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The Calculated Power Output from a Thin Iron-Seeded Plasma

by

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THE CALCULATED POWER OUTPUT FROM A THIN IRON-SEEDED PLASMA

by

A. L. Merts, Robert D. Cowan, and N. H. Magee, Jr.

ABSTRACT

Ionization equilibrium calculations are carried out for iron ions at a density of 10^{12} cm^{-3} in a (hydrogen) plasma with electron density 10^{14} cm^{-3} , at temperatures from 0.8 to 10 keV. The computed radiated power loss from this plasma due to the iron ions ranges from about 4 W/cm^3 at the lowest temperature to about 0.4 W/cm^3 at the highest temperature; loss rates for other electron and iron densities will scale approximately as $N_e N_{\text{Fe}}/10^{26}$. The losses are due principally to collisionally excited line radiation (especially $\Delta n = 0$ transitions) at low temperatures, and to collisionally excited $\Delta n \neq 0$ transitions and to continuum radiative recombination at high temperatures. Spectra are also computed for diagnostic x-ray K_{α} (1s - 2p) transitions; the change in spectral distribution as a function of temperature agrees well with observations in the ST Tokamak. Bound-bound radiative transitions and dielectronic recombination are discussed at length in appendices; the latter process is of great importance in the establishment of ionization equilibrium, and in the excitation of K_{α} radiation at the lower temperatures.

I. INTRODUCTION

In laboratory hydrogen plasma experiments, heavy element atoms from the walls and other parts of the container are sputtered into the plasma. These atoms become totally or partially ionized; the partially ionized atoms are especially effective emitters. The power loss due to line radiation from partially ionized ions becomes a serious problem when the concentration of heavy elements is as large as 1%. Here we will mean by heavy element any element with $Z \geq 26$.

We give a breakdown of the calculated power loss according to the mechanism producing it. It will be shown that, for the plasmas considered in this report, the most important process for producing radiation is electron collisional excitation followed by spontaneous radiative decay. However, the important processes involved in establishing the steady state of the plasma are electron impact ionization and dielectronic recombination. For very high stages of ionization (hydrogenic ions and He-

like ions), radiative recombination may become more important than dielectronic recombination.

The importance of bound-bound transitions and of dielectronic recombination is sufficiently great that we have devoted Appendices A and B to these matters. These Appendices are sufficiently comprehensive to give the reader an appreciation of the calculational methods used for these important processes.

II. COLLISIONAL IONIZATION

The experimental situation for cross sections for highly ionized atoms is at present a total absence of data. There do exist in the literature some data for a few ions in stages of ionization less than about ten. For lack of anything better at the moment we have used a formula due to Lotz.¹ For atoms and not too highly ionized ions, Lotz fit the rather skimpy experimental data with a three-parameter equation

$$Q(E) = \sum_j a_j \frac{q_j}{I_j E} \ln\left(\frac{E}{I_j}\right) \times \left\{ 1 - b_j \exp\left[-c_j \left(\frac{E}{I_j} - 1\right)\right] \right\}.$$

E is the energy of the incident electron, the summation is over all shells of the atom, and q_j and I_j are the electron occupation and ionization energy of the j^{th} shell. The three parameters can of course provide a satisfactory fit for any particular atom for which good experimental data are available. Lotz, however, presented tables of smoothed values for calculation for all elements; as a result we would expect errors up to roughly a factor of two.

For ions more highly ionized, for lack of anything better, we use the simpler formula (also due to Lotz²):

$$Q(E) = 4.5 \times 10^{-14} \sum_j \frac{q_j}{I_j E} \ln\left(\frac{E}{I_j}\right) \text{ cm}^2, \quad (1)$$

where E and I_j are in electron volts. The ionization rate coefficient is the Maxwellian average of $vQ(E)$:

$$\alpha_1 = 3.0 \times 10^{-6} \sum_j \frac{q_j}{I_j \sqrt{kT}} E_1\left(\frac{I_j}{kT}\right) \text{ cm}^3/\text{sec}, \quad (2)$$

where I_j and kT are in electron volts, and E_1 is the exponential integral of index one.

III. COLLISIONAL EXCITATION

Electron impact excitation cross sections for excitations in which the principal quantum number of the active electron does not change are the most important cross sections in determining the radiation loss from dilute plasmas. One equation for the excitation cross section is

$$Q(E) = \frac{8\pi}{\sqrt{3}} \frac{1}{E} \frac{1}{\Delta E} f_g^- \pi a_0^2, \quad (3)$$

where E is the energy of the incident electron in rydbergs, ΔE is the excitation energy for the

transition in rydbergs, f is the optical oscillator strength, and $\bar{g}$ is the effective Gaunt factor which brings about agreement with experiment or any correct theory. Van Regemorter³ used experimental data for the $1s-2p$ transition of the H atom to obtain a curve for $\bar{g}$ vs energy. For excitation of light ions by electrons with E less than about three times threshold, he used data from distorted-wave calculations by Vainstein; although there was much variation in $\bar{g}$ between various ions, the variation in energy was somewhat slow, and Van Regemorter chose a constant value of 0.2 for $\bar{g}$, for F up to about three times threshold. For higher energies he used the same $\bar{g}$ values obtained for the hydrogen atom.

The value of 0.2 proposed by Van Regemorter was believed to be accurate to within a factor of about two.

Bely carried out a study of various lithium-like ions using a Coulomb-Born approximation. His cross-section results agreed moderately well with various other calculations including one done with a strong-coupling method, but differed from the Van Regemorter prediction. For example, with the $\bar{g} = 0.2$ method the cross section appears to be too small by a factor of about 4 for the $2s + 2p$ transition in N V, and too large by an equal factor for $2s + 3p$.

Bely⁴ has fit his cross-section results to obtain $\bar{g}$. His expression for $\bar{g}$ is given by the three-parameter expression

$$\bar{g} = \frac{6\sqrt{3}}{8\pi} A \left[1 + B \log\{1 + C(X - 1)\} \right], \quad (4)$$

where X is the energy in units of ΔE , the threshold energy, and the parameters A , B , C show a smooth dependency on the ionic charge z . This formula appears to be reliable, and we have used the Bely formula to correct the Van Regemorter rate coefficients by a factor of 4 for $2s-2p$ transitions and to obtain a correction factor varying linearly between 0.5 (for $n = 2-3$) to 1.0 (for $n = 2-8$).

The collisional excitation rate can be obtained by averaging the cross section multiplied by the velocity of the electron over a Maxwellian distribution. Van Regemorter obtains for the deexcitation rate coefficient of an electric-dipole-allowed transition

$$\alpha_{n'n} = 20.60 \lambda_{\text{cm}}^3 T^{-1/2} P(\Delta E/kT) A_{n'n} \quad (5) \quad \alpha_r = 2.6 \times 10^{-14} \frac{1}{g_1}$$

Here λ_{cm} is the wavelength in cm, T is the electron temperature in $^{\circ}\text{K}$, $A_{n'n}$ is the Einstein coefficient (sec^{-1}) for the transition and $P(\Delta E/kT)$ is a slowly varying function given in Table II of the Van Regemorter paper. Note that Eq. (5) still must be multiplied by the above-mentioned correction. From detailed balancing arguments one gets a relation between the collisional deexcitation coefficients $\alpha_{n'n}$ and the collisional excitation coefficients $\alpha_{nn'}$:

$$\alpha_{n'n} = \alpha_{nn'} (g_n/g_{n'}) \exp(E_n - E_{n'}/kT) \quad (6)$$

IV. FREE-BOUND RECOMBINATIONS

The interaction between a free electron and a positively charged ion can lead to capture of the electron. Energy released in this recombination process by the emission of a prompt or delayed photon may escape and therefore represent an energy loss from the plasma. For dilute plasmas, the radiative free-bound and dielectronic recombination processes are also important ones which counterbalance collisional ionization in determining the steady state of the plasma; therefore, these processes should be considered in energy loss calculations.

A. Radiative Recombination

The radiative free-bound rate coefficients are calculated by performing the thermal average $\langle v \sigma_{f-b}(v) \rangle$, where σ_{f-b} is the cross section for radiative capture of the free electron, v is the thermal velocity of the free electron, and the average is over a Maxwellian distribution of velocities for the free electrons.

The cross section σ_{f-b} can be obtained from calculations of bound-free absorption cross sections and the use of detailed balance arguments. However, for present calculations it proved adequate to use the Kramers formula which leads to the following rate coefficient:

$$\times \sum_{n=n_0} g_n \frac{(\epsilon_n)^2}{(kT)^{3/2}} e^{\epsilon_n/kT} E_1\left(\frac{\epsilon_n}{kT}\right) \text{ cm}^3/\text{sec} \quad (7)$$

where g_1 and g_n are the statistical weights of the ground state of the recombining ion and the excited state n of the recombined ion respectively, ϵ_n and kT are the binding energy of state n and the electron temperature of the plasma in rydbergs, and E_1 is the exponential integral of index one. In Table I we show a comparison of typical rate coefficients given by Eq. (7) with those calculated numerically using cross sections obtained from the PELEC code.^{5,6} Although the ratios for individual transitions deviate considerably from unity, they lie within about a factor two of unity. We shall see later (Table II) that radiative recombination is small compared to dielectronic recombination. Therefore, for present calculations we have used the simpler rates arising from the Kramers cross sections.

B. Density Effects on Dielectronic Recombination

The conditions of the plasma that we wish to consider for the present idealized calculations are

TABLE I

COMPARISON OF RADIATIVE RECOMBINATION RATE COEFFICIENTS TO Fe XXI FOR A TEMPERATURE OF 1 keV, AS COMPUTED BY THE PELEC CODE AND THE KRAMERS FORMULA.^a

Sub-shell	α_{PELEC} (cm^3/sec)	$\alpha_{\text{PELEC}}/\alpha_{\text{Kramers}}$
1s	1.59-12	0.96
2s	1.75-13	1.30
2p	7.27-13	1.11
3s	1.04-13	1.79
3p	2.67-13	1.61
3d	1.62-13	0.62
4s	4.50-14	2.41
4p	1.19-13	2.20
4d	9.97-14	1.16
4f	3.88-14	0.33

^aThe calculations were carried out by W. D. Barfield.⁶

as follows: the electron density is 10^{14} cm^{-3} , the electron temperature is 800 to 5,000 eV, and the hydrogen plasma is seeded with Fe nuclei of density 10^{12} cm^{-3} .

