{1/2}$ state of W^{71+} where there is a 10% discrepancy between the total energy differences (with respect to the $2s_{1/2}$ state) and the eigenvalue differences. The computed oscillator strengths for the $2s$-$2p_{1/2,3/2}$ transitions agree with those calculated by Armstrong, Fielder, and Lin,[13] except for a 3% discrepancy in the case of the $2p_{1/2}$ state of W^{71+}.

The wave functions from Desclaux's program are given with $\ln r$ as the independent variable. A six-point Lagrangian interpolation procedure was used to generate wave functions on a grid with r as the independent variable. The grid spacing was chosen to scale approximately as $1/Z$. The number of doublings of the interval and the number of points obtained were adjusted to permit numerical integrations into a region where the scattering wave functions agreed with their asymptotic expressions.

The scattering calculations were performed in the coupled representation in which states of the scattering system are defined with the total angular momentum J a good quantum number. This is the simplest procedure to employ if one is interested, as here, only in the total cross section.[9] The radial wave functions for the scattering electron were obtained numerically as solutions of the Dirac equations for a Coulomb field whose charge is that of the ion. This program was checked by comparison of the wave functions with their analytical expressions as given, for example, by Rose.[14]

The cross sections are calculated in the following way: We consider a transition from an initial atomic state (n_a, l_a, j_a) to a final state (n_f, l_f, j_f). The cross section is given by

$$\sigma(n_a l_a j_a \to n_f l_f j_f) = \frac{2\pi}{p^2} \frac{1}{2j_a+1} \sum_J (2J+1) \times |\langle j_f l_f j_q l_q J | T | j_a l_a j_p l_p J \rangle|^2 . \qquad (2)$$

The indices p and q are used to refer to the inci-

dent and final scattering states, respectively. The sum in (2) includes not only J as noted but all those values of j_q, l_q, j_p, and l_p which are permitted for a fixed value of J. The operator T refers to the usual T matrix. Since we are neglecting exchange, unitarization, and the Breit interaction, the T matrix element above is just the matrix element of the electrostatic potential, e^2/r_{12}. It has been shown by Grant[15] that this matrix element can be expressed as a sum of products of radial integrals and coefficients which depend on the angular momenta involved. We write

$$\begin{aligned}\langle j_f l_f j_q l_q J \,|T|\, j_a l_a j_p l_p J\rangle &= e^2\langle j_f l_f j_q l_q J \,|r_{12}^{-1}|\, j_a l_a j_p l_p J\rangle \\ &= \sum_\nu R_\nu(J, j_f, j_q, j_a, j_p) V_\nu(fq, ap) \end{aligned} \quad (3)$$

in which

$$\begin{aligned}V_\nu(fq,ap) = e^2 \int_0^\infty dr_1 \int_0^\infty dr_2 \,[P_f(r_2)P_a(r_2) + Q_f(r_2)Q_a(r_2)] \\ \times [P_q(r_1)P_p(r_1) + Q_q(r_1)Q_p(r_1)] \\ \times \left(\frac{r_<^\nu}{r_>^{\nu+1}} - \frac{\delta_{\nu 0}}{r_2}\right)\end{aligned} \quad (4)$$

and

$$\begin{aligned}R_\nu(J, j_f, j_q, j_a, j_p) &= (-1)^{j_F + j_A + J}[(2j_a+1)(2j_f+1)(2j_p+1)(2j_q+1)]^{1/2} \\ &\times \begin{pmatrix} j_f & \nu & j_a \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix} \begin{pmatrix} j_p & \nu & j_q \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix} \begin{Bmatrix} j_a & j_p & J \\ j_q & j_f & \nu\end{Bmatrix}.\end{aligned} \quad (5)$$

The radial functions P_a, Q_a, P_f, Q_f which appear in (4) are solutions of the radial Dirac-Fock equations for the atomic states a and f. The function P is the large component, Q the small component. The corresponding functions P_p, Q_p, P_q, Q_q are continuum solutions of the radial Dirac equation for a pure Coulomb potential $-Ze^2/r$. The modifications of the scattering wave functions due to the finite size of the nucleus have been ignored.

