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Effect of resonances on 2*s*-2*p* and 2*l*-3*l*′ excitation of Li-like ions by electron impact

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Collision strengths are calculated in a five-state close-coupling approximation for excitation of C^{3+}, O^{5+}, Ne^{7+}, and Ar^{15+} by electron impact for energies less than the 3*d* threshold. Resonance contributions enhance the allowed 2*p*-3*s* collision strength by larger factors than the enhancement of the forbidden 2*s*-3*s* collision strength. The resonance enhancement is approximately independent of nuclear charge Z for 2*s*-3*s*, 2*s*-3*p*, and 2*p*-3*p*, and increases nearly linearly with Z for 2*p*-3*s*. The average effect of resonance contributions to $\Omega(2s,2p)$ is only 4%.

Electron-impact excitation processes for multiply charged ions of the lithium isoelectronic sequence are of considerable interest in astrophysical[1] and magnetically confined[2] plasmas. Impurity ions in fusion plasmas, for example, play an important role in the overall energy balance of the high-temperature plasma, since they can cause significant energy losses in the form of line radiation.

Experimental measurements of 2*s*-2*p* cross sections for electron-impact excitation of Be^+, C^{3+}, and N^{4+} have been reported recently.[3–5] No evidence of significant resonance structure is present in these experiments on the strong optically allowed 2*s*-2*p* transition. Calculations by Callaway *et al.*[6] for C^{3+} at energies below the $n=3$ states confirmed that the average effect of resonances on 2*s*-2*p* cross sections is about 4%. Presnyakov and Urnov[7] used analytical properties of the Coulomb Green's function to obtain solutions to the scattering problem which have the correct asymptotic expansion in powers of the reciprocal of the ion charge. Their illustrative calculations for the 2*s*-3*s* and 2*p*-3*s* transitions in O^{5+} showed large enhancements of 2 and 30, respectively, due to resonances converging to 3*p* and 3*d* states. Our close-coupling calculations give the first definitive results for a multiply-charged ion where there is a very large resonance enhancement of allowed excitation process.

There are two factors which limit the accuracy of a close-coupling calculation for the collision strength. They are the description of the target function and the number of states included in the close-coupling approximation. For lithiumlike ions, a Hartree-Fock description is sufficiently accurate. We use orbitals obtained by Weiss.[8] We retain the 2*s*, 2*p*, 3*s*, 3*p*, and 3*d* states in the close-coupling expansion. Higher states will not significantly affect the collision strengths in the energy region below the 3*d* states. Collision strengths are related to cross sections by

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

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 integro-differential equations which arise in the close-coupling approximation are solved using a noniterative integral equation method.[9] Exchange terms are neglected at radial distances where the longest-ranged orbital has fallen to less than 10^{-3}. These equations are solved at five energies above the excitation energy for the 3*d* state.

In order to obtain the detailed resonance structures, the collision strengths are needed at a large number of energy points. Since direct computations are very expensive, we use the program RANAL[10] to yield detailed and averaged collision strengths. This program uses quantum-defect theory[11] to analyze the reactance matrix elements.

The collision strengths are computed for each different total spin and angular momenta and parity ($SL\pi$) states of the (electron plus ion) system which result on coupling the incident-free-electron partial wave l with the target state S_iL_i of the ion. The collision strength for a given transition is obtained on summing over all contributing $SL\pi$ states. A direct computation is made for O^{5+} for $SL\pi={}^1G$ in the energy range 5.85 to 5.92 Ry. Individual resonances at 5.851 and 5.91 Ry and groups of resonances near 5.88 Ry are obtained for this partial wave. The same positions are obtained from pro-

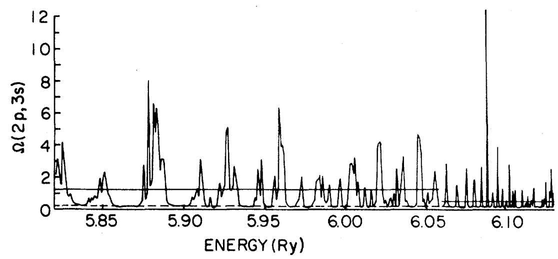

FIG. 1. $\Omega(2p,3s)$ vs k^2 (Ry). Dashed lines, nonresonance background; straight solid lines, Gailitis-average; solid line, unaveraged.

gram RANAL and the shape of the collision strength is similar.

The average effect of resonance contributions to $\Omega(2s,2p)$ is found to be only 4%. This is due to the fact that nonresonance contributions are dominated by large values of the orbital momentum of the scattered electron. Resonances due to the large l will be confined to a very narrow energy range just below the threshold energy of the closed channel, since their position will be $25/n^2$ below this channel and $n > l+1$ will be large. Further, the 2s and 2p states are more strongly coupled to each other than to the closed channels 3p or 3d, and so resonance enhancement is small.

