Z dependence of atomic parameters for selected autoionizing states of two-electron ions

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X-ray and Auger transition rates from doubly excited $2p^2\,{}^1D_2$, $2s^2\,{}^1S_0$, $2p3p\,{}^1D_2$, $2p^2\,{}^3P_2$, and $2p4d\,{}^1F_3$ states of heliumlike ions are presented for $Z=10$, 14, 18, 20, 22, 24, 26, and 28. Intensity factors of x-ray satellites originating from dielectronic recombination of ground-state hydrogenic ions via the above autoionizing states are also calculated. The calculations are performed in the intermediate-coupling scheme with the inclusion of configuration interaction using the Hartree-Fock-Slater atomic model.

I. INTRODUCTION

In recent years there has been a considerable interest in doubly excited states of two-electron ions.[1-16] Such states have been observed in ion-atom collisions,[1-3] in single-photon or multiphoton absorptions of atoms,[4] and in laboratory[5-7] and astrophysical[8] plasmas. Theoretical investigations of doubly excited states of heliumlike ions, leading to identification and analysis of dielectronic satellite spectra obtained in tokamaks, solar flares, and fusion microballoons have been reported by a number of authors.[5,9-11] There has been also a continuing interest in such systems by many-body theorists. The identification and classification of doubly excited states of heliumlike ions with new sets of quantum numbers have been proposed by Cooper *et al.*,[12] Macek,[13] Lin,[14] and others.[15] Calculations of energies and widths of doubly and triply excited autoionizing states in helium isoelectronic sequence for $Z=5-10$ have been reported by Bachau.[16]

Multiply excited states of two-electron ions may be formed during collisions of atoms with highly stripped ions by double electron capture,[3] or by the process of electron transfer and excitation.[17] An atom in its ground state can be doubly excited by multiphoton absorption.[4] Dielectronic capture of electrons by hydrogenlike ions in high-temperature plasmas populates such states. The radiative deexcitation of such states produces satellite lines that lie on the higher-wavelength side of the Lyman-α ($2p\rightarrow 1s$) line. The ratio of intensity of satellite lines to resonance lines has been used[5] for diagnostic purposes.

We report here on a multiconfiguration Hartree-Fock-Slater calculation of radiative and autoionization transition rates for selected doubly excited states of two-electron ions with $Z=10$, 14, 18, 20, 22, 24, 26, and 28. Intensity factors of x-ray satellites which result from dielectronic recombination of ground-state hydrogenlike ions via these intermediate resonance states are also reported.

II. THEORY

The autoionization transition rates are given by

$$\Gamma_a=(2\pi/\hbar)\left|\left\langle\psi_f\left|\sum_{i>j}V_{ij}\right|\psi_i\right\rangle\right|^2\rho(\epsilon)\ . \tag{1}$$

Here, ψ_i and ψ_f are, respectively, the antisymmetrized many-electron wave functions of the initial and final states, $\rho(\epsilon)$ is the density of final state, and $V_{ij}=\sum 1/r_{ij}$ is the two-electron electrostatic operator. The matrix element of V_{ij} can be expressed as a weighted sum of radial Slater integrals,

$$\langle\psi_f\mid V_{ij}\mid\psi_i\rangle=\sum_k a_k R^k(n_1l_1,n_2l_2;n_3l_3,n_4l_4)\ , \tag{2}$$

where n_il_i represents the appropriate one-electron orbital. The derivation of angular coefficients a_k for doubly excited two-electron ions has been reported elsewhere by Karim and Bhalla.[10]