We hope that the conditions are sufficiently realistic that the numbers resulting from present energy loss calculations can serve to guide thinking on the importance of radiation loss resulting from the presence of high-Z impurities in a high-temperature plasma machine. The importance of dielectronic recombination can hardly be overemphasized for the plasma conditions we have set for ourselves in this report. The existence of this process as an important mechanism in the steady state of plasmas was established by Burgess^{7,8} in 1964. He pointed out that the then existing discrepancies between the electron temperature inferred from continuum processes and that arrived at from line intensity measurements in the solar corona were largely removed with the inclusion of dielectronic recombination.

Burgess⁹ gave a simple and useful formula for the rate of recombination into a given ion by dielectronic recombination. This formula was derived for low electron densities less than about 10^{-8} cm^{-3} where collisional effects are unimportant; however, as the density is increased one must investigate the importance of competing processes. The most important of these are direct collisional ionization from the excited state and collisional excitation followed by collisional ionization. Burgess' formula is unsuitable for the estimation of competing processes; here we need the individual contributions from the various excited states involved in dielectronic recombination. We also need the spontaneous radiative deexcitation rate to all available lower levels.

The hydrogenic approximation affords us with a reasonable model for estimating the value of the principal quantum number n above which collisional processes play an important role in the total recombining process. The spontaneous radiative deexcitation rate to all available lower levels is given by Eq. (A.29). Here, as in Appendix A-6, we are interested in sufficiently large n that collisional processes statistically distribute the population to all possible quantum states of the ions.

For present purposes it is convenient to rewrite Eq. (A.29) with the aid of (A.27) as follows:

$$\tilde{A}_{n_j} = \bar{A}_{n_j, n_{j-1}} \ln \left[\frac{n_j^3}{(n_o - \frac{1}{2})^2} \right] \quad (8)$$

Consider the collisional deexcitation rate as given by Eq. (5):

$$N_e \alpha_{j+1, j} = \left\{ 20.6 \lambda_{\text{cm}}^3 N_e T^{-1/2} P\left(\frac{\Delta E}{kT}\right) \right\} \bar{A}_{j+1, j} \quad (9)$$

Then the ratio of the collisional deexcitation rate ($\Delta n = -1$) to the spontaneous radiative deexcitation rate (to all lower states) is given by

$$\frac{N_e \alpha_{j+1, j}}{\tilde{A}_{n_{j+1}}} = \frac{20.6 \lambda_{\text{cm}}^3 N_e T^{-1/2} P\left(\frac{\Delta E}{kT}\right)}{\ln \left(\frac{n_{j+1}^3}{(n_o - \frac{1}{2})^2} \right)} \quad (10)$$

In this expression the numerator is approximately proportional to n_j^9 while the denominator has only a logarithmic dependence on n_j . This strong dependence on n_j makes Eq. (10) easy to solve for the value of n_j for which the radiative deexcitation rate is equal to the collisional deexcitation rate. The collisional excitation rate is approximately equal to the collisional deexcitation rate.

Let n_c be the value of the principal quantum number n for which Eq. (10) is equal to unity; any larger value of n will be said to be in the collisionally dominated region. This value of n along with the effective ionization limit n_t given by Eq. (19) define the region of interest in the study of the effects of density on the dielectronic recombination.

The question of radiative stabilization is discussed in detail in Appendix B-2. In that section, one is concerned with the competition arising from autoionization. It is also apparent that stabilization (and destabilization) may also arise as the result of collisional processes. Some of these processes are discussed by Burgess and Summers¹⁰ and more recently by Summers.¹¹ At relatively low density, one process apparently not discussed is that

in which the collisional processes simply redistribute the population among all available angular momentum states having the same principal quantum number. From Fig. B-4 it is seen that dielectronic recombination occurs primarily into states of small l . The collisional redistribution will be predominantly into states of high l because of their large statistical weight. Since these high l states have a very low autoionization probability, and since the radiative stabilization rate is independent of l , the effect of collisional redistribution is to increase the branching ratio (B.2). It is important to note that this may happen even when the collisional excitation (or deexcitation) rates for $\Delta n \neq 0$ are small compared to autoionization rates. These effects are discussed further in Appendix C.

After the stabilizing radiation has taken place, one is left with the recombined ion in a highly excited state. For example, the first three entries of Table B-III show the recombined ion in a state with principal quantum number $n = 10$. For high enough density the collisional ionization rate exceeds the radiative deexcitation rate. For such cases the ion has never truly recombined.

For the case where collisional ionization is an important mechanism competing with radiative deexcitation, one must in principle solve the complete set of coupled rate equations for all ions and excited states present in the plasma. However, a simplification which proves adequate for present Tokamak plasmas is the Bates-Kingston-McWhirter¹² (BKM) quasistationary approximation, or a generalization of it given by Burgess and Summers.¹⁰ Introducing this approximation, the rate equations for the excited state j of an ion of charge $+z$ can be written in the form

$$0 \equiv \frac{\partial N_j^{+z}}{\partial t} = C_{ji}^{+z} N_i^{+z} + C_{j1}^{+z} N_1^{+z} + r_j^{+z} N_1^{+(z+1)} \quad (11)$$

for $j \neq 1$ and $i \neq 1$. Here a repeated index (except for 1) denotes a summation, C_{ji}^{+z} is the collisional rate coefficient connecting levels i and j , the subscript 1 denotes the ground state, and r_j^z is the recombination coefficient from the ground state of ion $(z+1)$ to state j of ion (z) . Following the convention of Summers,¹¹ the term $C_{jj}^{+z} N_j^{+z}$ represents

the total rate of decrease of N_j^{+z} from level j to all other levels, both bound and free. The rate equation for the ground state of ion (z) is of the form

$$\begin{aligned} \frac{\partial N_1^{+z}}{\partial t} = & -A^z N_1^z + \left(B_1^z N_1^{z-1} + \bar{E}_1^z N_1^{z-1} \right) \\ & + C_{1i}^z N_i^{+z} + r_1^z N_1^{z+1}, \end{aligned} \quad (12)$$

$i \neq 1$

A^z is the sum of the rate coefficient r_1^{z-1} and the ionization rate coefficient from the ground state of ion $(+z)$. The B 's are ionization rate coefficients for ion $(z-1)$, C_{1i} is the deexcitation rate coefficient from level i of ion $(+z)$, and r_1^z is the recombination rate coefficient from the ground state of ion $(z+1)$ to z . The homogeneous equations for the excited states can be solved for the N_i^z , and the solutions used to eliminate the excited states from Eq. (12). Following this procedure one obtains

$$\frac{\partial N_1^z}{\partial t} = S_{cd}^{z-1} N_1^{z-1} - \left(\alpha_{cd}^{z-1} + S_{cd}^z \right) N_1^z + \alpha_{cd}^z N_1^{z+1}, \quad (13)$$

where the S_{cd} and α_{cd} are the effective ionization and recombination coefficients, which are closely related to the "collisional-dielectronic recombination coefficients" of Burgess and Summers.¹⁰ This set of coupled equations can be solved by transforming it to diagonal form. This is most simply done by rewriting the system of equations in matrix form:

$$\dot{\vec{N}}_1 = R \vec{N}_1, \quad (14)$$

where R is the matrix formed from the coefficients given above. Let us set

$$\vec{N}_1 = Q \vec{Y}, \quad (15)$$

where Q is a constant nonsingular matrix. Then there exists an inverse Q^{-1} such that

$$Q^{-1}Q = I \quad , \quad (16)$$

and therefore we can write from Eqs. (14) and (15)

$$\dot{\vec{Y}} = Q^{-1}R Q \vec{Y} = \Lambda \vec{Y} \quad . \quad (17)$$

By forming columns of Q from the normalized eigenvectors of matrix R , we see that Λ is diagonal so that the diagonal elements are the eigenvalues of R . The eigenvalues of the rate matrix R are real and positive, and the reciprocal of the smallest eigenvalue is the characteristic relaxation time scale for approach to the steady state.¹³ For the plasma under consideration, the computed relaxation times at temperatures up to 2 keV are 2 to 3 ns. At higher temperatures the times are somewhat longer (5 to 7 ns) because of the presence of Fe XXV, which involves ionization from the tightly bound 1s shell.

The question of how the density affects the dielectronic recombination rates is handled directly in the formulation given above. However, it is not very transparent: it is simply one part of the recombination term. Moreover, numerical calculations are time consuming because of the large size of the matrix (C_{ij}) in Eq. (11)--120 × 120 in our case.

A mathematically simpler way of handling density effects was suggested by Burgess. He introduced a correction factor

$$D = \sum_{n=n_0}^{n_c} \alpha_d(n) / \sum_{n=n_0}^{\infty} \alpha_d(n) \quad . \quad (18)$$

Here $\alpha_d(n)$ is the dielectronic recombination coefficient for an outer electron $n\ell$ (summed over ℓ), n_0 is the smallest principal quantum number allowed, and n_c is the effective continuum limit. Excited states having $n > n_c$ are equivalent to ionization.

Wilson¹⁴ has defined n_c to be the principal quantum number above which collisional excitation and ionization rates are greater than the collisional and radiative deexcitation rates. Using his approximate rate coefficients he found

$$n_c^7 = 1.4 \times 10^{+15} z^6 T_e^{1/2} N_e^{-1} \quad , \quad (19)$$

where z is the charge of the ion, T_e is the electron temperature in °K, and N_e is the electron density in cm^{-3} . The exact form of this equation depends on the approximation made for the various rate coefficients. Other forms can be found in a textbook by Griem.¹⁵ In any case, the value of n_c is not sensitive to which formula is used in computing it.

