Effects of radiative cascades on hydrogenlike dielectronic satellite spectra

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Effects of radiative cascades from higher-level satellite states on the intensities of dielectronic satellite lines of lower-lying states are investigated for selected hydrogenlike ions. The ratio of intensities of a particular satellite line from radiative cascades and from direct transitions is found to depend on the atomic number of the ion and the plasma temperature. For the most prominent satellite lines the increase in intensity is $\leq 6\%$. Results are reported for hydrogenlike Ne, Si, Ar, Ca, Ti, Cr, Fe, and Ni at various plasma temperatures.

I. INTRODUCTION

Consider a hydrogenlike ion in ground state $|g\rangle$; a free electron with energy ε collides with it and excites the 1s electron to a higher orbital n. In this process the electron may lose enough energy and is captured to form a heliumlike ion in an excited state $|s\rangle$. This state may either autoionize, reemitting an electron, or it may decay radiatively to some lower-energy state $|f\rangle$. The dielectronic recombination (DR) is achieved if the state $|f\rangle$ lies sufficiently low in energy and cannot autoionize,

$$1s+e \rightarrow nln'l' \rightarrow 1snl+h\nu \ . \qquad (1)$$

In the above process the final state $|f\rangle$ of the electron configuration $1snl$, which is stable against autoionization, may be reached in a series of radiative casdcades from some higher-energy state $|s\rangle$ of electron configurations $nln'l'$ with $n,n' \geq 2$. These higher-order processes boost up populations of all lower-lying intermediate states, increase intensities of dielectronic satellite lines which proceed directly as in Eq. (1), and add to the theoretical values of dielectronic recombination rate coefficients obtained in calculations which neglect such effects.

Dielectronic satellite spectra of hydrogenlike ions have been observed in tokamaks,[1,2] fusion microballoons,[3,4] and in solar flares.[5-8] The ratios of intensities of the resonance to satellite lines have been used to determine electron temperature and ion densities in the plasmas. Theoretical studies of intensities of dielectronic satellite lines and dielectronic recombination rate coefficients of hydrogenlike Mg, Fe, and Ti have been performed by Dubau *et al.*;[9,10] similar calculations have been done by Blanchet *et al.*[11] for Ca^{19+}. The multiconfiguration Thomas-Fermi model is used in both these calculations. Bitter *et al.*[12] have used the Z expansion technique to calculate the dielectronic satellite spectrum of hydrogenlike titanium. The effects of radiative cascades have been neglected in all these calculations except for Fe^{25+}, where Dubau *et al.*[10] report on the cascade contribution to dielectronic line intensities at a plasma temperature of 2×10^7 K. Gau *et al.*[13] have performed a calculation of dielectronic recombination rate coefficients of neonlike molybdenum which includes the effects of radiative cascades. While the effects of radiative cascades is estimated by Gau *et al.* to be of order 30% for neonlike molybdenum at $kT_e = 2.8$ keV; Dubau *et al.*[10] have reported this contribution for prominent satellite lines of hydrogenlike iron to be less than 5% at $kT_e = 1.7$ keV.

Here we report on a calculation of dielectronic satellite line intensities of selected hydrogenlike ions through a formulation which includes the effects from radiative cascades. The ions with atomic number 10, 14, 18, 20 22, 24, 26, and 28 have been considered; these elements are usually present in the laboratory and astrophysical plasmas as impurities or are injected purposely into laboratory plasmas for diagnostic reasons. The dependence of cascade contributions as a function of atomic number and plasma temperature is investigated. Calculations are done in intermediate coupling scheme with the inclusion of effects of configuration interaction.