The angular factor R, Eq. (5), is a straightforward generalization of a similar quantity which appears in nonrelativistic calculations. The quantities (:::) are Wigner 3-j symbols, while $\{:::\}$ denotes a 6-j symbol.

In addition, the matrix element is restricted by selection rules which correspond to parity conservation.[15] Let

$$a_j = \begin{cases} +1 & \text{if } j = l + \frac{1}{2} \\ -1 & \text{if } j = l - \frac{1}{2}. \end{cases} \quad (6)$$

Then for a nonzero contribution, it is required that

$$\begin{aligned} &j_f + \nu + j_a = \text{even} \quad \text{if} \quad a_a \neq a_f; \\ &j_f + \nu + j_a = \text{odd} \quad \text{if} \quad a_a = a_f; \\ &j_p + \nu + j_q = \text{even} \quad \text{if} \quad a_p \neq a_q; \\ &j_p + \nu + j_q = \text{odd} \quad \text{if} \quad a_p = a_q. \end{aligned} \quad (7)$$

It is typical of optically allowed s-p transitions that the sum over J in Eq. (2) converges rather slowly. It is highly desirable for this reason to have closed expressions for the quantity R given by Eq. (5), which will avoid complications introduced by factorials of large numbers. Analogous expressions for the nonrelativistic case were given by Percival and Seaton.[16] In the present instance, the possible values of ν are limited to 0, 1, 2 by the triangular condition on the 3j symbols, and from there, only $\nu = 1$ is allowed by the conditions of Eq. (7). The necessary values of R can then be calculated using analytical expressions for the 3-j and 6-j symbols. The relevant formulas for R are presented in Table II. Cases not listed are either zero, or do not occur in the problem under consideration.

The computation of the radial integrals V_ν [Eq. (4)] also presents some problems. Since we are concerned with $\nu = 1$, the integrand in the final step decays as r^{-2} (times an oscillatory function) at large r. In order to obtain more accurate values for the matrix elements, we have carried the numerical integral out to large enough values of r for the Coulomb waves in (4) to be represented by their asymptotic forms. The contribution from the tails can then be estimated by an integration by parts. Thus, for example,

$$\int_{R_m}^\infty \frac{\sin kr}{r^2} dr = \frac{1}{kR_m^2} \cos kR_m + O\left(\frac{1}{kR_m^3}\right).$$

TABLE II. Selected values of the coefficient R [Eq. (5)].

j_a	j_f	j_p	j_q	$R_1(Jj_fj_qj_aj_p)$
$\frac{1}{2}$	$\frac{1}{2}$	$J-\frac{1}{2}$	$J-\frac{1}{2}$	$1/[3(2J+1)]$
$\frac{1}{2}$	$\frac{1}{2}$	$J-\frac{1}{2}$	$J+\frac{1}{2}$	$-2[J(J+1)]^{1/2}/[3(2J+1)]$
$\frac{1}{2}$	$\frac{1}{2}$	$J+\frac{1}{2}$	$J-\frac{1}{2}$	$-2[J(J+1)]^{1/2}/[3(2J+1)]$
$\frac{1}{2}$	$\frac{1}{2}$	$J+\frac{1}{2}$	$J+\frac{1}{2}$	$-1/[3(2J+1)]$
$\frac{1}{2}$	$\frac{3}{2}$	$J-\frac{1}{2}$	$J-\frac{3}{2}$	$[(J-1)/3(2J-1)]^{1/2}$
$\frac{1}{2}$	$\frac{3}{2}$	$J-\frac{1}{2}$	$J-\frac{1}{2}$	$[2/3(2J+1)]\,[(J+1)/(2J-1)]^{1/2}$
$\frac{1}{2}$	$\frac{3}{2}$	$J-\frac{1}{2}$	$J+\frac{1}{2}$	$-[(J+1)(2J+3)]^{1/2}/[3(2J+1)]$
$\frac{1}{2}$	$\frac{3}{2}$	$J+\frac{1}{2}$	$J-\frac{1}{2}$	$[J(2J-1)]^{1/2}/[3(2J+1)]$
$\frac{1}{2}$	$\frac{3}{2}$	$J+\frac{1}{2}$	$J+\frac{1}{2}$	$[2/3(2J+1)]\,[J/(2J+3)]^{1/2}$
$\frac{1}{2}$	$\frac{3}{2}$	$J+\frac{1}{2}$	$J+\frac{3}{2}$	$-[(J+2)/3(2J+3)]^{1/2}$

