PHYSICAL REVIEW A VOLUME 16, NUMBER 3 SEPTEMBER 1977

Excitation of lithiumlike ions by electron impact*

J. N. Gau and Ronald J. W. Henry

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803

(Received 11 April 1977)

Collision strengths Ω for electron-impact excitation of C IV and Ar XVI are calculated in a five-state close-coupling approximation for energies up to 3 times threshold energy. These results are combined with previous calculations for N V and Ne VIII and isoelectronic fits are given for $\Omega(2s,2p)$ and $\Omega(2s,3l)$, where $l = 0,1,2$. In addition, polarization of the resonance $2s,2p$ line is calculated for Li-like C, N, Ne, and Ar up to 12 times threshold. A common feature is that the polarization changes from positive to negative at about 9 times threshold energy.

I. INTRODUCTION

An accurate knowledge of collision strengths for contaminant ions is important for an understanding of their effect in controlled thermonuclear plasmas.[1,2] Lithiumlike ions are of particular importance, especially those with high nuclear charge Z which are present due to evaporation of some of the wall material of the plasma container. From a knowledge of the properties of lower-Z ions, it is possible to extrapolate along the isoelectronic sequence to obtain information about higher-Z ions. These ions are also of importance in determining temperatures of the solar corona.[3]

We present calculated collision strengths at energies from 1.4 to about 3.0 times threshold energy for $n=2$ to $n=3$ transitions in C IV and Ar XVI. Calculations are made in a five-state close coupling with exchange approximation in which the eigenstates $1s^22s$, $1s^22p$, $1s^23s$, $1s^23p$ and $1s^23d$ are retained in the close-coupling expansion. Collision strengths are related to cross sections by

$$\Omega(i,j)=\omega_i k_i^2 Q_{i\to j}, \qquad (1)$$

where ω_i is the statistical weight of level i, k_i^2 is the energy in Ry of the electron relative to level i, and $Q_{i\to j}$ is the cross section in πa_0^2 units for excitation from level i to level j.

The coupled integro-differential equations which result in the close-coupling approximation are integrated by a noniterative integral equation method used by Sams and Kouri[4] and developed further by Smith and Henry.[5]

The ionic wave functions for the five lowest states of the ion are presented by Hartree-Fock-type wave functions given by Weiss[6] for C, N, and Ne. Similar wave functions for Ar are obtained with the computer code of Hibbert.[7]

As noted previously,[8,9] the $2s$-$2p$ collision strength is quite insensitive to the method of calculation for energies above the $n=3$ thresholds. For example, for N V, calculations in a unitarized Coulomb-Born two-state close-coupling and five-state close-coupling approximations agree to within 10%. This result is not surprising since additional states beyond $2p$ are well removed in energy and the inclusion of these states in a close-coupling expansion is not expected to have a significant effect. However, below the $3s$ threshold, if a two-state close-coupling approximation is used, the effect of closed channels is omitted. Will this omission have a significant impact on the averaged values of $\Omega(2s,2p)$?

While resonances may contribute substantially to electron impact collision strengths for some multiply charged positive ions, they are probably not as important for $\Omega(2s,2p)$, since the nonresonant contributions come mainly from large values of the orbital momentum l of the scattered electron. Positions of the resonances for large l will be z^2/n^2 below the closed channel threshold, since the quantum defect will be negligible. Further, since $n \geq l+1$, n will be large for large l and the resonances will lie just below the threshold energy of the closed channel. Thus the resonances will be confined to a very narrow energy range. Further, agreement between nonresonant theories and recent crossed-beam experiments of Taylor *et al.*[10] for C IV and Taylor *et al.*[11] for Be II provides indirect evidence that resonances are unimportant for averaged values of $\Omega(2s,2p)$.

