Cross Sections for Photoionization from Valence-Electron States

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IN order to study recombination processes in gaseous nebulae, one requires the coefficients for radiative recombination to many excited states of neutral atoms and positive ions. These may be calculated as functions of electron temperature once the corresponding photoionization cross sections are known.[1] For photoionization from valence-electron states a general formula has been obtained using a method which is an extension of that used by Bates and Damgaard[2] for bound-bound transition probabilities.

Rydberg energy units are used (13.60 ev or 109737 cm^{-1}). Let I_{nl} be the threshold energy for ejection of electron nl; k^2 the kinetic energy of the ejected electron; the photon energy is then $(I_{nl}+k^2)$. The effective quantum number n_l^* is defined by $I_{nl}=Z^2/n_l^{*2}$ and the quantum defect by $\mu_l(-I_{nl})=n_l^*-n$, Z being the residual charge on the ion. For the continuum states put $k^2=Z^2/\theta^2$. The photoionization cross section is

$$a_r(nl)=8.57\times10^{-19}\frac{(I_{nl}+k^2)}{I_{nl}^2}\sum_{l'=l\pm1}C_{l'}|g(n_l^*;\theta,l')|^2\ \text{cm}^2,$$

where, for alkali-like systems, $C_{l-1}=l/(2l+1)$ and $C_{l+1}=(l+1)/(2l+1)$. The matrix element is

$$g(n_l^*;\theta,l')=I_{nl}\int_0^\infty P(n_l^*;r)rF(k,l',Z;r)dr,$$

$P(n_l^*;r)$ being the normalized bound-state radial function and $F(k,l',Z;r)$ the continuum radial function having the asymptotic form

$$F(k,l',Z;r)\sim k^{-\frac{1}{2}}\sin\left[kr-\tfrac{1}{2}l'\pi+\frac{Z}{k}\ln(2kr)+\arg\Gamma\left(l'+1-\frac{iZ}{k}\right)+\delta_{l'}(k^2)\right].$$

The phase $\delta_{l'}(k^2)$ is zero for the pure Coulomb field.

The general formula depends on the relation $\delta_{l'}(k^2)=\pi\mu_{l'}(k^2)$, valid for $k\ll(2\pi Z)$, where $\mu_{l'}(k^2)$ is the quantum defect for the $n'l'$ series extrapolated as a function of energy.[3,4] The Bates and Damgaard functions $P(n_l^*;r)$ have been used together with approximate analytic functions $F(k,l',Z;r)$ having

TABLE I.

l	l'	$a_{ll'}$	$b_{ll'}$	$c_{ll'}$	$\alpha_{ll'}$	$\beta_{ll'}$
0	1	−0.147	+0.2515	−0.078	+0.310	0.000
1	0	−0.216	−0.171	0.000	0.000	0.000
1	2	−0.120	+0.600	0.000	+0.362	+0.0535
2	1	−0.247	−0.272	0.000	−0.010	−0.019
2	3	−0.117	+1.170	0.000	+0.321	+0.106
3	2	−0.362	+0.599	−2.432	−0.390	+0.050

TABLE II.

n_l^* \ $(l,l')=$	(0,1)	(1,0)	(1,2)	(2,1)	(2,3)	(3,2)
	$\gamma_{ll'}(n_l^*)$					
1	1.754	...	...	...	...	...
2	1.605	1.667	1.574	...	...	...
3	1.591	1.667	1.582	1.819	1.447	...
4	1.590	1.667	1.579	1.771	1.535	1.850
5	1.591	1.667	1.582	1.741	1.544	1.908
6	1.594	1.667	1.587	1.722	1.549	1.918
7	1.596	1.667	1.593	1.707	1.556	1.920
8	1.599	1.667	1.598	1.697	1.564	1.921
9	1.601	1.667	1.603	1.688	1.573	1.922
10	1.603	1.667	1.608	1.682	1.581	1.924
11	1.605	1.667	1.614	1.676	1.589	1.926
12	1.607	1.667	1.618	1.672	1.596	1.928

TABLE III.

n_l^* \ $(l,l')=$	(0,1)	(1,0)	(1,2)	(2,1)	(2,3)	(3,2)
	$G_{ll'}(n_l^*)$					
1	2.723	...	...	...	...	...
2	2.095	1.028	2.840	...	...	...
3	1.856	1.117	2.264	0.669	3.000	...
4	1.718	1.152	2.010	0.818	2.413	0.468
5	1.623	1.168	1.856	0.899	2.139	0.599
6	1.553	1.175	1.749	0.952	1.971	0.704
7	1.498	1.177	1.666	0.988	1.854	0.793
8	1.452	1.176	1.601	1.014	1.765	0.868
9	1.414	1.173	1.546	1.033	1.694	0.933
10	1.381	1.170	1.501	1.047	1.635	0.991
11	1.352	1.165	1.461	1.058	1.585	1.041
12	1.327	1.161	1.427	1.065	1.543	1.085

[1] M. J. Seaton, Monthly Notices Roy. Astron. Soc. **111**, 368 (1951).

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[3] M. J. Seaton, Compt. rend. **240**, 1317 (1955); Proc. Phys. Soc. (London) **A70**, 620 (1957).

[4] F. S. Ham, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1955), Vol. 1, p. 127.

correct asymptotic form. Extensive numerical calculations have been made for $(l,l')=(0,1)$, $(1,0)$, $(1,2)$, $(2,1)$, $(2,3)$, and $(3,2)$ and $(l+1)\leqslant n_l^*\leqslant 12$. The results obtained may be fitted to expressions of the form

$$g(n_l^*;\theta,l')=G_{ll'}(n_l^*)[1+(n_l^*/\theta)^2]^{-\gamma_{ll'}(n_l^*)}\times\cos\pi[n_l^*+\mu_{l'}(k^2)+\chi_{ll'}(n_l^*,\theta)],$$

$$\chi_{ll'}(n_l^*,\theta)=a_{ll'}+\frac{b_{ll'}}{n_l^*}+\frac{c_{ll'}}{n_l^{*2}}+\frac{(n^*/\theta^2)\alpha_{ll'}}{1+(n_l^*/\theta^2)}+\frac{(n^*/\theta)^2\beta_{ll'}}{1+(n_l^*/\theta)^2}.$$

In the approximation used g depends on θ^2 and on the effective quantum numbers but is otherwise independent of Z. The coefficients $a_{ll'}$, $b_{ll'}$, $c_{ll'}$, $\alpha_{ll'}$ and $\beta_{ll'}$ are given in Table I. The functions $G_{ll'}(n_l^*)$ and $\gamma_{ll'}(n_l^*)$ vary slowly with n_l^* and may be interpolated from the values for integer n_l^* given in Tables II and III.

The bound-bound matrix elements

$$\rho(n_l^*,n_{l'}^*)=\int P(n_l^*;r)rP(n_{l'}^*;r)dr$$

may be calculated for $n_{l'}^*\gg n_l^*$ using the relation

$$\rho(n_l^*,n_{l'}^*)=(n_l^{*2}/Zn_{l'}^{*\frac{3}{2}})(2/\pi)^{\frac{1}{2}}g(n_l^*;in_{l'}^*,l').$$

For $n_{l'}^*\geq(n_l^*+1.5)$ this gives results not differing significantly from those obtained by Bates and Damgaard. The accuracy of the photoionization general formula should be comparable with that of the Bates and Damgaard calculations for bound-bound transition probabilities.

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