The transition probability for spontaneous emission of a photon of angular frequency ω is[18]

$$\Gamma_r(\gamma'J'-\gamma J)=\frac{4\omega^3}{3\hbar c^3}\frac{1}{2J+1}\mid\langle\gamma'J'\|D\|\gamma J\rangle\mid^2\ , \tag{3}$$

where γJ and $\gamma'J'$ represent, respectively, the initial and final states of the system, D is the electric-dipole operator, and $\langle\gamma'J'\|D\|\gamma J\rangle$ is the reduced matrix element. The reduced matrix element can be written as[19]

$$\langle S'L'J'\|D\|SLJ\rangle=(-1)^{l_>-l}(l_>)^{1/2}[(2J+1)(2J'+1)]^{1/2}(-1)^{S+L+J'+1}\begin{Bmatrix}J' & 1 & J\\ L & S & L'\end{Bmatrix}I(n'l'-nl)R_{\text{mult}}(L'-L)\ , \tag{4}$$

where

$$I(n'l'-nl)=\int_0^\infty P(nl,r)r^3P(n'l',r)dr \tag{5}$$

and $l_>$ is the larger of l and l'. A two-electron ion in configuration $nln'l'$ can decay radiatively by any of the following transitions:

$$nln'l'\rightarrow n_0l_0n'l',\quad n_0\le n\le n'\ , \tag{6a}$$

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$$nln'l' \rightarrow n_0 l_0 nl, \quad n_0 \le n \le n' , \tag{6b}$$

and

$$nln'l' \rightarrow nln''l'', \quad n \le n'' \le n' . \tag{6c}$$

The multiplet factors for each of the above transitions have been reported by Karim and Bhalla.[20]

The satellite intensity factor $F_2^*(f-i)$ is defined as[10]

$$F_2^*(f-i) = \frac{2J_i+1}{2J_f+1} \frac{\Gamma_a(i)\Gamma(j-i)}{\Gamma(i)} . \tag{7}$$

Here $|i\rangle$ is the intermediate resonance state formed as a result of dielectronic capture of an electron by a ground-state hydrogenlike ion, and $|f\rangle$ is a state to which this autoionizing state decays radiatively. For the dielectronic recombination process, the state $|f\rangle$ must lie below the first ionization threshold of the corresponding heliumlike ion. The total transition rate $\Gamma(i)$ is given by

$$\Gamma(i) = \sum \Gamma_a(i) + \sum_f \Gamma_r(f-i) . \tag{8}$$

III. NUMERICAL CALCULATION

The Hartree-Fock-Slater[21] atomic model was used to generate one-electron orbitals. Uncorrelated configuration state functions $\phi_i(\gamma SLJ)$ were used to construct a matrix representation of the nonrelativistic Hamiltonian including the spin-orbit interaction. Atomic-state functions were obtained by diagonalizing this Hamiltonian. A configuration $nln'l'$ was allowed to mix with all configurations $mlm'l'$ if $n+n'=m+m'$. Diagonal matrix elements $\langle \phi_i | H | \phi_i \rangle$ were corrected for relativistic effects.

IV. RESULTS AND DISCUSSIONS

Table I lists the radiative rates $\Gamma_r(j-i)$ for selected doubly excited states of heliumlike ions for $Z=10$, 14, 18, 20, 22, 24, 26, and 28. The autoionization rates $\Gamma_a(i)$ and satellite intensity factors $F_2^*(f-i)$ are listed, respectively, in Tables II and III. We have included those transitions which are either the dominant channels in dielectronic recombination, or are expected to exhibit significant variation in atomic parameters as a function of atomic number Z. The radiative transitions $2p^2\,{}^1D_2-1s2p\,{}^1P_1$, $2s2p\,{}^1P_1-1s2s\,{}^1S_0$, and $2p^2\,{}^3P_2-1s2p\,{}^3P_2$ of the $2l2l'$ complex constitute the dominant dielectronic satellite lines. The radiative transitions $2p^2\,{}^1D_2-1s2p\,{}^3P_2$, $2p^2\,{}^3P_2-1s2p\,{}^1P_1$, and $2s^2\,{}^1S_0-1s2p\,{}^3P_1$ are spin forbidden. The state $2s^2\,{}^1S_0$ can decay to the $1s2p\,{}^3P_1$ state by the configuration mixing with $2p^2\,{}^1S_0$. The transitions $2p3p\,{}^1D_2-1s3p\,{}^1P_1$, $2p3s\,{}^1P_1-1s3s\,{}^1S_0$, $2p4p\,{}^1D_2-1s4p\,{}^1P_1$, and $2p4d\,{}^1F_3-1s4d\,{}^1D_2$ are the dominant recombination channels in their respective complexes.