The error commited by retaining only the leading term is of the order R_m^{-3}, and R_m was chosen to be large enough for satisfactory accuracy. This argument is not affected by the presence of logarithmic phase factors in the asymptotic forms of the Dirac-Coulomb waves.

An additional problem arises for large angular momenta J which make an appreciable contribution to the cross section. In such cases (4) becomes

$$V_\nu = A\int [P_a(r_1)P_b(r_1)+Q_a(r_1)Q_b(r_1)]r_1^{-2}\,dr_1\,, \qquad (8a)$$

where

$$A = e^2\int [P_f(r_2)P_a(r_2)+Q_f(r_2)Q_a(r_2)]r_2\,dr_2\,. \qquad (9)$$

The constant A can be computed quite easily, but the remaining integral, Eq. (8), is difficult because of the presence of Dirac wave functions of large angular momentum. In the nonrelativistic case, the integral can be performed analytically with Coulomb wave functions,[17] but the corresponding results are not known for the relativistic radial functions. We have therefore made the approximation that for J larger than a set value (generally ~12) the integral (8a) is replaced by

$$V_\nu = A\int R_{la}(r_1)R_{lb}(r_1)r_1^{-2}\,dr_1 \qquad (8b)$$

where R_{lb} and R_{la} are nonrelativistic Coulomb wave functions. The value is then obtained analytically.[17]

This approximation seems to be reasonably well justified both physically and mathematically provided that the kinetic energy of the scattering electron is much smaller than mc^2. The physical reason for adopting (8b) is that for large angular momenta, the electron remains outside the region of strong potential energy, and is not accelerated to relativistic speeds. Mathematically it is straightforward and to show that as long as

$$l(l+1) \gg (Z\alpha)^2$$

(α is the fine-structure constant) and

$$W = E - mc^2 \ll mc^2\,,$$

the large radial component of the Dirac wave function approaches the nonrelativistic Coulomb wave function and the small component is reduced by a factor of $W/2mc^2$, which we ignore.

III. RESULTS AND DISCUSSION

The cross sections for the $2s_{1/2}$ to $2p_{1/2}$ and $2p_{3/2}$ transitions were obtained at energies ranging from close to threshold to ten (or more) times threshold. The approximation of Eq. (8b) was used to enable inclusion of enough angular momenta (ranging from 20 near the $2p_{1/2}$ threshold to 110 at the highest energies considered) to insure convergence. Our computed results are presented in

TABLE III. Computed cross sections (units πa_0^2). (KE stands for kinetic energy.)