In contrast to the situation for $2s$-$2p$, resonances may have an important effect on collision strengths for those cases which are dominated by smaller values of l. For example, Presnyakov and Urnov[12] find that their results for $\Omega(2s,3s)$ and $\Omega(2p,3s)$ for O VI exhibit large resonance contributions. We are presently carrying out additional calculations in a five-state close-coupling approximation in the energy region below the $3d$ threshold. Results will be presented in due course.[13]

In addition to the effect of resonances on excitations to the $n=3$ level there is a question con-

TABLE I. Collision strengths for C IV. Energy k^2 (Ry) is the electron energy relative to the 2s level. ΔE (Ry) is the threshold energy for each transition.

k^2(Ry)	$(2s, 2p)$	$(2s, 3s)$	$(2s, 3p)$	$(2s, 3d)$	$(2p, 3s)$	$(2p, 3p)$	$(2p, 3d)$
0.8	9.3[a]						
1.4	10.5[a]						
2.2	11.7[a]						
4.0	13.5	0.392	0.253	0.656	0.332	1.15	4.52
6.0	15.2	0.420	0.281	0.780	0.330	1.12	6.03
8.0	16.6	0.432	0.327	0.864	0.374	1.14	7.29
16.0	20.1	0.448	0.560	1.024	0.566	1.20	10.91
ΔE(Ry)	0.592	2.752	2.910	2.951	2.160	2.318	2.359

[a] Calculated in a two-state close-coupling approximation.

cerning the convergence of the close-coupling expansion. In previous studies,[8,9] we concluded that for energies less than three times the excitation threshold energy, coupling to all the $n = 2$ and $n = 3$ levels must be included in order to obtain results accurate to 10%. This conclusion is based on the addition of pseudostates in the close-coupling expansion and on a comparison made between calculations obtained in a five-state no-exchange approximation and an eight-state no-exchange approximation. The pseudostates were chosen to be degenerate in energy with their energy level corresponding approximately to the ionization threshold for the ion. Their function is primarily to represent on average all states of symmetries s, p, and d which have been omitted from a five-state close-coupling expansion, so that there are other channels to be excited.

In Sec. II we present our results for lithiumlike carbon and argon. Our results are combined with previous five-state close-coupling calculations for N V and Ne VIII of van Wyngaarden and Henry[8,9] and isoelectronic fits are given in Sec. III for collision strengths $\Omega(2s, 2p)$ and $\Omega(2s, 3l)$, $l = 0, 1, 2$. In Sec. IV, we present results for the percentage polarization of the resonance $2p \rightarrow 2s$ line in Li-like C, N, Ne, and Ar in the energy region up to 12 times threshold energy.

II. COLLISION STRENGTHS FOR C IV AND AR XVI

Collision strengths for C IV and Ar XVI are given in Tables I and II, respectively, as a function of electron energy k^2 relative to the 2s threshold; ΔE is the threshold energy for each transition. Calculations are made in a five-state close-coupling approximation, except as indicated in the tables.

Results for $\Omega(2s, 2p)$ for C IV are in excellent agreement with a two-state close-coupling calculation of Robb,[15] who used an R-matrix method to solve the scattering equations. Figure 1 compares our results for $Q_{2s\rightarrow 2p}$ for C IV with preliminary measurements obtained in a recent crossed-beam experiment by Taylor *et al.*[10] The error bars given for the experimental points represent only uncertainties which are statistical, and do not include possible systematic uncertainties which are not yet evaluated. Agreement between theory and experiment is very good.

A compendium of data for collision strengths for all ions of carbon has been compiled by Magee *et al.*[14] Comparisons with other approximate methods are given there and will not be repeated here. No other results for collision strengths exist for Ar XVI.

TABLE II. Collision strengths for Ar XVI. Energy k^2 (Ry) is the electron energy relative to the 2s level. ΔE (Ry) is the threshold energy for each transition.

k^2 (Ry)	$(2s, 2p)$	$(2s, 3s)$	$(2s, 3p)$	$(2s, 3d)$	$(2p, 3s)$	$(2p, 3p)$	$(2p, 3d)$
3.14	0.98[a]						
4.62	1.02[a]						
6.93	1.06[a]						
13.86	1.16[a]						
54.0	1.33	0.0307	0.0337	0.0634	0.0086	0.0738	0.369
70.0	1.41	0.0319	0.0416	0.0680	0.0085	0.0727	0.415
116.0	1.59	0.0341	0.0619	0.0802	0.0103	0.0709	0.525
ΔE (Ry)	2.309	37.838	38.495	38.718	35.529	36.186	36.408

[a] Calculated in a two-state close-coupling approximation.