The variations of radiative and Auger transition rates with Z for a few autoionizing states of heliumlike ions are

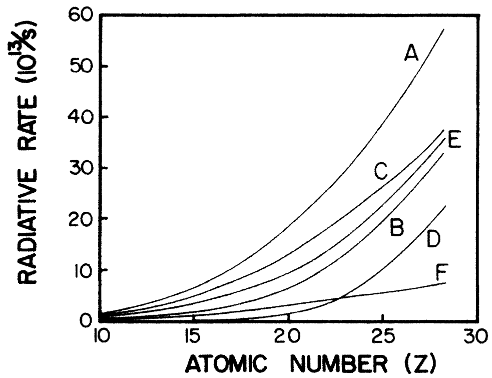

FIG. 1. Radiative transition rates for selected autoionizing states of heliumlike ions as a function of Z. The lines are identified as A, $2p^2\,{}^1D_2-1s2p\,{}^1P_1$; B, $2p3p\,{}^1D_2-1s3p\,{}^1P_1$; C, $2p^2\,{}^3P_2-1s2p\,{}^3P_2$; D, $2p^2\,{}^1D_2-1s2p\,{}^3P_2$; E, $2p4d\,{}^1F_3-1s4d\,{}^1D_2$; and F, $2s^2\,{}^1S_0-1s2p\,{}^1P_1$.

TABLE I. X-ray transition rates (in units of $10^{13}\ \mathrm{s}^{-1}$) for selected states of doubly excited heliumlike ions of atomic number ($Z=$) 10, 14, 18, 20, 22, 24, 26, and 28. The configurations considered here are of the type $2lnl'$, $n=2$, 3, and 4.

Transitions $\lvert i\rangle$ $\lvert f\rangle$	10	14	18	20	22	24	26	28
$2p^2\,{}^1D_2-$ $1s2p\,{}^1P_1$	1.14	4.49	12.11	18.10	25.42	34.06	43.43	55.95
$2s2p\,{}^1P_1-$ $1s2s\,{}^1S_0$	0.55	2.20	6.15	9.45	13.89	19.70	27.09	36.25
$2p^2\,{}^3P_2-$ $1s2p\,{}^3P_2$	0.86	3.38	8.99	13.29	18.29	23.86	29.29	36.70
$2p^2\,{}^1D_2-$ $1s2p\,{}^3P_2$	0.00	0.00	0.54	1.36	3.32	6.98	13.52	21.29
$2p^2\,{}^3P_2-$ $1s2p\,{}^3P_1$	0.29	1.15	3.31	5.23	8.00	11.93	17.35	24.83
$2s2p\,{}^3P_2-$ $1s2s\,{}^3S_1$	0.54	2.18	6.14	9.48	14.03	20.08	27.94	37.94
$2s2p\,{}^3P_1-$ $1s2s\,{}^3S_1$	0.54	2.17	6.10	9.37	13.77	19.53	26.84	35.90
$2s^2\,{}^1S_0-$ $1s2p\,{}^1P_1$	0.24	0.93	2.27	3.17	4.16	5.18	6.03	7.28
$2p^2\,{}^1S_0-$ $1s2p\,{}^1P_1$	0.93	3.67	10.49	16.39	24.63	35.82	50.87	70.15
$2p^2\,{}^3P_2-$ $1s2p\,{}^1P_1$	0.00	0.00	0.40	1.00	2.50	5.26	10.30	15.60
$2s2p\,{}^3P_0-$ $1s2s\,{}^3S_1$	0.54	2.17	6.12	9.43	13.95	19.94	27.70	37.57
$2s^2\,{}^1S_0-$ $1s2p\,{}^3P_1$	0.00	0.00	0.23	0.53	1.20	2.39	4.76	7.28
$2p3p\,{}^1D_2-1s3p\,{}^1P_1$	0.36	1.17	3.82	6.44	10.43	16.14	23.30	32.01
$2p4p\,{}^1D_2-1s4p\,{}^1P_1$	0.29	0.78	5.08	8.45	12.95	18.69	25.82	34.61
$2p3s\,{}^1P_1-$ $1s3s\,{}^1S_0$	0.28	1.06	3.31	5.16	8.00	12.13	17.73	25.04
$2p3d\,{}^1F_3-1s3d\,{}^1D_2$	0.61	2.13	4.92	6.89	9.32	12.30	15.93	20.36
$2p4d\,{}^1F_3-1s4d\,{}^1D_2$	0.64	2.39	6.30	9.43	13.60	19.06	26.01	34.75