	C^{3+}			Fe^{23+}	
KE (Ry)	$\sigma(2p_{1/2})$	$\sigma(2p_{3/2})$	KE (Ry)	$\sigma(2p_{1/2})$	$\sigma(2p_{3/2})$
1.0	1.895	3.789	4.0	1.968(−2)	
2.2	0.985	1.969	6.0	1.34(−2)	2.58(−2)
4.0	0.616	1.229	10.0	8.63(−3)	1.603(−2)
6.0	0.451	0.901	15.0	5.82(−3)	1.110(−2)
8.0	0.361	0.722	20.0	4.53(−3)	8.61(−3)
12.0	0.262	0.523	30.0	3.22(−3)	6.08(−3)
16.0	0.207	0.414	40.0	2.54(−3)	4.79(−3)
			50.0	2.12(−3)	3.99(−3)
	Mo^{39+}			W^{71+}	
KE (Ry)	$\sigma(2p_{1/2})$	$\sigma(2p_{3/2})$	KE (Ry)	$\sigma(2p_{1/2})$	$\sigma(2p_{3/2})$
8.0	3.63(−3)		16.0	5.05(−4)	
12.0	2.51(−3)		25.0	3.34(−4)	
17.0	1.81(−3)	3.24(−3)	50.0	1.745(−4)	
24.0	1.32(−3)	2.34(−3)	100.0	9.36(−5)	
32.0	1.022(−3)	1.79(−3)	150.0	6.59(−5)	9.39(−5)
50.0	6.96(−4)	1.193(−4)	200.0	5.17(−5)	7.22(−5)
75.0	4.96(−4)	8.37(−4)	400.0	2.92(−5)	3.90(−5)
100.0		6.55(−4)	600.0		2.76(−5)
130.0		5.245(−4)	800.0		2.19(−5)
160.0		4.41(−4)	1000.0		1.83(−5)
			1500.0		1.32(−5)

Table III. The cross sections relating to Fe^{23+} and W^{71+} are shown in Figs. 1 and 2.

The cross sections for C^{3+} add to a total cross section for the excitation of the $2p$ state which agrees rather well with that obtained from a five-state close-coupling calculation above the ionization threshold.[1] Even at the relatively low energy of 2.2 Ry, the discrepancy between the Coulomb-Born and the results of more elaborate calculations is not large: Our value of $2.95\pi a_0^2$ is to be compared with the two-state close-coupling result (with exchange) of $2.66\pi a_0^2$ and with a five-state close-coupling value (subtracting resonances) of $2.56\pi a_0^2$.[5] The difference is only 15%. A somewhat similar comparison can be made with a two-state close-coupling calculation with exchange for Fe^{23+}.[18] Here the maximum discrepancy is 6% at threshold, with quite good agreement from twice threshold energy upwards, when the effects of spin-orbit coupling are removed.

Examination of the results in Table III (and Figs. 1 and 2) shows that the relativistic cross sections have the same general shape and energy dependence as is obtained in a nonrelativistic calculation. As we pointed out in the Introduction, the most important relativistic effects result from the spin-orbit splitting of the $2p$ states of the target atom. In fact, it seems that the use of Dirac continuum radial wave functions produces only a minor effect, even for W^{71+}. This was established in the following way. The calculations for W^{71+} were repeated using the relativistic target wave functions and the relativistic angular momentum coupling rules, but simply substituting nonrelativistic Coulomb

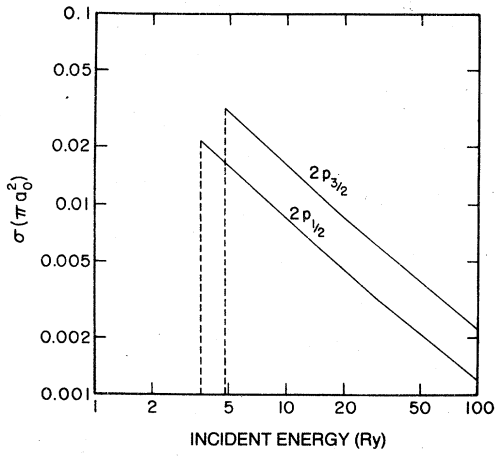

FIG. 1. Cross sections for the $2s \rightarrow 2p_{1/2,\,3/2}$ transitions in Fe^{23+} (units πa_0^2) are shown as a function of the kinetic energy of the incident electron (units Ry). The dashed lines indicate the thresholds.