In order to evaluate D , we need an expression for the effective (radiatively stabilized) dielectronic recombination rate coefficient α_d . For a given recombined state j in Fig. B-1, α_d may be found from the expression (B.19) for the rate of radiative decays $j \rightarrow k$, summed over all lower levels k . Let us consider all possible states j that can be formed by adding an electron $n\ell$ to a "core" configuration j_0 . As an example, consider the first six entries in Table B-III for Fe XXI: the configurations j are all of the form $1s^2 2s 2p^2 n\ell$, and the core configuration j_0 is $1s^2 2s 2p^2$ in each case. For a given core j_0 , the total rate coefficient (assuming the initial ions to be statistically distributed among all levels m of the ground configuration) is given from Eq. (B.20) by

$$\alpha_d(j_0) = \frac{4\pi^{3/2} a_0^3}{T_e^{3/2}} \sum_{n\ell} e^{-E_s/T_e} \bar{F}^t \quad , \quad (20)$$

where the electron temperature T_e and the free-electron kinetic energy E_s are in rydbergs. In place of the detailed expression (B.22) for $\bar{F}^t$ we here use the approximation (B.36), the summations in Eqs. (B.29)-(B.30) being over all levels j of the configuration $j = j_0 n\ell$. If $n\ell$ is not equivalent to any electron of the core j_0 then $G_j = (4\ell + 2)G_{j_0}$, where G_{j_0} is the statistical weight of the core configuration; also, the radiative decay rate of the inner excited electron is from (A.21) or Table B-II essentially independent of $n\ell$, and we factor out this rate, $A_r^{j_0}$. We abbreviate $\bar{A}_{at} \equiv \bar{A}_{at}^{j_0 n\ell}$ to $A_a^{n\ell}$. Then if n_0 is the minimum n for autoionization,

$$\alpha_d(j_0) = \frac{8\pi^{3/2} a_0^3}{T_e^{3/2}} e^{-E_s/T_e} \frac{G_{j_0} A_r^{j_0}}{G_m} \sum_{n=n_0}^{\infty} B_n \quad , \quad (21)$$

where G_m is the statistical weight of the ground

configuration of the recombining ion, E_s^∞ is the value of $E_s = E_s^{n\ell}$ for $n = \infty$, and

$$B_n(T_e) = \sum_{\ell} C_g^{n\ell} C_r^{n\ell} e^{(E_s^\infty - E_s)/T_e} \frac{(2\ell + 1) A_a^{n\ell}}{A_a^{n\ell} + C_r^{n\ell} A_r^{j_o}} \quad (22)$$

The quantity $C_g^{n\ell}$ is unity except for that single term (if any) for which $n\ell$ is equivalent to electrons of the core configuration j_o , where it corrects for the fact that $G_j \neq (4\ell + 2)C_{j_o}$. For this $n\ell$, $C_r^{n\ell}$ corrects for the fact that $\bar{A}_{rt} \neq A_r^{j_o}$; for the present we assume all other $C_r^{n\ell} = 1$, but in Appendix C we will use $C_r^{n\ell} > 1$ to allow for contributions to $\bar{A}_{rt}$ by decay of the outer excited electron.

For configurations j_o that differ from n by a $\Delta n = 0$ excitation, n_o is necessarily so large that the exponential in Eq. (22) is always close to unity; for $\Delta n > 0$ excitations, the exponential is significantly greater than unity for small n . Some computed values of B_n for Fe XXI are shown in Fig. 1. To obtain these results we carried out the summation over n in three sections: (1) explicitly in detail from the minimum allowed $n = n_o$ to some value

Fig. 1. Plot of B_n in Eq. (22) for three cases in Fe XXI (plain curve $T_e = \infty$, *** $T_e = 1$ keV). The difference in shape between curves for $\Delta n = 0$ and $\Delta n > 0$ excitations is pronounced. For $\Delta n > 0$, B_n becomes negligible at such small values of n that plasma-density effects are unimportant for $N_e = 10^{14} \text{ cm}^{-3}$.

$n = n_1$; (2) from n_1 to n_t , using the asymptotic dependence $A_a^{n\ell} = A_a^{1\ell} (n_1/n)^3$ discussed in Sec. B-8:

$$\sum_{n=n_1}^{n_t} B_n = \sum_{\ell} \sum_{n=n_1}^{n_t} \frac{(2\ell + 1) e^{(E_s^\infty - E_s)/T_e}}{\left[1 + \left(\frac{A_r^{j_o}}{A_a^{1\ell}} \right) \left(\frac{n}{n_1} \right)^3 \right]} \quad (23)$$

and (3) from n_t to ∞ using an integral approximation to the sum:

$$\begin{aligned} \sum_{n=n_t}^{\infty} B_n &\cong \sum_{\ell} n_1^3 \int_{n_t}^{\infty} \frac{(2\ell + 1) dx}{\left(\frac{A_r^{j_o}}{A_a^{1\ell}} \right) x^3} \\ &= \sum_{\ell} \frac{n_1^3 (2\ell + 1)}{2n_t^2} \left(\frac{A_a^{1\ell}}{A_r^{j_o}} \right) \end{aligned} \quad (24)$$

Clearly, if n_t is not so large that $A_r/A_a \gg 1$, then the integral approximation will be too large and the calculated value of D will be too small, thus overestimating the density effects.

In practice, we have carried the summations over ℓ no higher than $\ell = 8$. It may be seen from Fig. B-4 that this is valid for large A_r or for large n . Any error present at small n has only a small effect on the computed value of D because the major contributions to the summations in Eq. (18) arise from the large- n terms, and because the errors in numerator and denominator tend to cancel out.

An example of the variation of D with n_t is shown in Fig. 2. It is important to note that the density effects decrease in going to higher z along an isoelectronic sequence. This is because A_a is nearly constant whereas A_r varies approximately as z^4 , and because n_t increases with z ; thus the contribution (24) decreases rapidly with increasing z , so that D tends rapidly to unity. For the ions and electron density considered here the density effect is only about 8%, and we have neglected it in all our calculations.

The total dielectronic recombination rate is given by summing the expression (20) over all core

Fig. 2. Plot of D in Eq. (18) vs the effective ionization limit n_i . Because n_i decreases as density increases the dielectronic recombination coefficient decreases. (Curves correspond to those in Fig. 1.)

configurations j_0 . We have carried out calculations of this type, using the approximation (22), for a large variety of cases. The results have shown that it is sufficiently accurate for our power loss calculations to use a much simpler approach suggested by Burgess.⁹ His approximate formula is

$$\alpha_d = 3.0 \times 10^{-12} T_e^{-3/2} B(z) \sum_{m=i+1} \bar{f}_{im} A(x) e^{-\bar{E}/kT_e} \quad (25)$$

The quantities appearing in this expression are:

T_e = electron temperature in units of 10^6 °K ;

z = the charge number of the recombining ion ;

i = the initial state of the recombining ion ;

m = a state of the excited core configuration j_0 of the recombined ion (before radiative stabilization) ;

$\bar{f}_{im}$ = oscillator strength of the transition $i \rightarrow m$ of the recombining ion [see Eq. (A.19)] ;

$\bar{E}/kT_e = 0.158(z+1)^2(n_i^{-2} - n_m^{-2})/T_e a$, where n_i and n_m are effective quantum numbers ;

$$a = 1.0 + 0.015 z^3/(z+1)^2 ;$$

$$B(z) = z^{1/2}(z+1)^{5/2}/(z^2 + 13.4)^{1/2} ;$$

$$A(x) = x^{1/2}/(1 + 0.105x + 0.015x^2) , \quad \text{where}$$

$$x = (z+1)(n_i^{-2} - n_m^{-2}) .$$

For $\Delta n \neq 0$ transitions, we have modified this formula in that $A(x)$ has been replaced by

$$A'(x) = 0.5x^{1/2}/(1 + 0.210x + 0.030x^2) .$$

This was done to obtain a better analytical fit to our detailed numerical calculations. Appendix C discusses this point in greater detail.

V. POWER LOSS CALCULATIONS

In this section we give the calculation for the power loss when the rates for the processes described in Secs. I through IV are used. Three-body (radiationless) recombination rate coefficients can be calculated from the expression¹⁶

$$b = 8.75 \cdot 10^{-27} z^3 T_e^{-9/2} N_e \text{ cm}^3/\text{sec} , \quad (T_e \text{ in eV}). \quad (26)$$

However, this process contributes less than one percent to the total recombination rate in our plasma, and we have omitted it. The calculated collisional ionization and collisional excitation cross sections used have large uncertainties. The power loss reflects these uncertainties. In view of these uncertainties the power loss probably cannot be believed to better than a factor of two. The accuracies of the radiative and dielectronic processes are discussed in the appendices.

Power losses from our Fe-seeded plasma for temperatures from 0.8 to 10 keV are given in Table II. This table shows the breakdown in power loss according to the mechanism producing it. By collisional excitation we mean the radiative deexcitation

TABLE II
POWER LOSS FROM Fe-SEEDS PLASMA

$$(N_e = 10^{14} \text{ cm}^{-3}; N_{\text{Fe}} = 10^{12} \text{ cm}^{-3})$$

T_e (keV)	Total Power Loss (W/cm ³)	Coll. Excitation		Recombination		Free- Free
		$\Delta n = 0$	$\Delta n \neq 0$	Diel.	Rad.	
0.8	4.109	2.194	1.081	0.774	0.042	0.017
1.0	4.074	2.738	0.713	0.536	0.065	0.023
1.2	2.922	2.115	0.402	0.293	0.083	0.029
1.5	1.546	1.104	0.195	0.123	0.089	0.035
1.7	1.100	0.749	0.145	0.081	0.088	0.038
2.0	0.757	0.463	0.116	0.053	0.084	0.042
2.5	0.534	0.256	0.111	0.037	0.081	0.047
3.0	0.455	0.165	0.123	0.032	0.083	0.052
5.0	0.420	0.045	0.167	0.024	0.114	0.070
10.0	0.423	0.004	0.144	0.010	0.160	0.115

following collisional excitation. The designation $\Delta n = 0$ means transitions that do not involve a change in the principal quantum number. Under recombination, the abbreviation Diel. denotes dielectronic recombination, and Rad. denotes radiative recombination from the continuum to all excited states and the ground state. Free-free is the bremsstrahlung radiation resulting from scattering of free electrons by the ions, considered as point charges.

Note that up to 1.5 keV the power loss resulting from dielectronic recombination exceeds that due to radiative recombination. Of the losses resulting from collisional excitation, those arising from $\Delta n = 0$ transitions are greater than those from $\Delta n \neq 0$ up to temperatures of 3 keV.

The ion abundances needed in these calculations are given in Table III. These were computed by standard methods, using our rate coefficients and the solar coronal model. Our results differ somewhat from those of Jordan,¹⁷ because of differences in the rate coefficients used.