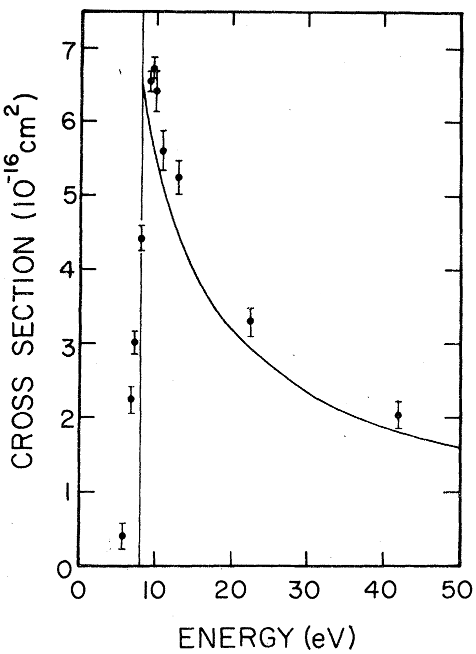

FIG. 1. Cross section for $2s\to 2p$ excitation of C IV vs impact electron energy. Solid curve: present results; solid circles, Taylor *et al.* (Ref. 10).

III. ISOELECTRONIC COLLISION STRENGTHS

Two-state close-coupling calculations for $\Omega(2s, 2p)$ for C IV and Ar XVI given in Sec. II are combined with similar calculations on N V and Ne VIII by van Wyngaarden and Henry.[8,9] For this dipole-allowed, spin-allowed collision strength, we fit the data to the following form

$$z^2\Omega(x) = c_0(z) + c_1(z)x^{-1} + c_2(z)\ln x, \tag{2}$$

where $x = k^2/\Delta E$ is the energy in threshold units, and where

$$\left.\begin{aligned} c_0(z) &= 282 - 800z^{-1},\\ c_1(z) &= 236z^{-1},\\ c_2(z) &= 18 + 204z^{-1}, \end{aligned}\right\} \text{ for } 2s, 2p \tag{3}$$

and $z = Z - 2$ is the net charge experienced by the active ionic electron. Note that the data are only generated up to $x = 5$.

Figure 2 gives $z^2\Omega(2s, 2p)$ vs z^{-1} for several values of x. Open circles represent calculated values for Li-like C, N, Ne, and Ar. Calculations of Robb[15] for Fe XXIV are given by open squares. The expression given in Eq. (2) with the parameters of Eq. (3) give agreement with Robb to within 3%. Note that for ions heavier than Fe, relativistic effects are expected to be important and that the present expression represents results calculated in a nonrelativistic approximation. We are presently carrying out calculations which include relativistic effects.

Five-state close-coupling calculations for $\Omega(2s, 3l)$, $l = 0, 1, 2$ for C IV and Ar XVI given in Sec. II are combined with similar calculations on N V and Ne VIII by van Wyngaarden and Henry.[8,9] For $\Omega(2s, 3p)$, we fit the data to Eq. (2). We obtain

$$\left.\begin{aligned} c_0(z) &= -10 + 72z^{-1} - 170z^{-2},\\ c_1(z) &= 19 - 117z^{-1} + 275z^{-2},\\ c_2(z) &= 24 - 151z^{-1} + 302z^{-2}, \end{aligned}\right\} \text{ for } 2s, 3p. \tag{4}$$

For the dipole-forbidden, spin-allowed collision strength, we fit the data to the following form:

$$z^2\Omega(x) = d_0(z) + d_1(z)x^{-1} + d_2(z)x^{-2}, \tag{5}$$

where

$$\left.\begin{aligned} d_0(z) &= 10.4 - 13.3z^{-1} + 6.3z^{-2},\\ d_1(z) &= -3.1 + 5.8z^{-1},\\ d_2(z) &= 0, \end{aligned}\right\} \text{ for } 2s, 3s$$

and

$$\left.\begin{aligned} d_0(z) &= 31.7 - 49.9z^{-1},\\ d_1(z) &= -33.8 + 65.3z^{-1},\\ d_2(z) &= 19.0 - 45.4z^{-1}, \end{aligned}\right\} \text{ for } 2s, 3d. \tag{6}$$

Note that the data are only generated up to $x = 3$. For larger values of x, we have found that a unitarized Coulomb-Born approximation gives collision strengths within 20% of those calculated in a five-state close-coupling approximation.