II. THEORY

The intensity of a dielectronic satellite line is given by

$$I_d(s\text{-}f) = n_e n_g \alpha_d(s\text{-}f) \ , \qquad (2)$$

where n_e and n_g, are, respectively, the density of electrons and hydrogenlike ions in the ground state $|g\rangle$ of the plasma, and $\alpha_d(s\text{-}f)$ is the DR rate coefficient. Assuming a Maxwellian electron energy distribution one can obtain[14,15]

$$\alpha_d(s\text{-}f) = 1.656\times 10^{-22}(kT_e)^{-3/2}F_2^*(s\text{-}f) \times \exp(-E_s/kT_e) \qquad (3)$$

where kT_e, the product of electron temperature T_e and Boltzmann's constant k, is in eV. The satellite intensity factor $F_2^*(s\text{-}f)$ is defined as

$$F_2^*(s\text{-}f) = (g_s/g_g)A_a(s)A_r(s\text{-}f)/A_T(s) \ . \qquad (4)$$

g_s and g_g are, respectively, the statistical weights of the autoionizing state $|s\rangle$ and ground state $|g\rangle$, $A_a(s)$ is the autoionization rate of $|s\rangle$, $A_r(s\text{-}f)$ is the rate for radiative transition for $|s\rangle \rightarrow |f\rangle$, and

$$A_T(s)=A_a(s)+\sum_f A_r(s\text{-}f) .$$

Consider autoionizing states $|i\rangle, |j\rangle, |k\rangle, \ldots,$ situated above the state $|s\rangle$; it is easy to see that the effects of radiative cascades can be included by multiplying the right-hand side of Eq. (2) by

$$C_{\text{cas}}=1+[1/\alpha_d(s\text{-}f)]\left[\sum_i \alpha_d(i\text{-}s)\omega(s\text{-}f)+\sum_{\substack{i,j\\(j>i)}}\alpha_d(j\text{-}i)\omega(i\text{-}s)\omega(s\text{-}f)+\sum_{\substack{i,j,k\\(k>j>i)}}\alpha_d(k\text{-}j)\omega(j\text{-}i)\omega(i\text{-}s)\omega(s\text{-}f)+\cdots\right], \tag{5}$$

where the line fluorescence yield $\omega(k\text{-}j)$ is defined as

$$\omega(k\text{-}j)\equiv A_r(k\text{-}j)/A_T(k) .$$

The autoionization transition rate of an excited state $|s\rangle=|n_1l_1n_2l_2SLJ\rangle$ to a state $|g\rangle=|n_0l_0\varepsilon l_cS'L'J'\rangle$ in atomic units is given by

$$A_a(s\text{-}g)=2\pi(2l_1+1)(2l_2+1)(2l_0+1)(2l_c+1)$$
$$\times\left[(-1)^p\sum_k a_kR^k(n_1l_1n_2l_2;n_0l_0n_cl_c)+(-1)^q\sum_k b_kR^k(n_1l_1n_2l_2;n_cl_cn_0l_0\right]^2 ,$$

where $R^k(n_1l_1n_2l_2;n_3l_3n_4l_4)$ are Slater integrals,

$$p=l_1+l_0+L ,$$
$$q=l_1+l_0+S ,$$
$$a_k=\begin{Bmatrix} l_1 & l_2 & L\\ l_c & l_0 & k\end{Bmatrix}\begin{pmatrix} l_1 & k & l_0\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_2 & k & l_c\\ 0 & 0 & 0\end{pmatrix}$$

and b_k is obtained from a_k by interchanging the quantum numbers l_c and l_0.

X-ray transition rates in atomic units can be written as[16]

$$A(S'L'J'\text{-}SLJ)=\tfrac{4}{3}(\Delta E/c)^3|\langle S'L'J'||D||SLJ\rangle|^2 ,$$

where $|SLJ\rangle$ and $|S'L'J'\rangle$ are, respectively, the initial and final states of the system, ΔE is the energy difference between these states, c is the speed of light, D is the electric dipole operator, and $\langle S'L'J'||D||SLJ\rangle$ is the reduced matrix element. The reduced matrix element can be written as

$$\langle S'L'J'||D||SLJ\rangle=(-1)^{l_>-l}[(2J+1)(2J'+1)]^{1/2}(-1)^{S+L+J'+1}(l_>)^{1/2}\begin{Bmatrix} J' & 1 & J\\ L & s & L'\end{Bmatrix}I(n'l'\text{-}nl)R_{\text{mult}}(L'-L) ,$$

where

$$I(n'l'\text{-}nl)=\int_0^\infty P(nl,r)r^3P(n'l',r)dr$$

and $l_>$ is the maximum of l and l' in the electron jump $nl-n'l'$. A doubly excited heliumlike ion can decay through electric-dipole emission by one of the following transitions:

(i) $nln'l'\text{-}n_0l_0n'l', \quad n_0\le n\le n'$

(ii) $nln'l'\text{-}n_0l_0nl, \quad n_0\le n\le n'$

(iii) $nln'l'\text{-}nln''l'', \quad n\le n''\le n'$.