To obtain a feel for the effects of uncertainties in the rate coefficients, we have arbitrarily multiplied the rate coefficients by various constant factors. The resulting power loss at $T_e = 1.2$ keV is shown in Table IV. The last four columns of this table show the change in power loss when the dielectronic rate coefficients for a single

ion have been varied in the manner shown. The variation of total power loss with temperature for three of the cases in the table is shown in Fig. 3.

It must be emphasized that all the above results refer only to our plasma with $N_e = 10^{14} \text{ cm}^{-3}$ and $N_{\text{Fe}} = 10^{12} \text{ cm}^{-3}$. Since all radiation rates are proportional to the product of electron and ion densities, the power loss for other iron densities may

Fig. 3. Total power loss calculated using the normal rate coefficients, the dielectronic rate coefficients multiplied by a factor of 2, and the collisional ionization rates multiplied by 2.

TABLE III
ION ABUNDANCE USED FOR POWER LOSS CALCULATIONS IN TABLE II^a

T_e (keV)	Ion Species											
	XVI	XVII	XVIII	XIX	XX	XXI	XXII	XXIII	XXIV	XXV	XXVI	XXVII
0.8	0.021	0.072	0.151	0.218	0.227	0.172	0.094	0.038	0.012			
1.0		0.010	0.031	0.077	0.141	0.196	0.202	0.163	0.108	0.072		
1.2				0.015	0.042	0.092	0.153	0.204	0.229	0.259		
1.5						0.020	0.056	0.131	0.261	0.525		
1.7							0.028	0.088	0.237	0.635		
2.0							0.011	0.050	0.194	0.732	0.010	
2.5								0.022	0.139	0.801	0.034	
3.0								0.012	0.103	0.807	0.076	
5.0									0.035	0.596	0.327	0.040
10.0										0.167	0.496	0.333

^aAbundances less than 1% ignored.

TABLE IV
POWER LOSS FOR ALTERED RATE COEFFICIENTS AT 1.2 keV

Power Loss (W/cm ³)	Ionization and Recombination Rate Changes									
	Normal	Coll.×2	Coll./2	Diel.×2	Diel./2	Be→B Diel.×2	Be→B Diel./2	He→Li Diel.×2	He→Li Diel./2	
Total	2.92	1.37	4.28	4.47	2.06	3.37	2.61	2.92	2.93	
Coll. Exc.	2.52	1.11	3.68	3.40	1.83	2.86	2.28	2.51	2.53	
Diel. Recomb.	0.29	0.13	0.53	0.97	0.10	0.41	0.21	0.29	0.30	
Rad. Recomb.	0.08	0.11	0.05	0.05	0.10	0.08	0.09	0.08	0.08	
Free-Free	0.03	0.03	0.02	0.02	0.03	0.03	0.03	0.03	0.03	

be obtained by multiplying the numbers in Table II by $N_{Fe}/10^{12}$. For $N_e \approx 10^{14}$, power loss for other electron densities will scale as $N_e/10^{14}$; however, this is only a first approximation because the ionization equilibrium changes with N_e and because density effects rapidly become more important with increasing electron density.

Some comments are appropriate concerning the approximations and fundamental atomic data used in the calculations. For $N_e \leq 10^{14}$ and the high ionization stages involved here, excitation rates due to both collisions and recombination are much smaller than electric-dipole radiative decay rates up to rather high principal quantum numbers. Hence at

least 99% of all ions lie in the ground configuration; for simplicity, we have assumed that all ions lie in the ground state. Required ionization energies were obtained from experimental data (AEL) or from the estimates of Lotz.¹⁸ Power losses were calculated under the assumption that collisionally excited atoms lose 100% of their excitation energy by radiative decay, and that recombining ions radiate the ionization energy of the recombining ion plus the kinetic energy of the recombining electron. [Losses due to reionization of the doubly excited atom have already been allowed for through the branching ratio in (22), which is implicitly included in the Burgess formula (25).] Because of bookkeeping limitations,

excited levels were considered only for $n' \leq 10$ [except of course that higher n' contributions are included in the Burgess formula (25)]; the results in Table II show this to be a good approximation, the large $\Delta n \neq 0$ contributions above $T_e = 3$ keV arising mainly from $1s-2p$ transitions. Energy levels were obtained from experimental data for iron or nearby elements, where possible; otherwise from the theoretical HX calculations described in Appendix A. Energies were assumed to depend only on the electron configuration ($n\ell$) up to principal quantum numbers of 4, and only on n for $n > 4$; experimental data were correspondingly averaged as appropriate. Theoretical array-averaged oscillator strengths, Eq. (A.19), were used for transitions $n\ell-n'\ell'$ where both n and n' were no greater than 4. For $n' > 4$ hydrogenic values (A.24) were used; these values include the occupation number w_i from (A.20).

VI. X-RAY DIAGNOSTICS

A. Excitation of $1s-2p$ Radiation

Information on the density of high-Z impurity atoms and on their distribution as to ionization stage (and thereby information on the electron temperature) can be obtained by measuring the absolute intensity of energy radiated by these atoms in, say, the region of $1s-2p$ transitions. Preliminary measurements of this type for iron atoms in the ST Tokamak have been made by the Princeton group,¹⁹ and the results are shown in Fig. 4. Various intensity maxima were observed at photon energies ranging from somewhat above 6.4 keV (which corresponds to the ordinary K_{α_1} and K_{α_2} x-ray lines of singly ionized iron, Fe II) up to about 6.7 keV (corresponding to transitions in helium-like iron, Fe XXV $1s^2\ ^1S_0-1s2p\ ^1P_1, ^3P_1$); the intermediate maxima were identified as arising from intermediate ions, Fe XIX to XXIV, as indicated in the figure.

The deduction from these data of abundances of the various ions can be made only with the aid of theoretical calculations of the radiation rates to be expected from each ion, as functions of electron density and temperature. In this section we discuss methods of making such calculations, and give preliminary results for iron.

In the low-density plasmas of interest here, essentially all ions lie in the ground level, or at

Fig. 4. Observed X-ray spectrum of the Princeton ST Tokamak in the region of Fe $1s-2p$ transitions (1.94 to 1.85 Å).

least in some level of the ground configuration. Emission of $1s-2p$ radiation can arise only if an ion is momentarily raised to an excited configuration that has a $2p$ electron and a $1s$ hole. Excitation by absorption of radiation is unimportant in low-density sources. There are then three possible mechanisms by which such an excited configuration can be produced; we illustrate these using Fe XXII as an example.

(a) Collisional excitation out of the $1s$ shell:

where the first step involves a collisional-excitation rate coefficient α_e and the second involves the transition probability rate A_r for $2p \rightarrow 1s$ radiative decay. For ions having (as here) more than four electrons, an additional possibility is

(b) Dielectronic recombination involving excitation out of the 1s shell:

(c) For ions with more than four electrons, collisional ionization out of the 1s shell:

For iron atoms at the temperatures of interest here ($T_e \lesssim 10$ keV), a simple calculation using Eq. (2) shows that (c) is unimportant relative to (a) and (b), and so we henceforth ignore it.

Each of the radiative processes indicated in Eqs. (27) to (30) involves several different spectrum lines because each configuration generally possesses more than one energy level. However, each set of lines ("transition array") covers only a relatively small wavelength range. The spectral resolution used in the Princeton experiment (Fig. 4) was low enough that individual lines were not observed--only a single spectral maximum for each transition array. On the other hand, we shall see in Sec. VI-D that any specific observed maximum does not in general arise from a single ionization stage: the labeling (Fe XIX, Fe XX, ...) in the figure applies to the "basic" collisionally excited arrays of the type (27). The Fe XXII array (28) for $n > 2$ lies essentially at the position labeled Fe XXIII for the basic array $1s 2s^2 2p \rightarrow 1s^2 2s^2$. Similarly, the arrays (29) and (30) arise from what were initially

Fe XXII ions, but lie at the basic positions of Fe XXI for (29) with $n = 2$, of Fe XXII for (29) with $n > 2$, and of Fe XXIII for (30) with $n'' \geq n' > 2$.

B. Dielectronic Recombination

A detailed discussion of dielectronic recombination is given in Appendix B, and it is shown there that the rate of radiative transitions $j \rightarrow k$ resulting from this process (j and k being, respectively, autoionizing and nonautoionizing states) is given by (B.9). At electron densities of 10^{14} cm^{-3} and temperatures up to 10 keV practically all ions will lie in the ground configuration, but excited states of this configuration may be more or less uniformly populated. Thus as shown in Sec. B-5, the rate of emission of $2p \rightarrow 1s$ photons in the spectrum line $j \rightarrow k$ is, from Eq. (B.19),*

$$R(j \rightarrow k) = n_e n_{N-1} \frac{4\pi^{3/2} a_0^3}{T_e^{3/2}} e^{-E_s/T_e} \bar{F}^{jk}, \quad (32)$$

where T_e is the electron temperature in rydbergs, E_s is an average value of the kinetic energy $E^j - E^m$ of the recombining electron, and

$$\bar{F}^{jk} = \frac{g_j \left(\sum_m A_a^{jm} \right) A_r^{jk}}{\left(\sum_m g_m \right) \left(\sum_{m'} A_a^{jm'} + \sum_{k'} A_r^{jk'} \right)}. \quad (33)$$

Here m is a level of the ground configuration of the recombining ion; j is an autoionizing state of the recombined ion, and g_j is the statistical weight of the corresponding level; k is any level reached from j by a $2p \rightarrow 1s$ radiative decay; m' and k' are any levels below j reachable, respectively, by autoionizing and radiative decay transitions. The total rate of emission of $2p \rightarrow 1s$ photons resulting from dielectronic recombination is

$$R_d = n_e n_{N-1} \frac{4\pi^{3/2} a_0^3}{T_e^{3/2}} e^{-E_s/T_e} \bar{F}^t, \quad (34)$$

* In this section and in the appendices, we shall use n instead of N to denote particle densities, reserving the symbol N to represent the number of electrons in the ion.

where

$$\bar{F}^t = \sum_{j,k} \bar{F}^{jk}, \quad (35)$$

the summations being over all upper levels j and lower levels k of the appropriate configurations.