TABLE II. Auger transition rates (in units of 10^{13} s^{-1}) for selected states of doubly excited heliumlike ions of atomic number ($Z=$) 10, 14, 18, 20, 22, 24, 26, and 28.

Autoionizing states	10	14	18	20	22	24	26	28
$2p^2\,{}^1D_2$	30.28	33.56	32.95	30.91	29.87	28.15	24.87	23.23
$2s2p\,{}^1P_1$	16.19	17.44	18.07	18.12	18.24	18.62	18.57	18.45
$2p^2\,{}^3P_2$	0.04	0.34	1.95	3.14	5.38	8.16	11.38	13.35
$2s2p\,{}^3P_2$	1.25	1.32	1.34	1.31	1.34	1.37	1.37	1.37
$2s2p\,{}^3P_1$	1.26	1.33	1.41	1.45	1.58	1.76	1.96	2.21
$2s^2\,{}^1S_0$	29.15	31.01	31.38	30.83	31.51	31.39	31.01	30.72
$2p^2\,{}^1S_0$	1.23	1.69	2.21	2.35	2.81	3.33	3.83	4.27
$2s2p\,{}^3P_0$	1.25	1.32	1.34	1.31	1.34	1.37	1.37	1.37
$2p3p\,{}^1D_2$	7.85	7.16	9.91	10.53	11.58	12.29	12.08	12.61
$2p4p\,{}^1D_2$	2.30	2.15	4.80	4.97	5.15	5.14	5.08	5.00
$2p3s\,{}^1P_1$	0.02	0.05	7.90	7.73	7.79	7.81	7.64	7.28
$2p3d\,{}^1F_3$	1.81	2.08	2.14	2.08	2.11	2.07	2.02	1.96
$2p4d\,{}^1F_3$	1.05	1.12	1.11	1.06	1.07	1.06	1.05	1.04

shown, respectively, in Figs. 1 and 2. The satellite intensity factors for hydrogenlike ions that proceed via these doubly excited states are plotted as a function of Z in Fig. 3. The selected transitions are identified in Fig. 1 and Fig. 3 as

$$
\begin{aligned}
&(\mathrm{A})\quad 2p^2\,{}^1D_2-1s2p\,{}^1P_1\ ,\\
&(\mathrm{B})\quad 2p3p\,{}^1D_2-1s3p\,{}^1P_1\ ,\\
&(\mathrm{C})\quad 2p^2\,{}^3P_2-1s2p\,{}^3P_2\ ,\\
&(\mathrm{D})\quad 2p^2\,{}^1D_2-1s2p\,{}^3P_2\ ,\\
&(\mathrm{E})\quad 2p4d\,{}^1F_3-1s4d\,{}^1D_2\ ,\\
&(\mathrm{F})\quad 2s^2\,{}^1S_0-1s2p\,{}^1P_1\ .
\end{aligned}
\tag{9}
$$

The electric dipole transitions are A, B, C, and E. The transition rates for these lines are seen to increase rapidly with Z. This behavior is expected: Transition energies increase approximately as $(Z-\sigma)^2$ where σ is a screening parameter, whereas the radial dipole integrals $I(n'l'-nl)$ in Eq. (5) decrease roughly as Z; the radiative transition rates in Eq. (3) therefore should increase approximately as $(Z-\sigma)^6/Z^2$. The transition D is spin forbidden and is seen to have negligible strength up to $Z=22$, after which it rises steeply. Inclusion of the spin-orbit interaction in evaluating atomic parameters for heliumlike ions is therefore warranted for $Z\geq 22$. Both the spin-orbit coupling and configuration interaction are responsible in the creation of the line F; the strength of this line is seen to increase slowly but steadily with Z.