The multiplet factors $R_{\text{mult}}(L'\text{-}L)$ for these transitions are, respectively,

$$R(\text{i})=(-1)^{l_0+l'+L}[(2L+1)(2L'+1)]^{1/2}\times\begin{Bmatrix} l_0 & L' & l'\\ L & l & 1\end{Bmatrix},$$

$$R(\text{ii})=(-1)^{l_0+l'-S}[(2L+1)(2L'+1)]^{1/2}\times\begin{Bmatrix} l_0 & L' & l\\ L & l' & 1\end{Bmatrix},$$

and

$$R(\text{iii})=(-1)^{l+l'+L'}[(2L+1)(2L'+1)]^{1/2}\times\begin{Bmatrix} L' & l & l''\\ l' & 1 & L\end{Bmatrix}.$$

III. NUMERICAL CALCULATION

The radial one-electron orbitals were generated using the nonrelativistic Hartree-Fock-Slater atomic model. Doubly excited heliumlike configurations considered were $nln'l'$ with $n=2$, and 3; $n'=2$, 3, 4; and with all allowed values of l and l'. A total of 133 initial uncorrelated configuration state functions ϕ_i were obtained from angular momentum coupling. These ϕ_i served as the basis set for constructing a matrix representation of the total Hamiltonian

$$H=\sum_i[-\hbar^2/2m)\nabla_i^2-(Ze^2)/r_i-\xi(r_i)l_i\cdot s_i]+\sum_{\substack{i,j\\(i>j)}}(e^2/r_{ij}) .$$

TABLE I. The contributions of radiative cascades to intensities of satellite lines of $2l2l'$ configurations from higher-lying states for heliumlike ions of atomic number 10, 14, 18, 20, 22, 24, 26, and 28 at plasma temperatures corresponding approximately to maximum dielectronic recombination for the respective elements. The temperature T_e is in keV. The satellites are arranged in order of decreasing intensity (for heavier elements).

Array	Z / T_e / Key[a]	10	14	18	20	22	24	26	28
	T_e	0.6	1.1	1.8	2.1	2.6	3.0	3.6	4.0
		$100I_{cas}/I_{tot}$							
$2p^2(^1D_2)$-$1s2p(^1P_1)$	J	0.31	0.66	0.95	1.05	1.15	1.20	1.32	1.36
$2s2p(^1P_1)$-$1s2s(^1S_0)$	T	0.54	1.86	3.79	4.50	5.13	5.23	5.25	5.22
$2P^2(^3P_2)$-$1s2p(^3P_2)$	A	12.71	5.05	1.95	1.53	1.22	0.96	0.84	0.77
$2p^2(^1D_2)$-$1s2p(^3P_2)$	K			0.95	1.05	1.15	1.20	1.32	1.36
$2p^2(^3P_2)$-$1s2p(^3P_1)$	B	12.71	5.05	1.95	1.53	1.22	0.96	0.84	0.77
$2s2p(^3P_2)$-$1s2s(^3S_1)$	Q	1.18	1.66	2.37	2.74	4.33	6.10	8.12	10.84
$2s2p(^3P_1)$-$1s2s(^3S_1)$	R	1.40	4.46	9.70	10.28	9.82	8.80	9.08	9.37
$2s^2(^1S_0)$-$1s2p(^1P_1)$	O			1.11	1.21	1.29	1.37	1.45	1.52
$2p^2(^1S_0)$-$1s2p(^1P_1)$	M	4.40	3.86	2.29	1.54	1.06	0.62	0.50	0.43
$2p^2(^3P_2)$-$1s2p(^1P_1)$	G	12.71	5.05	1.95	1.53	1.22	0.96	0.84	0.77
$2s2p(^3P_0)$-$1s2s(^3S_1)$	S	1.05	1.25	0.82	0.86	0.99	1.13	1.47	1.45
$2s^2(^1S_0)$-$1s2p(^3P_1)$	P			1.11	1.21	1.29	1.37	1.45	1.52

[a]See Ref. 1.