The photon-energy distribution of the total radiation rate (34) is given by the energy distribution of the various spectrum lines, each with an intensity proportional to $\bar{F}^{jk}$. Each spectrum line covers a finite energy interval, because of the finite lifetime of the upper state and because of Doppler broadening. We assume all lines to have the same shape and the same width, represent each by a distribution function with area $\bar{F}^{jk}/\bar{F}^t$, and thereby obtain for the sum total of all lines a photon-energy distribution function $w(E)$, where

$$\int w(E) dE = 1; \quad (36)$$

the photon-radiation-rate distribution function is

$$\frac{dR}{dE} = R w(E). \quad (37)$$

Sample calculations (Table B-II) indicate that auto-ionization lifetimes are considerably greater than radiative lifetimes, and that the latter are $\geq 3 \cdot 10^{-15}$ sec, leading to half-widths at half maximum of only

$$\Gamma_L = \frac{1}{4\pi c \Delta t} \leq \frac{1}{12 \cdot 3 \cdot 10^{10} \cdot 3 \cdot 10^{-15}} = 10^3 \text{ cm}^{-1} = 1 \text{ kK}.$$

Doppler halfwidths are given by

$$\Gamma_D = 1.22 \cdot 10^{-3} (T_{\text{keV}}/A)^{1/2} \sigma_0; \quad (38)$$

for 1s-2p transitions in Fe ($A = 56$, $\sigma_0 = 54000 \text{ kK}$), this gives $\Gamma_D = 9 \text{ kK}$ at $T = 1 \text{ keV}$ and $\Gamma_D = 20 \text{ kK}$ at 5 keV , so that Γ_L as well as Γ_a is negligible. Judging from Fig. 4, the total half-width in the Princeton experiment (including instrumental effects) was about $\Gamma = 70 \text{ kK} = 0.0087 \text{ keV}$. Illustrative

computed distribution functions $w(E)$ are shown in Fig. 5 for Gaussian line shapes with $\Gamma = 10, 20$, and 70 kK , respectively. The last value ($\Gamma = 70$) will be assumed in all that follows (except for Fig. 11); it is evident that this half-width has almost completely washed out any structure within a transition array, as mentioned in Sec. VI-A.

C. Collisional Excitation

Analogously to the dielectronic recombination rate coefficient in (B.2), we can define a collisional excitation rate coefficient $\alpha_x^{k_0 j}(T_e)$ such that

$$n_e n_N \alpha_x^{k_0 j}(T_e) \quad (39)$$

is the rate (per unit volume of plasma) of excitation of ions (Z, N) from some state k_0 to all states of level j . For excitations that would be allowed by absorption of electric-dipole radiation, we assume the rate coefficient to be given by the van Regemorter expression (5) and (6), which may be written in the form

$$\begin{aligned} \alpha_x^{k_0 j}(T_e) &= 3 \sqrt{\pi/3} \frac{h a_0}{m} \frac{f_{k_0 j}}{E_0 T_e^{1/2}} P e^{-E_0/T_e} \\ &= 3.15 \cdot 10^{-7} \frac{f_{k_0 j}}{E_0 T_e^{1/2}} P e^{-E_0/T_e} \text{ cm}^3/\text{sec}, \end{aligned} \quad (40)$$

where E_0 and T_e are the excitation energy and the electron temperature in rydbergs, $f_{k_0 j}$ is the optical oscillator strength (A.12) for the transition in question, and the value of the effective Gaunt factor P varies from 0.2 for $E_0/T \gg 1$ to about 1.0 for $E_0/T \ll 1$. Assuming as for dielectronic recombination that the ions (Z, N) are uniformly distributed among the states of the ground configuration, $n_N^{k_0} = n_N g_{k_0} \sum g_{k_0}$, then the total excitation rate to level j (per cm^3 of plasma) is

$$3.15 \cdot 10^{-7} n_e n_N \frac{\sum_{k_0} g_{k_0} f_{k_0 j}}{g_{k_0} E_0 T_e^{1/2}} P e^{-E_0/T_e}, \quad (41)$$

Fig. 5. Computed dielectronic-recombination distribution functions $w(E)$, in units of $(\text{keV})^{-1}$, for the transition array Fe XXI $1s^2 2s^2 2p^2 - 1s 2s^2 2p^3$, assuming Gaussian line shapes with (from top to bottom) HWHM of 10, 20, and 70 kK. The 20 reasonably strong lines of this 35-line array are not fully resolved even for $\Gamma = 10$ kK.

where $G_{k_0} = \sum g_{k_0}$ is the statistical weight of the ground configuration, and the summations are carried over all levels k_0 of the ground configuration.

Application of this expression to $1s-2p$ excitations of Fe XXVI and Fe XXV is straightforward. In each case, the ground configuration ($1s$ and $1s^2$, respectively) contains only one level. Since collisional deexcitation is negligible, ions excited to the state j can only decay radiatively back to the ground state, and so the rate of emission of $2p+1s$ photons is also given by (41). [In the helium-like ion case, the excited configuration $1s2p$ has four levels, only two of which ($^1P_1, ^3P_1$) are connected to the ground level by electric-dipole transitions. Collisional excitation to 3P_0 and 3P_2 , which is not included in Eq. (41), followed by collisional transfer to 1P_1 or 3P_1 , could result in additional contributions to the calculated $1s-2p$ radiation. We have neglected this radiation completely, even though on the basis of statistical-weight arguments it could be just as important as that which we have included.]

For Fe XXIV and lower ionization stages, excitation out of the $1s$ shell produces levels j that lie above the first ionization limit. The rate of emission of $2p+1s$ photons will then be less than the collisional excitation rate because some excited ions will decay by autoionization rather than by radiative deexcitation. In addition, Fe XXII and lower stages possess more than one level in the ground configuration; excited ions in level j can in general then decay radiatively by more than one path, so that radiative decays $j \rightarrow k$ can no longer be placed in one-to-one correspondence with excitations $k \rightarrow j$. For simplicity, we handle these branching-ratio problems by making use of the calculations of Sec. VI-B on dielectronic recombination excitation. That is, we assume that the total collisional excitation rate is given by the summation of Eq. (41) over j , but that the relative populations of excited states are the same as for dielectronic recombination. Thus the total rate of collisionally excited $2p+1s$ radiation (for a given excited configuration) is

$$R_x = 3.15 \cdot 10^{-7} n_e n_N \frac{\bar{f} \bar{B}}{E_0 T_e^{1/2}} P e^{-E_0/T_e}, \quad (42)$$

where

$$\bar{f} = \frac{\sum_j \sum_{k_o} g_{k_o} f_{k_o,j}}{G_{k_o}} \quad (43)$$

is the averaged total oscillator strength (A.19) for the transition array in question and $\bar{f}$ is the mean branching ratio (B.31), which allows for losses due to autoionization and/or non $2p \rightarrow 1s$ radiative decays. The photon-radiation-rate energy distribution is given by Eq. (37), where $w(E)$ is the same distribution function that was calculated for the dielectronic recombination case, examples of which were given in Fig. 5.

All collisional excitation cases considered are given in Table V, along with values of $\bar{f}$ [obtained from detailed spectral calculations, rather than from the approximation (A.19)] and of $\bar{B}$ (from Table B-II). Excitations of the type $1s-3s$ and $1s-3d$ are, of course, not electric-dipole allowed; effective values of $\bar{f}$ for these cases were estimated by assuming the value of $\bar{f} \bar{B}/\bar{f}$ to be the same as for $1s-3p$ excitations. (This leads to collisional excitation cross sections for the optically forbidden cases that are 1/4 to 1/6 of that for $1s-3p$, which is not unrealistic.) Where the excited configuration contains both a $2p$ and an np electron, the decay has been assumed to be only via $2p \rightarrow 1s$ even though the branching ratio may be as small as 0.8 (Table B-I).

For Fe XXIII to XXVI, which have no $2p$ electron in the ground configuration, K_α radiation could be produced by collisional excitation of $1s$ to $3s$ or $3d$, followed by radiative decay to $2p$; these processes have been neglected because of their low excitation probability and because of the possibility of collisional transfer from $3s$ or $3d$ to $3p$ followed by radiative decay directly to $1s$.

D. Results

Figure 6 shows the K_α radiation spectrum computed to arise from what initially were ground-configuration Fe XXII ions in a plasma at $T_e = 1$ keV. The dotted curve represents collisionally excited radiation; the main peak at $h\nu = 6.59$ keV results from $1s \rightarrow 2p$ excitation followed by $2p \rightarrow 1s$ radiative decay, whereas the minor feature at $h\nu = 6.63$ is

Fig. 6. Computed $1s-2p$ spectrum resulting from Fe XXII atoms in the plasma: dotted curve, as a result of collisional excitation; solid curve minus dotted curve, from excited Fe XXI ions produced by dielectronic recombination. The ordinate scale corresponds to 10^{12} Fe XXII ions per cm^3 at $T_e = 1$ keV. (A small constant background has been added for computer-plotting convenience.)

due to $1s \rightarrow n\ell$ excitation ($n = 3$ to 5) followed by $2p \rightarrow 1s$ decay. The difference between the solid and dotted curves represents radiation from excited Fe XXI ions produced by dielectronic recombination of electrons with Fe XXII ions; the major contribution at $h\nu = 6.55$ results from recombination into the configuration $1s2s^2 2p^3$, and the remaining contribution arises from recombination into configurations $1s2s^2 2p^2 n\ell$ ($n = 3 - 5$). As discussed in Sec. VI-A, the three peaks in the solid curve lie essentially at the positions of radiation emitted by $1s-2p$ collisionally excited Fe XXI, XXII, and XXIII, in the order of increasing photon energy.