Figures 1 and 2 give, respectively, collision strengths $\Omega(2p,3s)$ and $\Omega(2s,3s)$ for O^{5+} versus energy for the region between the 3s and 3d threshold. Dashed lines represent the nonresonant background collision strength, straight solid lines give the Gailitis-averaged[12] collision strength, and solid lines give the unaveraged collision strength. The dominant nonresonance contributions to $\Omega(2l,3s)$ come from partial waves $^1F^o$ and $^1P^o$. While these partial waves contribute significantly to the resonance part of $\Omega(2l,3s)$, other partial waves $^3P^o$, ^1D, ^1G, and ^3G also contribute substantially.

In Figs. 1 and 2, the enhancement of the allowed excitation $\Omega(2p,3s)$ is larger than that of the forbidden excitation $\Omega(2s,3s)$, in qualitative agreement with Presnyakov and Urnov.[7] This result is unexpected since other calculations suggest that forbidden excitations are affected more by resonances than allowed ones (e.g., Pradhan *et al.*[13] on heliumlike ions, Berrington *et al.*[14] on berylliumlike ions, van Wyngaarden and Henry[15] on *SV*). A simple explanation for the large enhancement is as follows. When the initial or final states are more strongly coupled to the closed channel than to each other, then the resonance effects will be large. The strength of coupling may be gauged by considering collision strengths for energies just above threshold for the highest state included in the close-coupling expansion.

This explanation is implicit in the Gailitis formula which may be used to obtain a qualitative estimate of the effect of resonances. Following the approach of Gailitis[12] and Seaton,[11] collision strengths may be averaged over resonances. Three assumptions are that the closed channels are degenerate, that the resonance widths are narrow compared with the resonance separations, and that the collision strengths are energy independent over the energy range of extrapolation. Then, the Gailitis formula, as given by Hershkowitz and Seaton,[16] is

$$\bar{\Omega}(i,j)=\Omega^{>}(i,j)+\sum_{i'}\frac{\Omega^{>}(i,i')\Omega^{>}(i',j)}{\sum_{i''}\Omega^{>}(i',i'')}\,, \quad (2)$$

where the sum i' is over degenerate closed channels of the new threshold, and i'' is summed over all open channels. Collision strengths $\Omega^{>}(i,j)$ are calculated above the new threshold and extrapolated to energies below this threshold.

The Gailitis formula differs from the Gailitis-averaged collision strengths obtained from program RANAL in that the program includes an interference term in the Gailitis expression[11,12] in addition to those terms given in Eq. (2).

Table I compares the resonance enhancement factor $\bar{\Omega}(i,j)/\Omega^{>}(i,j)$ for O^{5+} as calculated using RANAL and the Gailitis formula (2). For this case, interference effects are significant only for $\Omega(2s,3p)$ and $\Omega(2p,3p)$. We conclude that the simple Gailitis

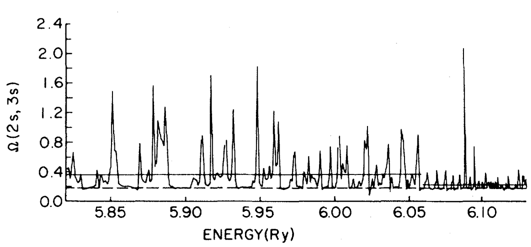

FIG. 2. $\Omega(2s,3s)$ vs k^2 (Ry). Legend as in Fig. 1.

TABLE I. Enhancement factors for O^{5+}.

	Below 3p threshold		Below 3d threshold	
	RANAL	Eq. (2)	RANAL	Eq. (2)
$\Omega(2s,3s)$	2.0	1.9	1.2	1.2
$\Omega(2p,3s)$	6.8	6.6	2.8	2.6
$\Omega(2s,3p)$			2.1	2.9
$\Omega(2p,3p)$			2.2	3.8

formula given by Eq. (2) gives a good qualitative estimate of the effect of resonances.

Collision strengths are given in Table II for O^{5+} at $k^2=6.25$ Ry (the $3d$ threshold is at 6.13 Ry). Consider the Gailitis formula applied to $\bar{\Omega}(2p,3s)$ below the $3p$ threshold,

$$\bar{\Omega}(2p,3s)=\Omega^{>}(2p,3s)+\frac{\Omega^{>}(2p,3p)\Omega^{>}(3p,3s)}{[\Omega^{>}(2s,3p)+\Omega^{>}(2p,3p)+\Omega^{>}(3s,3p)]}+\frac{\Omega^{>}(2p,3d)\Omega^{>}(3d,3s)}{[\Omega^{>}(2s,3d)+\Omega^{>}(2p,3d)+\Omega^{>}(3s,3d)+\Omega^{>}(3p,3d)]}\ .$$