The autoionization of the doubly excited states involves the transition $2lnl'-1s\epsilon l''$ where $\epsilon l''$ represents the continuum electron. The identification of Auger lines

TABLE III. Satellite intensity factors $F_2^*(f-i)$ (in units of 10^{13} s^{-1}) of dielectronic recombination for ground-state hydrogenlike ions with $Z=10$, 14,18, 20, 22, 24, 26, and 28 which proceed via selected autoionizing states of heliumlike ions.

Stabilizing transitions $\vert i\rangle$ $\vert f\rangle$	10	14	18	20	22	24	26	28
$2p^2\,{}^1D_2-$ $1s2p\,{}^1P_1$	2.75	9.90	21.88	27.77	32.39	34.63	32.96	32.30
$2s2p\,{}^1P_1-$ $1s2s\,{}^1S_0$	0.79	2.92	6.88	9.29	11.75	14.19	16.19	17.76
$2p^2\,{}^3P_2-$ $1s2p\,{}^3P_2$	0.07	0.59	2.99	4.60	7.20	9.89	12.19	13.54
$2p^2\,{}^1D_2-$ $1s2p\,{}^3P_2$	0.00	0.00	0.97	2.08	4.23	7.09	10.26	12.29
$2p^2\,{}^3P_2-$ $1s2p\,{}^3P_1$	0.02	0.20	1.10	1.81	3.15	4.95	7.22	9.16
$2s2p\,{}^3P_2-$ $1s2s\,{}^3S_1$	0.94	2.05	2.75	2.87	3.06	3.21	3.27	3.32
$2s2p\,{}^3P_1-$ $1s2s\,{}^3S_1$	0.57	1.24	1.72	1.87	2.10	2.38	2.66	2.99
$2s^2\,{}^1S_0-$ $1s2p\,{}^1P_1$	0.12	0.45	1.05	1.42	1.78	2.09	2.24	2.36
$2p^2\,{}^1S_0-$ $1s2p\,{}^1P_1$	0.26	0.58	0.91	1.03	1.26	1.52	1.78	2.01
$2p^2\,{}^3P_2-$ $1s2p\,{}^1P_1$	0.00	0.00	0.13	0.35	0.98	2.18	4.29	5.75
$2s2p\,{}^3P_0-$ $1s2s\,{}^3S_1$	0.19	0.41	0.55	0.57	0.61	0.64	0.65	0.66
$2s^2\,{}^1S_0-$ $1s2p\,{}^3P_1$	0.00	0.00	0.11	0.24	0.51	0.96	1.76	2.49
$2p2p\,{}^1D_2-1s3p\,{}^1P_1$	0.85	2.37	6.13	8.56	11.34	13.82	15.05	16.48
$2p4p\,{}^1D_2-1s4p\,{}^1P_1$	0.60	1.01	5.50	6.87	7.91	8.43	8.66	8.72
$2p3s\,{}^1P_1-$ $1s3s\,{}^1S_0$	0.02	0.05	3.0	3.79	4.73	5.65	6.29	6.54
$2p3d\,{}^1F_3-1s3d\,{}^1D_2$	1.53	3.15	3.70	3.56	3.49	3.28	3.06	2.85
$2p4d\,{}^1F_3-1s4d\,{}^1D_2$	1.36	2.52	2.95	2.92	2.97	2.95	2.92	2.88