TABLE II. Contributions from radiative cascades to the intensity of the J line of heliumlike titanium at a plasma temperature of 2.6 keV. The higher-energy states in column 1 decay radiatively to $2p^2(^1D_2)$ state with wavelengths given in column 2, and with a radiative transition rate given in column 4. The autoionization rate is presented in column 3, total x-ray rates in column 5, satellite intensity functions F_2^* in column 6, and dielectronic recombination rate coefficients in column 7. In the event these states decay radiatively to the $2p^2(^1D_2)$ state, they have a 43.36% chance of making it to the $1s2p(^1P_1)$ state, boosting up the intensity of the J line. Integers in square brackets in the last five colunms indicate powers of 10, e.g., $0.784[13]=0.784\times10^{13}$.

Higher state $\vert i\rangle$	Wavelength (Å)	Auger rate (sec^{-1})	X-ray rate $A_r(i\text{-}s)$ (sec^{-1})	Total x ray $\sum_f A_r(i\text{-}f)$ (sec^{-1})	$F_2^*(i\text{-}s)$ (per sec)	$\alpha_d(i\text{-}s)$ (10^{-13} cm^3/sec)
$2s3p(^3P_1)$	14.6525	0.784[13]	0.375[11]	0.633[14]	0.619[10]	0.149[−4]
$2p3d(^3P_1)$	14.1899	0.198[12]	0.219[12]	0.161[15]	0.404[9]	0.961[−6]
$2s3p(^1P_1)$	14.7450	0.868[12]	0.292[12]	0.997[14]	0.378[10]	0.911[−5]
$2p3s(^1P_1)$	14.2952	0.779[14]	0.128[13]	0.120[15]	0.759[12]	0.181[−2]
$2p3d(^1P_1)$	14.0493	0.102[13]	0.866[12]	0.159[15]	0.831[10]	0.197[−4]
$2p3d(^3D_1)$	14.3454	0.795[13]	0.389[11]	0.154[15]	0.287[10]	0.686[−5]
$2s3p(^3P_2)$	14.6201	0.531[13]	0.399[12]	0.566[14]	0.854[11]	0.205[−3]
$2p3s(^3P_2)$	14.4963	0.136[13]	0.175[12]	0.147[15]	0.399[10]	0.957[−5]
$2p3d(^3P_2)$	14.2409	0.458[11]	0.568[12]	0.155[15]	0.421[9]	0.100[−5]
$2p3d(^3F_2)$	14.4443	0.207[13]	0.796[12]	0.155[15]	0.262[11]	0.628[−4]
$2p3d(^3D_2)$	14.2493	0.102[13]	0.179[13]	0.160[15]	0.284[11]	0.679[−4]
$2p3d(^1D_2)$	14.3887	0.148[13]	0.374[13]	0.145[15]	0.954[11]	0.226[−3]
$2p3d(^3F_3)$	14.4244	0.496[13]	0.184[12]	0.152[15]	0.204[11]	0.489[−4]
$2p3d(^3D_3)$	14.2360	0.123[13]	0.639[12]	0.168[15]	0.163[11]	0.389[−4]
$2p3d(^1F_3)$	14.0777	0.211[14]	0.253[14]	0.177[15]	0.944[13]	0.224[−1]
$2s4p(^3P_1)$	10.7916	0.411[13]	0.334[11]	0.370[14]	0.502[10]	0.108[−4]
$2p4s(^3P_1)$	10.8056	0.732[12]	0.110[12]	0.987[14]	0.121[10]	0.260[−5]
$2p4d(^3P_1)$	10.7179	0.559[12]	0.910[11]	0.143[15]	0.530[9]	0.113[−5]
$2s4p(^1P_1)$	10.7569	0.104[14]	0.634[10]	0.854[14]	0.103[10]	0.221[−5]
$2p4s(^1P_1)$	10.6689	0.244[14]	0.429[12]	0.135[15]	0.988[11]	0.211[−3]
$2p4d(^1P_1)$	10.6021	0.177[11]	0.309[11]	0.154[15]	0.351[7]	0.747[−8]
$2p4d(^3D_1)$	10.6294	0.104[12]	0.567[11]	0.156[15]	0.567[8]	0.121[−6]
$2s4p(^3P_2)$	10.7832	0.235[13]	0.171[12]	0.407[14]	0.233[11]	0.500[−4]
$2p4s(^3P_2)$	10.6867	0.318[12]	0.294[12]	0.146[15]	0.159[10]	0.983[−5]
$2p4d(^3P_2)$	10.7287	0.242[12]	0.831[12]	0.120[15]	0.418[10]	0.893[−5]
$2s4f(^3F_2)$	10.7187	0.256[12]	0.685[11]	0.361[14]	0.120[10]	0.257[−5]
$2p4d(^3F_2)$	10.7401	0.803[12]	0.899[11]	0.139[15]	0.129[10]	0.275[−5]