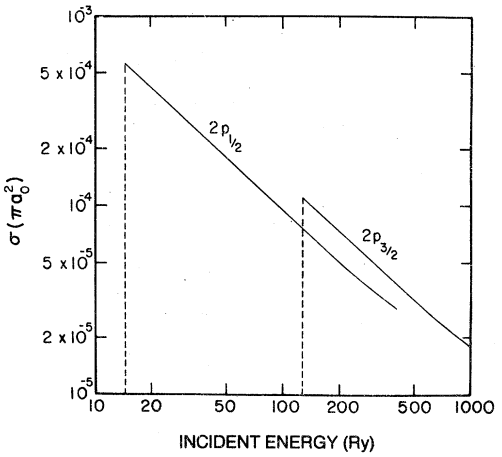

FIG. 2. Similar to Fig. 1 but for W^{71+}.

wave functions for the Dirac radial functions. The resulting semirelativistic cross sections are slightly smaller (by a factor ranging from about 5% to 9%) than the fully relativistic ones.

In addition, a parallel set of completely nonrelativistic Coulomb-Born calculations were performed for comparison. The nonrelativistic results are much too large (a factor of 3) below the $2p_{3/2}$ threshold, since the spin-orbit splitting of the $2p_{1/2}$ and $2p_{3/2}$ states has not been included. Immediately above this threshold, the nonrelativistic cross sections are a reasonable approximation (typically better than 5%) to the sum of the $2p_{1/2}$ and $2p_{3/2}$ excitations. The agreement worsens markedly as the energy increases, with the nonrelativistic results becoming significantly smaller than the relativistic ones. In addition, we should note that the nonrelativistic energy for the $2p$ threshold is always lower than the relativistic value for the $2p_{1/2}$ threshold. This discrepancy is quite serious (more than 4 Ry) for W^{71+}. Hence, a nonrelativistic calculation predicts that transitions occur at energies below their actual onset.

The following procedure was developed in order to analyze our results and to permit interpolation for ions not specifically studied: A least-squares fit to each cross section was made using a three-term nonrelativistic empirical formula[19]

$$\sigma = c_1/x^2 + c_2/x + (c_3/x)\ln x \qquad (10)$$

in which $x = E/\Delta E_t$, E being the kinetic energy of the incident electron and ΔE_t the excitation energy. The fits had rather good accuracy (~2% or better) except possibly at the lowest energy for which calculations were made. These fits enable one to compare cross sections at corresponding

TABLE IV. Scaled interpolated cross sections. The quantity $(Z+1)^3\,\sigma/100$ (units πa_0^2) is given as a function of the ratio of the kinetic energy of the incident electron to the excitation energy (Z is the ionic charge).

	C^{3+}		Fe^{23+}		Mo^{39+}		W^{71+}	
x	$2p_{1/2}$	$2p_{3/2}$	$2p_{1/2}$	$2p_{3/2}$	$2p_{1/2}$	$2p_{3/2}$	$2p_{1/2}$	$2p_{3/2}$
1.0	1.92	3.88	3.26	4.62	3.19	2.28	2.34	0.422
1.5	1.32	2.64	2.09	3.02	2.03	1.51	1.45	0.280
2.0	1.032	2.065	1.58	2.29	1.52	1.15	1.071	0.215
3.0	0.744	1.49	1.076	1.58	1.036	0.798	0.724	0.151
5.0	0.500	0.998	0.690	1.019	0.659	0.513	0.459	0.0992
10.0	0.292	0.583	0.385	0.570	0.365	0.285	0.255	0.0567
15.0	0.212	0.424	0.275	0.406	0.259	0.202	0.182	0.0407
20.0	0.169	0.337	0.216	0.319	0.204	0.159	0.143	0.0312

values of x, and thus to compare our results with nonrelativistic calculations, such as that for Fe^{23+} mentioned previously.[18]

Our results for the interpolated cross sections, multiplied by $(Z+1)^3$ ($Z+1$ is the charge of the heliumlike core) are given in Table IV. It will be seen that $(Z+1)^3\sigma$ is a slowly varying function of Z, compared to the cross section itself. In fact, for the transition to the $2p_{1/2}$ state, the maximum change in this quantity seldom exceeds 50% for all of the ions studied, whereas for the $2p_{3/2}$ transition there is a pronounced decrease for large Z. The difference in the behavior of these cross sections results from the different dependences of the excitation energies on Z: the excitation energy of the $2p_{1/2}$ state increases only slightly faster than $Z+1$ whereas that of the $2p_{3/2}$ state varies roughly as $(Z+1)^4$ when Z is large. The scaled interpolated cross sections are shown in Fig. 3 as functions of $Z+1$ for $x=10$ and $x=20$. It is evident from Table IV that qualitatively similar curves are obtained from other values of x.