In an actual plasma at any given temperature of interest, iron atoms exist in a number of different ionization stages. The spectrum radiated by the iron in the plasma is a simple superposition of spectra like Fig. 6 for the various ions, each weighted by the fractional ion abundances given in Table III. Computed spectra for various electron temperatures are shown in Fig. 7 on a logarithmic vertical scale. (The noticeably low point on each

TABLE V
COLLISIONAL EXCITATION OF 1s-2p RADIATION

Ion	k_o	j	k	E_o (Ry)	$\bar{f}$	$\bar{B}$
Fe XXVI	1s	2p	1s	512	0.421	1.000
Fe XXV	$1s^2$	1s2p	$1s^2$	492	0.821	1.000
Fe XXIV	$1s^2 2s$	1s2s2p	$1s^2 2s$	489	0.809	0.319
Fe XXIII	$1s^2 2s^2$	$1s2s^2 2p$	$1s^2 2s^2$	486	0.795	0.110
Fe XXII	$1s^2 2s^2 2p$	$1s2s^2 2p^2$	$1s^2 2s^2 2p$	484	0.645	0.528
		$1s2s^2 2p3s$	$1s^2 2s^2 3s$	559	0.023	0.654
		3p	3p	561	0.143	0.761
		3d	3d	563	0.036	0.980
		4p	4p	587	0.052	0.654
		5p	5p	598	0.024	0.643
Fe XXI	$1s^2 2s^2 2p^2$	$1s2s^2 2p^3$	$1s^2 2s^2 2p^2$	481	0.504	0.529
		$1s2s^2 2p^2 3s$	$1s^2 2s^2 2p3s$	552	0.023	0.802
		3p	3p	554	0.137	0.887
		3d	3d	557	0.032	0.988
		4p	4p	578	0.050	0.906
		5p	5p	589	0.024	0.939
Fe XX	$1s^2 2s^2 2p^3$	$1s2s^2 2p^4$	$1s^2 2s^2 2p^3$	478	0.369	0.510
		$1s2s^2 2p^3 3s$	$1s^2 2s^2 2p^2 3s$	546	0.022	0.889
		3p	3p	548	0.132	0.913
		3d	3d	550	0.028	0.991
		4p	4p	569	0.048	0.942
		5p	5p	580	0.023	0.964
Fe XIX	$1s^2 2s^2 2p^4$	$1s2s^2 2p^5$	$1s^2 2s^2 2p^4$	476	0.240	0.489
		$1s2s^2 2p^4 3s$	$1s^2 2s^2 2p^3 3s$	539	0.021	0.958
		3p	3p	541	0.127	0.940
		3d	3d	545	0.024	0.993
		4p	4p	562	0.045	0.976
		5p	5p	571	0.022	0.988
Fe XVIII	$1s^2 2s^2 2p^5$	$1s2s^2 2p^6$	$1s^2 2s^2 2p^5$	473	0.117	0.469
		$1s2s^2 2p^5 3s$	$1s^2 2s^2 2p^4 3s$	533	0.021	0.966
		3p	3p	535	0.121	0.947
		3d	3d	539	0.020	0.994
		4p	4p	554	0.043	0.980
		5p	5p	562	0.021	0.990

Fig. 7. Computed 1s-2p spectra for equilibrium distributions of Fe ionization stages at the indicated electron temperatures. All spectra are plotted as in Fig. 6, except that the total iron ion density is 10^{12} cm^{-3} . The ionization-stage labeling of the various maxima follows the same convention used in Fig. 4.

dotted curve results from the very small branching ratio $\bar{B}$ for collisionally excited Fe XXIII in Table V.) The spectrum for $T_e = 1.2$ keV is repeated in Fig. 8 on a linear scale, to give a better comparison with the observed spectra in Fig. 4.

The basic similarity between the calculated spectra and the observed spectra of Fig. 4 is unmistakable, but there are two points of quantitative disagreement:

(1) The computed peaks (including the ordinary x-ray Fe II K_α peak) occur uniformly at energies about 0.015 keV greater than observed because of a systematic $\frac{1}{2}\%$ error in the theory.

(2) For each temperature, the observed spectrum corresponds to ionization stages somewhat lower than calculated. Thus for example, the observed spectrum for $T_e = 1.2$ keV corresponds most closely to that calculated for $T_e = 0.9$ keV. This discrepancy may be explained in several ways: (a) the observations are made along a tangential line of sight through the Tokamak that includes plasma at peak temperatures less than 1.2 keV; (b) the observations are time integrated, and temperatures at early and late times in the discharge are lower than 1.2; (c) the confinement time of the discharge is comparable with

the equilibration relaxation times dictated by the ionization and recombination rates of iron ions (see Sec. IV-B), so that the degree of ionization has not had time to reach the equilibrium abundances assumed in the calculations; (d) the calculated ion abundances may be incorrect because of errors in the rate constants used. As an illustration of this last point, Fig. 9 shows the effect of altered theoretical ion abundances when all ionization rate coefficients or all dielectronic rate coefficients are arbitrarily changed by a factor of 2; it is evident that agreement between calculated and observed spectra at $T_e = 1.2$ keV can be obtained either by decreasing the ionization rates by a factor of about 2 or by increasing the dielectronic recombination rates by a factor of about 2--either of which is well within the possible uncertainties of these quantities. It is evident that with our present uncertain knowledge of the basic atomic physics parameters involved, comparison of observed and theoretical spectra cannot be expected to give plasma temperatures with an uncertainty smaller than 25% or so.

The energy-integrated K_α radiation rates for each excitation process and each T_e are summarized in Table VI and Fig. 10. Collisional excitation for $n > 2$ is evidently unimportant; at low temperatures this is because of the Boltzmann factor and the high excitation energies involved, and at high temperatures it is because the predominant ionization stages (Fe XXIII to Fe XXVI) have no 2p electrons in their ground configurations, and because cascading from $n > 2$ states was neglected in the calculation. Dielectronic recombination predominates over collisional excitation at low temperatures* because the recombining-electron energies E_s [Eq. (34)] are considerably smaller than the collisional excitation energies E_0 [Eq. (42)]; at high temperatures, the Boltzmann factors are of much less consequence, and collisional excitation is the more important process.

Fig. 8. Computed 1s-2p spectrum (collisional plus dielectronic) for $T_e = 1.2$ keV, plotted on a linear vertical scale.

* Note that this is true only for 1s-2p radiation. The major contribution of line radiation to power loss from the plasma arises from transitions $n \rightarrow n'$ with both n and n' greater than one, and here collisional excitation is the dominant process.

Fig. 9. Computed 1s-2p Fe spectra with (left) all collisional ionization rate coefficients and (right) all dielectronic recombination rate coefficients multiplied by (top) a factor two and (bottom) a factor $\frac{1}{2}$. All curves are for $T_e = 1.2$ keV.

The radiation rates given in Table VI are for $n_e = 10^{14}$ electrons/cm³ and $n_i = 10^{12}$ iron atoms/cm³; approximate rates for other densities can of course be obtained by multiplying the tabulated rates by $n_e n_i / 10^{26}$. Deduction of experimental iron impurity atom concentrations by comparison of observed and calculated absolute K_α radiation rates is subject to large uncertainties, because the dielectronic recombination rates may be in error by a factor of two, and the collisional excitation rates may be in error by as much as an order of magnitude. However, deduction of total radiation-loss rates (at all photon energies) by means of absolute K_α rate measurements and Tables II and VI should be more accurate because the ratio of the

two sets of excitation rates involved should be less uncertain than the absolute rates separately.

Finally, we show in Fig. 11 the calculated K_α spectrum for $T_e = 1.2$ keV assuming Gaussian line shapes with $\Gamma = 20$ kK, instead of 70 kK. This is actually from a preliminary calculation omitting $n = 3 - 5$ contributions and certain other effects, but the complex spectral structure shows that it may be appreciably more difficult to try to make diagnostic K_α measurements with high instrumental resolution than with low resolution. In addition, the fine detail of the theoretical spectrum is considerably more uncertain than is the gross structure.

TABLE VI

TOTAL RADIATION RATE (W/cm^3) OF Fe IMPURITY ATOMS ($n_e = 10^{14}$, $n_{\text{Fe}} = 10^{12} \text{ cm}^{-3}$)
IN THE 1s-2p SPECTRAL REGION

T_e (keV)	Collisional		Dielectronic		Total
	$n = 2$	$n = 3 - 5$	$n = 2$	$n = 3 - 5$	
0.8	8.2-5	2.9-5	2.4-4	1.5-4	5.0-4
1.0	5.6-4	1.2-4	2.0-3	9.0-4	3.5-3
1.2	2.1-3	1.7-4	5.9-3	2.4-3	1.1-2
1.5	8.1-3	1.3-4	1.2-2	5.1-3	2.6-2
1.7	1.4-2	7.6-5	1.6-2	6.8-3	3.7-2
2.0	2.6-2	5.5-5	2.0-2	9.2-3	5.5-2
2.5	4.9-2		2.3-2	1.2-2	8.5-2
3.0	7.1-2		2.4-2	1.3-2	1.1-1
5.0	1.2-1		1.9-2	1.2-2	1.5-1
10.0	1.1-1		6.3-3	4.7-3	1.2-1

Fig. 10. Relative contributions of the various excitation processes to 1s-2p radiation from Fe ions. The distances between successive curves represent contributions of collisional excitation or of dielectronic recombination, for principal quantum numbers of the (outer) excited electron of $n = 2$ or of $n = 3$ to 5.

Fig. 11. Computed 1s-2p spectrum for Fe impurity ions at $T_e = 1.2$ keV, analogous to the corresponding section of Fig. 7 except with $\Gamma = 20$ instead of 70 kK.

APPENDIX A

ENERGY LEVELS AND RADIATIVE TRANSITIONS FOR BOUND STATES

A-1. BASIS WAVEFUNCTIONS

Detailed calculations of energy levels and of radiative and autoionization transition probabilities are made via the Slater-Condon theory of atomic structure, using an orthonormal set of antisymmetric N-electron basis functions constructed from products of one-electron functions. The basis functions $|b\rangle \equiv |\beta L S J M\rangle$ are fully coupled so as to be eigenfunctions of the total angular-momentum operators L^2 , S^2 , J^2 , and J_z . Most physical quantities of interest are independent of M, and this quantum number will usually be dropped from the notation. The label β includes the nuclear charge Z, the electron configuration

$$(n_1 \ell_1)^{w_1} (n_2 \ell_2)^{w_2} \dots (n_q \ell_q)^{w_q}, \quad \sum_{i=1}^q w_i = N, \quad (A.1)$$

and all intermediate quantum numbers such as $L_i S_i$ ($1 \leq i \leq q$).

The one-electron radial wavefunctions from which the basis functions are constructed are obtained by self-consistent-field solution of equations of the form

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V_{n\ell}(r) \right] P_{n\ell}(r) = \epsilon_{n\ell} P_{n\ell}(r). \quad (A.2)$$

The central-field potential-energy function $V(r)$ is calculated via the HX prescription,²⁰ which gives a good approximation to Hartree-Fock radial functions.