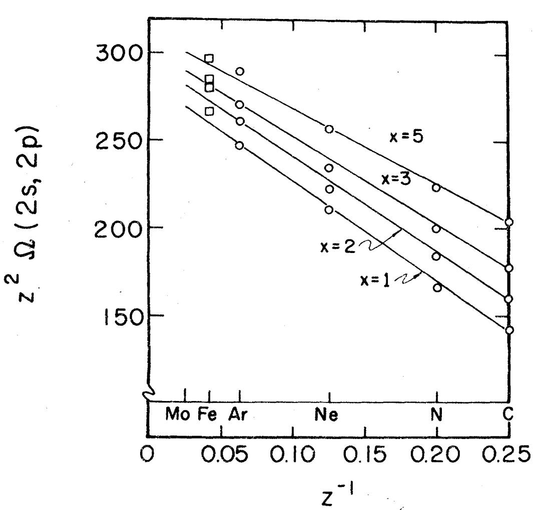

FIG. 2. $z^2\Omega(2s, 2p)$ vs z^{-1} for various x. Curves $x=1$; $x=2$; $x=3$; $x=5$. Open circles represent present calculations and those of van Wyngaarden and Henry (Refs. 8 and 9). Open squares represent calculations of Robb (Ref. 15).

The form chosen for the fits is similar to that given by Magee and Merts.[16] Equation (2) has the asymptotic behavior for large incident energy E of $Q_{i\to j} \sim E^{-1}\ln E$, which is the correct form for a dipole-allowed excitation cross section. In Eq. (5), $Q_{i\to j} \sim E^{-1}$, which is the correct form for a dipole-forbidden, spin-allowed excitation cross section. We emphasize that we have fitted by a least-squares procedure, data calculated primarily for $x \le 3$. The largest maximum error for the fit to the above functional forms is 4%. The forms chosen to represent the collision strengths are integrable analytically so that excitation rates may be derived easily.[16]

IV. POLARIZATION OF RESONANCE RADIATION

Figure 3 gives the theoretical percentage polarization P of the doublet resonance radiation in the direction at right angles to the direction of an incident electron beam. Two-state close-coupling results are used for Q_0 and Q_1, the excitation cross sections of the ^2P level with, respectively, the component $m=0$ and $m=1$ of the orbital angular momentum with respect to the beam axis. The expression used for P is[17]

$$P(\text{percent}) = \frac{300(9\alpha - 2)(Q_0 - Q_1)}{12Q_0 + 24Q_1 + (9\alpha - 2)(Q_0 - Q_1)}, \quad (7)$$

where the value of α depends on the ratio of the hyperfine structure energy separation to the natural linewidth, and is $\frac{4}{9}$ for C IV, Ne VIII, and Ar XVI since these ions have zero nuclear spin. For N V, we calculate 0.296 for α.

In Fig. 3, P is plotted as a function of x. The polarization changes sign near 9 times threshold energy. This behavior is similar to that for measurements on ions Ca^+, Ba^+, and Be^+ by Dunn and co-workers[11,18,19] and for neutral atoms. For example, Fano and Macek[20] connect the momentum transfer from an electron to the target with the collision-produced alignment of the excited target. At threshold, the momentum transfer should be along the electron direction and at high energy it should be dominantly transverse to the electron direction of motion. The corresponding polarization of emitted radiation should be positive near threshold and proceed to negative polarization at high energies. Near threshold energy,

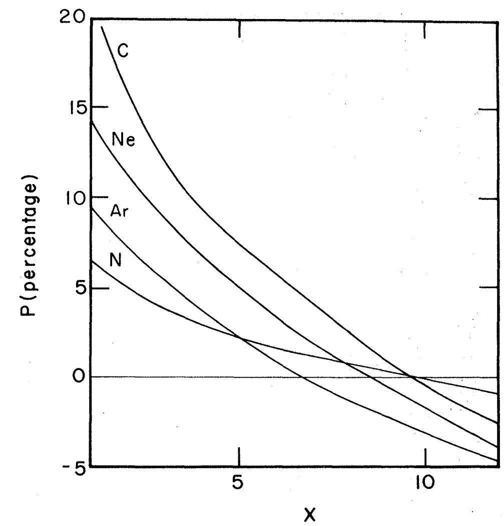

FIG. 3. Percentage polarization of resonance radiation vs energy in threshold energy units.