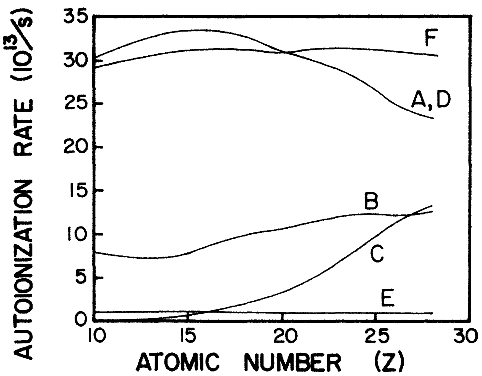

FIG. 2. Auger transition rates for selected autoionizing states of heliumlike ions as a function of Z. The states are identified as A and D, $2p^2\,^1D_2$; B, $2p3p\,^1D_2$; C, $2p^2\,^3P_2$; E, $2p4d\,^1F_3$; and F, $2s^2\,^1S_0$.

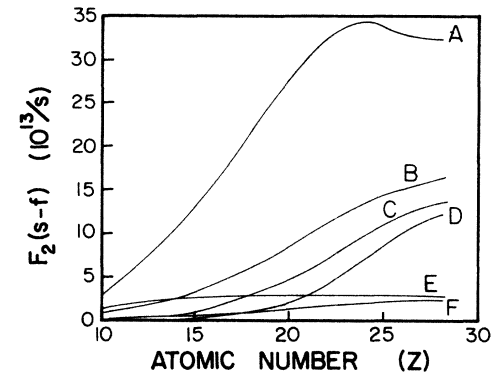

FIG. 3. Satellite intensity factors $F_2^*(f-i)$ for dielectronic recombination of ground-state hydrogenline ions which proceed via selected autoionizing states of heliumlike ions. For line identification see caption of Fig. 1.

in Fig. 2 is similar to those in Eq. (9); the final ionic state here, however, is always $1s\,^2S_{1/2}$. The radial Auger matrix elements $R^k(2l,nl';1s\epsilon l'')$ increase extremely slowly with Z so that the autoionization rate is nearly insensitive to the atomic number Z. This behavior is exhibited for the transitions E, B, and F, in Fig. 2. The transition C is possible because of the spin-orbit mixing of the state $2p^2\,^3P_2$ with $2p^2\,^1D_2$. The decrease in the intensity of line A and the increase in the intensity of C at about $Z=18$ are thus concerted: The spin-orbit interaction is switching part of the intensity of channel A to channel C.

The dependence of the satellite intensity factor $F_2^*(f-i)$ on the atomic number Z is rather involved and can be best understood by rewriting Eq. (7) as

$$F_2^*(f-i)=\frac{2J_i+1}{2J_f+1}\frac{\omega(f-i)a(i)}{T(i)}\ , \tag{10}$$

where $\omega(f-i)=\Gamma_r/\Gamma(i)$ is the line fluorescence yield for the transition $|i\rangle\rightarrow|f\rangle$, $a(i)=\Gamma_a/\Gamma(i)$ is the total Auger yield for the $|i\rangle$, and $T(i)$ is the lifetime of the state $|i\rangle$. Since

$$a(i)+\sum_f \omega(f-i)=1\ ,$$

Eq. (10) suggests that $F_2^*(f-i)$ will be large when the Auger and fluorescence yields are comparable, and when the lifetime of the state $|i\rangle$ is short. From Figs. 1 and 2 it is seen that autoionization is the dominant decay channel for $Z\leq 20$; for $Z=22-26$ the strengths of the two channels become comparable. For even higher Z the radiative channel becomes dominant. Accordingly, the satellite intensity functions A, B, C, and D in Fig. 3 increase with Z, reach a plateau near $Z=24$, and then fall off slowly. The autoionization channel for line E has a negligible strength which remains fairly constant with Z, whereas the radiative channel increases sharply with Z. The line F on the other hand has a strong and approximately Z-independent autoionization rate, and a very weak radiative channel which slowly gains strength with Z. The $F_2^*(f-i)$ functions for both these lines therefore remain small over the range of Z considered here. At even higher Z, the line E is expected to dip further while the line F will slowly pick up strength.

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