In order to make possible estimates of the excitation cross sections for lithiumlike ions not explicitly studied here, we have determined an expression which reproduces the coefficients c_i ($i=1,3$) in Eq. (10) as functions of Z. It is

$$[c_i(Z+1)^3]^{-1}=\sum_{n=0}^{3} d_{in}(Z+1)^n . \tag{11}$$

The coefficients d_{in} are listed in Table V. Unfortunately, there is not much independent information which can be used to determine the accuracy of the interpolation procedure, however, it seems reasonable to anticipate inaccuracies of the order of 20%. An interpolation procedure has greater difficulty in the presence of the strong Z dependence introduced by relativistic effects than in the nonrelativistic situation considered by Gau and Henry.[1]

The simple energy dependence of the empirical formula for the cross section, Eq. (10), makes possible an analytical calculation of the energy-loss rate from a plasma in which the electrons have a Maxwell distribution of speeds. Such calculations can be made for a wide range of Z with the aid of Eq. (11). We shall consider here a closely related quantity, the thermally averaged effective cross section, which we define as

$$\sigma_e=\frac{1}{v_A}\int P(v)\, v\sigma(v)\, d^3v , \tag{12}$$

in which $P(v)$ is the Maxwellian velocity distribution and v_A is the average thermal velocity. Let

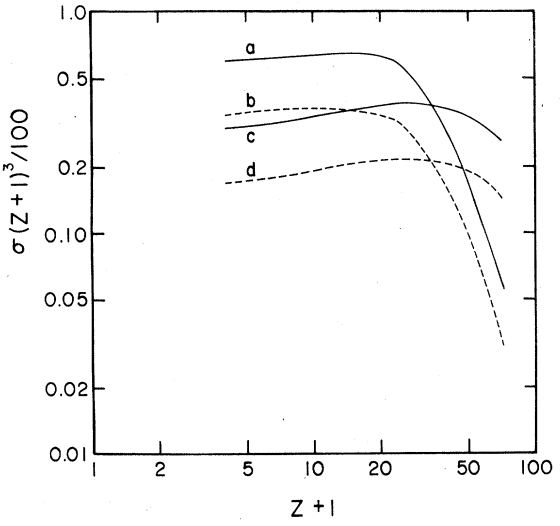

FIG. 3. Scaled interpolated cross section $(Z+1)^3\sigma$ is shown as a function of the charge of the ion, Z. Curve (a) $2p_{3/2}$ state, $x=10$; (b) $2p_{3/2}$, $x=20$; (c) $2p_{1/2}$, $x=10$; (d) $2p_{1/2}$, $x=20$.

TABLE V. Interpolating coefficients d_{in} [Eq. (11)] are given for the $2s$-$2p_{3/2}$ and $2s$-$2p_{1/2}$ transitions.

n	d_{1n}	$2p_{3/2}$ d_{2n}	d_{3n}	d_{1n}	$2p_{1/2}$ d_{2n}	d_{3n}
0	8.19(−3)	4.30(−3)	7.53(−3)	1.767(−2)	9.21(−3)	1.531(−2)
1	−4.10(−4)	−1.85(−5)	−1.535(−4)	−9.62(−4)	−2.77(−4)	−3.43(−4)
2	1.206(−5)	−4.71(−6)	5.42(−6)	2.78(−5)	5.03(−6)	1.216(−5)
3	5.90(−8)	1.59(−7)	1.49(−7)	−2.24(−7)	−1.88(−8)	−9.37(−8)

the electron temperature considered by denoted Θ. Then

$$v_A = (8K\Theta/\pi m)^{1/2},$$

in which K is Boltzmann's constant and m is the electron mass. The reader should note that we do not need to consider relativistic kinematics for the plasma electrons at the temperatures of principal interest here: the relativistic effects are confined to the ionic structure and, secondarily, to the rapid motion of an electron near a nucleus during a collision. The quantity σ_e can be expressed as in integral over the variable x used in (10):

$$\sigma_e = q^2 \int_0^\infty x e^{-qx} \sigma(x)\, dx \qquad (13)$$

in which $q = E_x/K\Theta$. A simple expression for σ_e can be obtained with the aid of (10):