TABLE II. (*Continued*).

Higher state $\lvert i \rangle$	Wavelength (Å)	Auger rate (sec^{-1})	X-ray rate $A_r(i\text{-}s)$ (sec^{-1})	Total x ray $\sum_f A_r(i\text{-}f)$ (sec^{-1})	$F_2^*(i\text{-}s)$ (per sec)	$\alpha_d(i\text{-}s)$ (10^{-13} cm^3/sec)
$2p4d(^3D_2)$	10.6405	0.396[12]	0.973[12]	0.157[15]	0.614[10]	0.131[−4]
$2p4d(^1D_2)$	10.6444	0.912[12]	0.496[11]	0.151[15]	0.745[9]	0.159[−5]
$2s4f(^3F_3)$	10.7175	0.678[12]	0.293[11]	0.321[14]	0.212[10]	0.452[−5]
$2p4d(^3F_3)$	10.7359	0.209[13]	0.934[11]	0.122[15]	0.552[10]	0.118[−4]
$2s4f(^1F_3)$	10.7148	0.861[11]	0.195[10]	0.703[13]	0.824[8]	0.176[−6]
$2p4d(^1F_3)$	10.6056	0.107[14]	0.802[13]	0.161[15]	0.175[13]	0.372[−2]
$2p4d(^3D_3)$	10.6423	0.115[13]	0.188[12]	0.156[15]	0.485[10]	0.103[−4]

Total DR rate coefficients from cascades $\sum \alpha_d(i\text{-}s)=0.290[-1]$
Total intensity contribution from cascades $I_{cas}=\sum \alpha_d(i\text{-}s)\omega(s\text{-}f)=0.126[-1]$
DR rate coefficient from direct transition $I_{dir}=0.108[+1]$
Percentage increase is $I_{cas}100/(I_{cas}+I_{dir})=1.15\%$

The mixing was allowed among configurations belonging to the same complex. Relativistic corrections were included in the diagonal terms $\langle \phi_i \mid H \mid \phi_i \rangle$. Atomic state functions $\psi_i=\sum_j c_{ij}\phi_j$ were obtained by diagonalizing the Hamiltonian. These wave functions were then used to calculate the transition rates and other atomic parameters through the formulations of Sec. II.

IV. RESULTS AND DISCUSSIONS

Contributions to intensities of satellite lines of $2l2l'$ configurations from higher-lying states are presented in Table I for heliumlike ions of atomic number 10, 14, 18, 20, 22, 24, 26, and 28 at plasma temperatures corresponding approximately to maximum dielectronic recombination for the respective ions. The satellite lines are listed in order of decreasing intensity for heavier elements. A systematic trend in satellite line intensities as a function of atomic number is clearly evident. For satellites *A*, *B*, *M*, and *G* the ratio of intensity from radiative cascades to the total intensity decreases with *Z*; for others there is an increase. The increase in intensity from radiative cascades is less than 10% for the prominent lines. For the *J* line, the strongest satellite corresponding to $2p^2(^1D_2)$-$1s2p(^1P_1)$ transition, the effect is only 0.3% for neon at plasma temperature 0.6 keV, increasing to about 1.4% for nickel at a temperature of 4 keV.