A-2. ENERGY LEVEL CALCULATIONS

Stationary states of the atom are found by solving the Schrödinger equation

$$H\psi^k = E^k \psi^k, \quad (A.3)$$

where H is a nonrelativistic Hamiltonian, including both Coulomb and spin-orbit interactions:

$$H = \sum_{i=1}^N \left(-\nabla_i^2 + \frac{2Z}{r_i} + \xi(r_i) \vec{\ell}_i \cdot \vec{s}_i \right) + \sum_{i < j} \frac{2}{r_{ij}}, \quad (A.4)$$

lengths being measured in Bohr units and energies in rydbergs (1 Ry = 13.605 eV). Solutions are obtained by expanding the wavefunction ψ^k in terms of the basis functions

$$|\psi^k\rangle = \sum_b |b\rangle \langle b|\psi^k\rangle, \quad (A.5)$$

where the sum extends over basis functions belonging to one or more configurations. The eigenvalue equation (A.3) then becomes replaced by the matrix equation

$$(H)_{bb'}^k = E^k \delta_{bb'}, \quad (A.6)$$

where the bb' component of the Hamiltonian matrix is

$$H_{bb'} = \langle b|H|b'\rangle \quad (A.7)$$

and the components of the eigenvector $\vec{Y}^k$ are the expansion coefficients in (A.5):

$$(\vec{Y}^k)_b = \langle b|\psi^k\rangle. \quad (A.8)$$

Routine computer methods for calculating the matrix elements (A.7), and for diagonalizing the matrix to obtain eigenvalues (energy levels) and eigenvectors (wavefunctions) are described elsewhere.²¹ First-order relativistic and correlation energy corrections²⁰ are included for improved accuracy.

A-3. STATISTICAL WEIGHTS

A quantum state of the atom is designated by $k \equiv \gamma J M$, and an energy level (in the absence of external fields) by γJ . To the approximation that the single-configuration approximation is valid, the portion γ of the level designation includes the configuration (A.1).

The statistical weight of a level is equal to the number of quantum states belonging to that level--i.e., the number of possible values of M:

$$g = 2J + 1 \quad (A.9)$$

The total statistical weight of all levels of the configuration (A.1) is

$$g = \prod_{i=1}^q \binom{4\ell_i + 2}{w_i} = \prod_{i=1}^q \frac{(4\ell_i + 2)!}{w_i! (4\ell_i + 2 - w_i)!} \quad (A.10)$$

A-4. RADIATIVE TRANSITIONS

Transitions between two levels γJ and $\gamma' J'$ associated with the emission or absorption of electric-dipole radiation are basically described in terms of the intermediate-coupling line strength

$$S = |\langle \gamma J \| \sum_{m=1}^N r_m^{(1)} \| \gamma' J' \rangle|^2$$

$$= \left| \sum_{bb'} \langle \gamma J \| b \rangle \langle b \| \sum_{m=1}^N r_m^{(1)} \| b' \rangle \langle b' | \gamma' J' \rangle \right|^2 \quad (A.11)$$

where $r_m^{(1)}$ is the tensor-operator form of the m^{th} electron coordinate (in Bohr units). Evaluation of the reduced dipole matrix element between basis functions is straightforward,²¹ and the expansion coefficients (A.8) are available from diagonalization of the pertinent energy matrices.

Absorption transitions from a state $k = \gamma J M$ of a level γJ to a state $k' = \gamma' J' M'$ of a higher level $\gamma' J'$ are usually described in terms of the component oscillator strength $f_c(k, k')$, and absorption from k to all states of the upper level by the (line) oscillator strength

$$f \equiv \sum_{M'} f_c(\gamma J M, \gamma' J' M')$$

The oscillator strength f is independent of M , and summation over M gives the weighted oscillator strength

$$gf \equiv \sum_M f = 3.0376 \cdot 10^{-6} S \sigma \quad (A.12)$$

where g is the statistical weight of the lower level, and

$$\sigma = E^{k'} - E^k \quad (A.13)$$

is the wavenumber of the spectrum line, σ and E being measured in cm^{-1} (kaysers).

The probability per unit time, A , that an atom in a state k' of the upper level $\gamma' J'$ spontaneously makes an electric-dipole transition to all states k of the lower level γJ is independent of M' , and is given by

$$gA \equiv \sum_{M'} A = 2.0260 \cdot 10^{-6} S \sigma^3 \text{ sec}^{-1}$$

$$= 0.66698 g f \sigma^2 \text{ sec}^{-1} \quad (A.14)$$

where g is the statistical weight of the initial level, and σ is again in cm^{-1} .

For simple cases in highly ionized atoms, it is usually reasonably accurate to limit the wavefunction expansion (A.5) to basis functions of a single configuration. A convenient line-strength sum rule then holds for all lines of a transition array; i.e., for all transitions between levels γJ of a configuration

$$\dots (n_i \ell_i)^{w_i} \dots (n_j \ell_j)^{w_j} \dots \quad (A.15)$$

and all levels $\gamma' J'$ of a configuration

$$\dots (n_i \ell_i)^{w_i} \dots (n_j \ell_j)^{w_j} \dots \quad (A.16)$$

where $\ell_j = \ell_i \pm 1$. It can be shown that²¹

$$\sum_{\gamma J} \sum_{\gamma' J'} S = \frac{w_i w_j}{2(\ell_i + 1)(\ell_j + 1)} \left[\prod_{m=1}^q \binom{4\ell_m + 2}{w_m} \right] \cdot p_{\ell_i \ell_j}^2 \quad (A.17)$$

where

$$P_{\ell\ell'} = \delta_{\ell', \ell \pm 1} (-1)^{\ell+\ell'} (\ell_>)^{\frac{1}{2}} \int_0^\infty P_{n\ell} r P_{n'\ell'} dr, \quad (A.18)$$

with $\ell_>$ equal the larger of ℓ and ℓ' , and r in Bohr units.

In highly ionized atoms it is usually true (if $\Delta n \neq 0$) that the energy spread of the levels of a configuration is small compared with the energy difference between configurations. All lines of an array then have nearly the same wavenumber, and the sum rule (A.17) can be applied to obtain a total (array) oscillator strength summed over all levels of the final configuration (A.16) and averaged over all states of the initial configuration (A.15). From (A.12) and the appropriate modification of (A.10),

$$\bar{f} \equiv \frac{\sum_{YJ} \sum_{Y'J'} g_{f'}^{8f}}{\sum_{YJ} g} = 3.0376 \cdot 10^{-6} \bar{\sigma} \frac{w_i (4\ell_i + 3 - w_i)}{2(2\ell_i + 1)(2\ell_j + 1)} P^2 \quad (A.19)$$

$$= \frac{w_i (4\ell_j + 3 - w_i)}{(4\ell_j + 2)} \bar{f}^{(1)}, \quad (A.20)$$

where $\bar{f}^{(1)}$ is the averaged total oscillator strength for a hypothetical one-electron atom ($w_i = w_j = 1$) having the same values of $\bar{\sigma}$ and P as for the real atom. Similarly, the total transition probability A to all levels of the final configuration (A.15) averaged over all states of the initial configuration (A.16) is

$$\bar{A} \equiv \frac{\sum_{Y'J'} \sum_{YJ} g_{f'}^{2A}}{\sum_{YJ} g} = 2.0260 \cdot 10^{-6} \bar{\sigma}^3 \frac{w_i (4\ell_i + 3 - w_i)}{2(2\ell_i + 1)(2\ell_j + 1)} P^2 \quad (A.21)$$

$$= \frac{w_i (4\ell_i + 3 - w_i)}{(4\ell_i + 2)} \bar{A}^{(1)}, \quad (A.22)$$

where $\bar{A}^{(1)}$ is the averaged total transition probability for the hypothetical one-electron atom.

A-5. ACCURACY

Computed wavelengths for highly ionized atoms are accurate to about 2 to 5% for $\Delta n = 0$ transitions, to about 0.2% for $1s-np$ transitions, and to about 0.2 to 1% for other $\Delta n \neq 0$ transitions.²² The accuracy of computed oscillator strengths is unknown because no experimental data exist for such ions, but is estimated to be ± 10 to 25% except for weak lines of no interest here. Averaged total values $\bar{f}$ and $\bar{A}$ are probably good to ± 5 to 10% in most cases.

A-6. HYDROGENIC APPROXIMATIONS

Hydrogenic (one-electron-atom) expressions are of course inapplicable to $\Delta n = 0$ transitions. However, for $\Delta n \neq 0$ transitions in highly ionized atoms, hydrogenic results are of adequate accuracy for many purposes. This is particularly true of the array-averaged oscillator strength $\bar{f}$ and transition probability $\bar{A}$, where details due to angular-momentum coupling are not involved, and for highly excited states (especially those of large ℓ), where core-penetration and relativistic effects are small.

For sufficiently large n of the excited electron, collisionally induced $\Delta n = 0$ transitions are much more probable than either radiative transitions or collisional $\Delta n \neq 0$ transitions. Thus, for any given such n , atoms will be statistically distributed among all quantum states, the number of atoms in configuration $n\ell$ being proportional to $2\ell + 1$. It is then of interest to consider mean quantities for transitions

$$n_i - n_j, \quad (A.23)$$

summed over all final ℓ and averaged over all initial ℓ :

$$\bar{f}_{n_i n_j} \equiv \frac{\sum_{\ell_i} (2\ell_i + 1) \sum_{\ell_j} \bar{f}_{n_i \ell_i, n_j \ell_j}}{\sum_{\ell_i} (2\ell_i + 1)}, \quad (A.24)$$

$$\bar{A}_{n_j n_i} \equiv \frac{\sum_{\ell_j} (2\ell_j + 1) \sum_{\ell_i} \bar{A}_{n_j \ell_j, n_i \ell_i}}{\sum_{\ell_j} (2\ell_j + 1)} \quad (\text{A.25})$$

Approximate nonrelativistic hydrogenic expressions for these quantities are²³

$$\begin{aligned} \bar{A}_{n_i n_j} &\approx \frac{2^5}{3\sqrt{3}\pi} \frac{1}{n_i^5 n_j^3} \left(\frac{1}{n_i^2} - \frac{1}{n_j^2} \right)^{-3} \\ &= \frac{1.96}{n_i^5 n_j^3} \left(\frac{1}{n_i^2} - \frac{1}{n_j^2} \right)^{-3}, \end{aligned} \quad (\text{A.26})$$

$$\begin{aligned} \bar{A}_{n_j n_i} &\approx \frac{1.57 \cdot 10^{10} Z_c^4}{n_i^3 n_j^5} \left(\frac{1}{n_i^2} - \frac{1}{n_j^2} \right)^{-1} \text{sec}^{-1} \\ &= \frac{1.57 \cdot 10^{10} Z_c^4}{n_i^3 n_j^3 (n_j^2 - n_i^2)} \text{sec}^{-1}, \end{aligned} \quad (\text{A.27})$$

where $Z_c = Z - N + 1$ is the effective core charge seen by the excited electron; these expressions are asymptotically accurate for $n_j \gg n_i \gg 1$, and are correct to within +40% for all $n_j > n_i \geq 1$. (Compared with these errors, relativistic corrections are negligible up to at least $Z_c = 30$.)