P may be expanded as follows

$$P = 42.9(1 - 2.57y + 4.04y^2 \cdots), \text{ for } \alpha = 0.444 \quad (8)$$

$$P = 15.7(1 - 2.84y + 5.24y^2 \cdots), \text{ for } \alpha = 0.296,$$

where $y = Q_1/Q_0$. For a neutral atom, only the s wave contributes at zero energy and so Q_1 vanishes. However, for a positive ion, more than one partial wave contributes at threshold due to the Coulomb interaction and so Q_1 does not vanish. Further, y increases with increasing z and this is consistent with Fig. 3, where we note that P decreases with increasing z at threshold for the same value of α.

ACKNOWLEDGMENTS

We are grateful for the computing facilities provided by the LSU Systems Network Computer Center. We calculated the polarization of resonance radiation using a program written by Dr. W. L. van Wyngaarden. We wish to thank Dr. W. L. van Wyngaarden, Dr. S. P. Rountree, Dr. D. Norcross, and Dr. J. Callaway for helpful conversations. We would like to thank P. O. Taylor *et al.* and the group at LASL for permission to cite their results prior to publication.

*Research supported in part by the U. S. Energy Research and Development Administration, Division of Physical Research, Contract No. AT-(40-1)-4881.

[1]E. Hinnov, J. Nucl. Matter 53, 9 (1974).
[2]D. M. Meade, Nucl. Fusion 14, 289 (1974).
[3]L. Heroux, Proc. Phys. Soc. Lond. 83, 121 (1964).
[4]W. N. Sams and D. J. Kouri, J. Chem. Phys. 51, 4809 (1969).
[5]E. R. Smith and R. J. W. Henry, Phys. Rev. A 7, 1585 (1973).

[6]A. W. Weiss, Astrophys. J. 138, 1262 (1963).
[7]A. Hibbert, Comput. Phys. Commun. 9, 141 (1975).
[8]W. L. van Wyngaarden and R. J. W. Henry, J. Phys. B 9, 1461 (1976).
[9]W. L. van Wyngaarden and R. J. W. Henry, Can. J. Phys. 54, 2019 (1976).
[10]P. O. Taylor, D. Gregory, G. H. Dunn, R. A. Phaneuf, and D. H. Crandall, Abstracts of Conf. on Atomic Processes in High Temperature Plasmas, 1977.
[11]P. O. Taylor, R. A. Phaneuf, and G. H. Dunn, quoted by M. A. Hayes, D. W. Norcross, J. B. Mann, and W. D. Robb, J. Phys. B (to be published).
[12]L. P. Presnyakov and A. M. Urnov, J. Phys. B 8, 1280 (1975).
[13]J. Callaway, D. Oza, J. N. Gau, and R. J. W. Henry, in Abstracts of the Tenth International Conference on the Physics of Electronic and Atomic Collisions, Paris (1977).
[14]N. H. Magee and A. L. Merts, J. B. Mann, and W. D. Robb, Los Alamos Scientific Laboratory report LA-6691-MS (1977).
[15]W. D. Robb (private communication).
[16]N. H. Magee and A. L. Merts, Abstracts of Conf. on Atomic Processes in High Temperature Plasmas, 1977.
[17]D. R. Flower and M. J. Seaton, Proc. Phys. Soc. Lond. 91, 59 (1967).
[18]P. O. Taylor and G. H. Dunn, Phys. Rev. A 8, 2304 (1973).
[19]D. H. Crandall, P. O. Taylor, and G. H. Dunn, Phys. Rev. A 10, 141 (1974).
[20]U. Fano and J. H. Macek, Rev. Mod. Phys. 45, 553 (1973).