Table II contains the details of contributions from cascades to the intensity of the *J* line for titanium at plasma temperature 2.2 keV. It can be seen that there are many cascade satellites, but only a few contribute significantly. The contributions from $2pnd(^1F_3)$ and $2pns(^1P_1)$ are by far the largest. The effect of cascades from the $2l3l'$ complex is about an order of magnitude greater than cascades from $2l4l'$ configurations. Contributions from $2l5l'$ and other higher-lying configurations will be negligible. The contribution from the second term in the

TABLE III. Effect of radiative cascades on dielectronic satellite lines of hydrogenlike iron as a function of electron temperature. Each entry represents (intensity from cascades/intensity from direct transition)×100. Satellites are arranged in order of decreasing intensity.

Array	Key	1.7 a	1.0 b	2.0 b	3.0 b	4.0 b	5.0 b	6.0 b
		Electron temperature T_e in keV						
$2p^2(^1D_2)$-$1s2p(^1P_1$	*J*	0.79	0.53	1.00	1.25	1.39	1.49	1.55
$2s2p(^1P_1)$-$1s2s(^1S_0)$	*T*	2.63	2.22	4.17	5.16	5.74	6.12	6.38
$2P^2(_3P^2)$-$1s2p(^3P_2)$	*A*	0.44	0.33	0.63	0.79	0.88	0.94	0.98
$2p(^1D_2)$-$1s2p(^3P_2)$	*K*	0.79	0.53	1.00	1.25	1.39	1.49	1.55
$2p^2(^3P_2)$-$1s2p(^3P_1)$	*B*	0.44	0.33	0.63	0.79	0.88	0.94	0.98
$2s2p(^3P_2)$-$1s2s(^3S_1)$	*Q*	6.09	3.28	6.51	8.19	9.19	9.85	10.32
$2s2p(^3P_1)$-$1s2s(^3S_1)$	*R*	7.13	3.82	7.42	9.28	10.37	11.09	11.60
$2s^2(^1S_0)$-$1s2p(^1P_1)$	*O*	0.35	0.54	1.08	1.36	1.53	1.64	1.72
$2p^2(^1S_0)$-$1s2p(^1P_1)$	*M*	1.18	0.20	0.38	0.47	0.52	0.56	0.58
$2p^2(^3P_2)$-$1s2p(^1P_1)$	*G*	0.44	0.33	0.63	0.79	0.88	0.94	0.98
$2s2p(^3P_0)$-$1s2s(^3S_1)$	*S*	0.38	0.58	1.11	1.39	1.55	1.65	1.73
$2s2(^1S_0)$-$1s2p(^3P_1)$	*P*	0.35	.054	1.08	1.36	1.53	1.64	1.72

[a]Calculation using the Thomas-Fermi model, Ref. 10.
[b]Present calculation.

large parentheses of Eq. (5) was estimated to be about 2 orders of magnitude less than is obtained from the first term.

In Table III we present the relative contributions to the intensities of dielectronic satellite lines of hydrogenlike iron from radiative cascades and from direct transitions as a function of plasma temperature. Dubau *et al.*[10] have used the Thomas-Fermi model to calculate relative intensities of hydrogenlike iron at 2×10^7 K; their values are also listed in Table III for comparison. It has been pointed out by Bhalla and Karim[17] that there are systematic and significant discrepancies in theoretical values of satellite intensity functions $F_2^*(s\text{-}f)$ obtained from the Thomas-Fermi model, the Z-expansion technique, and the Hartree-Fock-Slater model. For $2lnl'$ $n=3$ and 4 satellites, Z-expansion values of F_2^* functions are typically $(1-30)\%$ higher than the Hartree-Fock-Slater calculations, while the Thomas-Fermi estimates are about $(10-40)\%$ lower. As is shown in Table II, calculation of effects of radiative cascades involves summations of DR rate coefficients over many weak satellite lines where the discrepancy is expected to be large. The modest agreement in Table III between our results (at 2 keV) and of Dubau *et al.*[10] is rather reasonable. The monotonic increase with electron temperature in the ratio of intensities from cascades and direct transitions can easily be understood: The ratio contains the factor $\exp[-(\varepsilon_i-\varepsilon_s)/kT_e]$ where ε_s and ε_i are, respectively the Auger electron energies corresponding to direct and cascade autoionizing states. Since $\varepsilon_i>\varepsilon_s$ this factor increases with kT_e. The reason for the increase or decrease of cascade contributions with the atomic number, however, is rather involved and depends on the details of individual transition rates.

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