[We have included $\Omega^{>}(3p,3d)$ in the denominator to account for nondegeneracy of the $3p,3d$ channels.] This formula, which is strictly only applicable when the $3p$ and $3d$ channels are degenerate, shows the dependence of the resonance effects $\Omega(2p,3s)$ on the other collision strengths between $2p,3s$ and the closed $3p,3d$ levels. In particular, since $\Omega^{>}(3s,3p)$ is dominant in the second term, the effect of the closed $3p$ channel is approximately given by $\Omega^{>}(2p,3p)$. Similarly, $\Omega^{>}(3p,3d)$ dominates the third term and the effect of the closed $3d$ channel is approximately given by $\Omega^{>}(2p,3d)$, i.e.,

$$\bar{\Omega}(2p,3s)\simeq\Omega(2p,3s)+\Omega^{>}(2p,3p)+\Omega^{>}(2p,3d)\ .$$

Also, the average effect on $2s\rightarrow3s$ may be estimated as

$$\bar{\Omega}(2s,3s)\simeq\Omega^{>}(2s,3s)+\Omega^{>}(2s,3p)+\Omega^{>}(2s,3d)\ .$$

Thus, while the effect of resonances is considerable on all transitions, the dominating role of $\Omega^{>}(2p,3d)$ is apparent. Since this couples to the allowed $\Omega(2p,3s)$ in this example, we can understand readily why the allowed $\Omega(2p,3s)$ is enhanced more than the forbidden $\Omega(2s,3s)$.

TABLE II. Collision strengths for Li-like ions at $1.109\Delta E(2s,3d)$.

Ω	C^{3+}	O^{5+}	Ne^{7+}	Ar^{15+}
$2s,2p$	9.78	4.76	2.69	0.611
$2s,3s$	0.386	0.180	0.105	0.0304
$2s,3p$	0.269	0.132	0.0815	0.0283
$2s,3d$	0.543	0.302	0.192	0.0584
$2p,3s$	0.406	0.132	0.0594	0.0103
$2p,3p$	1.329	0.548	0.309	0.0865
$2p,3d$	3.426	1.863	1.138	0.317
$3s,3p$	40.64	26.30	15.53	3.782
$3s,3d$	7.21	3.54	1.87	0.479
$3p,3d$	56.71	25.82	13.39	3.019

Table II also gives collision strengths for C^{3+}, Ne^{7+}, and Ar^{15+} at the same relative energy as O^{5+}, i.e., $1.019\Delta E(2s,3d)$. Figure 3 gives the resonance enhancement factors versus Z^{-1}, where Z is the nuclear charge. The enhancements for collision strengths $\Omega(2s,3s)$, $\Omega(2s,3p)$, and $\Omega(2p,3p)$ are approximately independent of Z, whereas $\Omega(2p,3s)$ increases nearly linearly with Z. The different dependence on Z for the enhancement of $\Omega(2p,3s)$ is a consequence of the different nonresonant behavior of $\Omega^{>}(2p,3s)$ with Z. This collision strength behaves approximately as $(Z-3.9)^{-2}$, whereas the others behave as $(Z-1.4)^{-2}$. This functional form is anticipated since $(Z-s)^2\ \Omega$ is approximately constant with Z. However, the screening constant s is normally bounded by $s=0$ (no screening) and $s=2$ (complete screening for Li-like ions).

It has been shown in the present work that the resonance contribution to excitation cross sections or collision strengths can be very important for allowed transitions as well as for forbidden ones. It is conjectured that a measure of the effect of resonances on a given collision strength $\Omega(i,j)$ may be obtained by comparing $\Omega(i,j)$ with $\Omega(i,k)$ and $\Omega(j,k)$, where k is the intermediate state which supports Rydberg series of resonances, and $\Omega(i,k)$ and $\Omega(j,k)$ are calculated at an energy just above thresh-

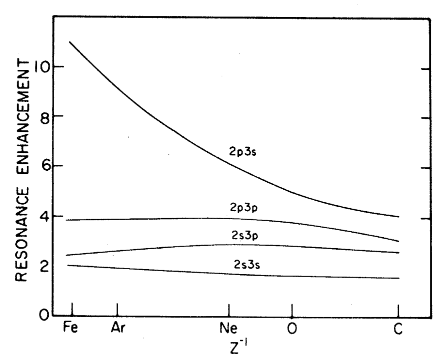

FIG. 3. Resonance enhancement vs Z^{-1}.

old for state k. Further, RANAL may produce an accurate representation of the detailed structure of resonances as evidenced by the agreement for positions and shapes of resonances obtained between a direct calculation and results from RANAL for one partial wave. Finally, the resonance enhancements along the Li-isoelectronic sequence are found to be independent of nuclear charge for $\Omega(2s,3s)$, $\Omega(2s,3p)$, and $\Omega(2p,3p)$ but the enhancement for $\Omega(2p,3s)$ increases approximately linearly with Z.

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