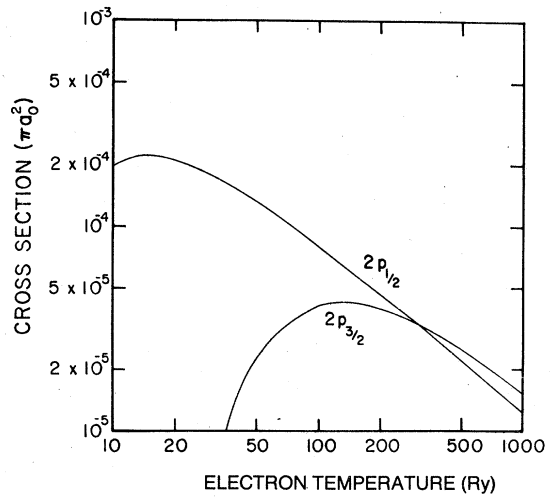

FIG. 4. Thermal average effective cross sections, Eq. (14), for the excitation of W^{71+} are shown as a function of electron temperature in Ry.

$$\sigma_e = q[c_2 e^{-q} + (c_3 + qc_1)E_1(q)], \qquad (14)$$

in which E_1 is an exponential integral function. The rates of interest in a macroscopic description of a plasma are proportional to σ_e.

Equations (11) and (14) enable calculation of σ_e for a large number of lithiumlike ions. As the calculation is quite straightforward and simple we show the results in only one case: that of W^{71+} (Fig. 4). The effective cross section for the excitation of the $2p_{1/2}$ state is larger than that for the $2p_{3/2}$ state for electron temperatures below about 300 Ry, and is quite large even at the low temperature of 10 Ry. However, the energy-loss rate from the plasma involves a product of the excitation energy and the effective cross section; the loss rate will therefore be larger from the $2p_{3/2}$ state than from the $2p_{1/2}$ state for temperatures above 50 Ry. The situation is similar for the other ions studied.

We conclude our discussion of the results with some additional remarks concerning reliability. In the nonrelativistic region (perhaps up to Fe^{23+}) we have pointed out that our results agree rather well with other calculations of $2s \rightarrow 2p$ transitions including, perhaps surprisingly some close-coupling studies. There are unfortunately no fully relativistic calculations at the present time with which our results can be compared, neither is there experimental data for the highly stripped ions which are our main interest.

Some comments can be made within the framework of the Born approximation. It appears from the work of Bely[20] that unitarization can make a difference to the Born approximation of the order of 10%–15% in the most unfavorable case considered here (C^{3+} at threshold), and that the effect of unitarization would cause a change of not more than 2%–3% in the other ions we have considered explicitly. The effect of inclusion of exchange can be roughly estimated by examination of the results of Walker[9] for the $2s \rightarrow 2p_{1/2}$ and $2s \rightarrow 2p_{3/2}$ transitions in hydrogenic ions as being of the order 6% near threshold, but decreasing to less than 1% at

about 5 times threshold (and not depending strongly on Z). Other studies of the excitation of C^{3+} by nonrelativistic calculations indicate that inclusion of exchange decreases the cross section by roughly 10% for $x < 5$. There is, of course, no guarantee that inclusion of exchange in a Born-approximation calculation necessarily leads to more accurate results in comparison with experiment.

In sum, it appears that the present calculations should be sufficiently accurate to permit realistic estimates of energy-loss rates associated with the excitation of highly stripped Li-like ions in a wide range of plasma conditions.

ACKNOWLEDGMENT

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