It is clear from (A.27) that for given n_j , $\bar{A}_{n_j n_i}$ is large for both small n_i and for large n_i ($= n_j - 1$), and has a minimum in between. This is illustrated by the dot-dash curve in Fig. A-1 for the case $n_j = 20$. The source of this behavior may be seen from the four solid curves, which are also for the case $n_j = 20$: for small ℓ_j , transitions are most probable to small n_i ; for large ℓ_j [which are weighted heavily in (A.25)] they are most probable for large n_i --being in fact restricted by selection rules to $n_i = n_j - 1$ in the limit $\ell_j = n_j - 1$.

Fig. A-1. Solid curves: nonrelativistic array transition probabilities for the indicated transitions $n\ell - n'\ell'$. Dash-dot curve: total transition probability for $n' = 20$, summed over ℓ and averaged over ℓ' .

The solid curve labeled "nℓ-20m" and the two dashed curves illustrate the downward radiative cascade process from high-angular-momentum states: starting from 20m ($n - \ell = 11$), the most probable transition is to 14ℓ ($n - \ell = 6$); from 14ℓ decay is most probable to 11k ($n - \ell = 4$); from there to 9i ($n - \ell = 3$); etc. Thus, the decay tends toward states with $n - \ell = 1$, after which the chain necessarily continues in steps of $\Delta n = \Delta \ell = -1$.

In ions having filled shells up through $n_0 - 1$, the mean lifetime of states in the shell n_j is given by the total transition probability from states n_j to all lower states $n_i \geq n_0$. From (A.27), this is

$$\begin{aligned}
T_{n_j}^{-1} &\equiv \tilde{A}_{n_j} \equiv \sum_{n_i=n_0}^{n_j-1} \bar{A}_{n_j n_i} \approx \frac{1.57 \cdot 10^{10} Z_c^4}{n_j^3} \int_{n_0 - \frac{1}{2}}^{n_j - \frac{1}{2}} \frac{dn_i}{n_i (n_j^2 - n_i^2)} \\
&= \frac{1.57 \cdot 10^{10} Z_c^4}{2n_j^5} \left[\ln \frac{n_j^2}{n_j^2 - n_i^2} \right]_{n_0 - \frac{1}{2}}^{n_j - \frac{1}{2}} \\
&= \frac{1.57 \cdot 10^{10} Z_c^4}{2n_j^5} \ln \left[\frac{(n_j - \frac{1}{2})^2}{(n_0 - \frac{1}{2})^2} \left(\frac{n_j^2 - (n_0 - \frac{1}{2})^2}{n_j^2 - \frac{1}{4}} \right) \right] \quad (A.28)
\end{aligned}$$

$$\approx \frac{1.57 \cdot 10^{10} Z_c^4}{2n_j^5} \ln \left[\frac{n_j^3}{(n_0 - \frac{1}{2})^2} \right], \quad n_0 \ll n_j \quad (A.29)$$

APPENDIX B

DIELECTRONIC RECOMBINATION

B-1. BASIC PROCESS

Figure B-1 shows a few of the possible states of a system consisting of a nucleus of charge Z plus

Fig. B-1. The dielectronic process for recombination of a free electron with an ion containing $N-1$ electrons to give an ion with N electrons. m_0 and m represent $(N-1)$ -electron states. All other levels, including the shaded continua that extend upward from m_0 and m , represent N -electron states.

N electrons, at most one of which is free. The state k_0 is one of the states of the ground level of the ion (Z, N) . The first ionization limit of this ion is also the ground-level energy of the next higher ion $(Z, N-1)$; m_0 is one of the states of this level. Excitation of one of the most weakly bound electrons of the ion (Z, N) gives rise to levels (such as k) lying below the ionization limit m_0 . Excitation of an inner-subshell electron (or of two electrons from the outermost subshell) may lead to a state j that lies above m_0 ; this state may autoionize—that is, it may spontaneously make a nonradiative transition to a state i consisting of the ion $(Z, N-1)$ in some bound state m of energy less than $E^i = E^j$, plus a free electron with kinetic energy

$$\epsilon = E^i - E^m \equiv E^{im} \quad (B.1)$$

*For simplicity, we shall use k to denote either a level or a specific one of the g_k states of that level. When necessary, it will be stated explicitly whether the level or a state is meant.

Dielectronic recombination is the inverse of the autoionization process. Thus, let i be an N -electron state consisting of the ion $(Z, N-1)$ in some bound state m ($E^m < E^j$) plus a free electron with kinetic energy $\epsilon = E^i - E^m$. If ϵ is such that $E^i \approx E^j$, the free electron may excite an electron of the ion $(Z, N-1)$, thereby losing enough kinetic energy to be captured into a bound orbit and producing the metastable state j of the ion (Z, N) .

Dielectronic recombination may be thought of as a resonance in a (radiationless) inelastic scattering process in which the incident free electron loses more than 100% of its kinetic energy, and thereby becomes captured. We shall not be interested in the energy-dependent cross-section $\sigma_d^{mj}(\epsilon)$ for this capture by the ion $(Z, N-1)$ in state m into (all states of) the level j of the ion (Z, N) , but only in a quantity related to the thermal average $\langle v \sigma_d^{mj} \rangle$. More specifically, we define a rate coefficient $\alpha_d^{mj}(T_e)$ such that

$$n_e n_{N-1}^m \alpha_d^{mj}(T_e) \quad (B.2)$$

is the rate of such captures (per unit volume of plasma) out of a sea of free electrons with uniform density n_e in thermal (Maxwell-Boltzmann) equilibrium at temperature T_e ; n_{N-1}^m is the density of ions $(Z, N-1)$ in the state m .

Rather than attempt to calculate the rate coefficient directly, we evaluate it in terms of the inverse (autoionization) process, using the principle of detailed balance. The rate (per unit volume) at which the inverse transitions take place is

$$n_N^j g_j \left(\frac{A_a^{jm}}{g_m} \right), \quad (B.3)$$

where n_N^j is the density of ions (Z, N) in each of the g_j states of the level j and A_a^{jm} is the probability per unit time that such an ion will autoionize, leaving an ion $(Z, N-1)$ in the level m . Under conditions of complete thermal equilibrium, (B.2) and (B.3) must be equal:

$$\alpha_d^{mj}(T) = \frac{n_N^j g_j}{n_e n_{N-1}^m g_m} A_a^{jm}. \quad (B.4)$$

But under such conditions

$$\begin{aligned} \frac{n_N^j}{n_e n_{N-1}^m} &= \frac{(n_N/u_N) e^{-(E^j - E^0)/kT}}{n_e (n_{N-1}/u_{N-1}) e^{-(E^m - E^0)/kT}} \\ &= \frac{n_N u_{N-1}}{n_e n_{N-1} u_N} e^{-(E^0 - E^0)/kT} e^{-(E^j - E^m)/kT}, \end{aligned}$$

where u_N and u_{N-1} are the partition functions for the two ions. From the Saha equation we obtain finally²⁴

$$\begin{aligned} \alpha_d^{mj}(T) &= \frac{h^3}{2(2\pi m kT)^{3/2}} \frac{g_j A_a^{jm}}{g_m} e^{-E^j m/kT} \\ &= \frac{4\pi^{3/2} a_0^3}{T^{3/2}} \frac{g_j A_a^{jm}}{g_m} e^{-E^j m/T}, \end{aligned} \quad (B.5)$$

where in the second expression $E^j m$ and T are in rydbergs ($1 \text{ keV} = 73.498 \text{ Ry} = 8065.47 \text{ kK} = 8.065 \text{ MK}$) and a_0 is the Bohr radius. This expression for the dielectronic recombination rate coefficient holds whether or not the ion populations correspond to equilibrium conditions, provided that the free electrons of uniform density n_e in (B.2) have a Maxwell-Boltzmann velocity distribution.

Some clarification of the relationship between the states i and m is appropriate. Before the dielectronic recombination process begins, the free electron will interact only weakly with the ion, and so the state m will be characterized by a well-defined total angular momentum J_m . The statistical weight g_m in (B.5) will therefore be $2J_m + 1$. The free electron will be described by a plane wave, which may be represented by the usual partial-wave expansion. Each term in this expansion corresponds to a definite angular momentum ℓ' of the free electron about the ion $(Z, N-1)$. The corresponding N -electron state can be represented as a superposition

of states i of the form

$$(J_m, \ell' s') J_i, \quad (B.6)$$

where s' is the spin of the free electron, and where dielectronic recombination to the state j can occur only if $J_i = J_j$ (because the angular momentum of the total system is conserved in the recombination process). Calculation of the transition probability A_a^{jm} in (B.5) involves a summation over all possible ways in which ℓ' and s' can be coupled to J_m to produce $J_i = J_j$, and also a summation over all possible values of ℓ' :

$$A_a^{jm} = \left(\sum_i A_a^{ji} \right)_{\text{fixed } m \text{ and } J_i}. \quad (B.7)$$

Ultimately, all states i are to be taken into account, each being given the usual statistical weight $2J_i + 1$. Note that for given m and ℓ' , the total statistical weight of the possible states i is

$$\sum_i (2J_i + 1) = (2J_m + 1)(2\ell' + 1)(2s' + 1);$$

this includes the familiar factor $(2\ell' + 1)$ that appears in the partial-wave expansion of the free-electron plane wave. Because of the selection rules that hold for the Coulomb interaction (no change in parity, L , S , nor J), then for any given configuration j , only a very limited number of terms ℓ' in this expansion make nonzero contributions to the summation in (B.7).

B-2. RADIATIVE STABILIZATION

Once the ion (Z, N) has been formed in the state j , there is the possibility that it may re-ionize at a rate A_a^{jm} (any energetically possible m). We cannot really consider the process of dielectronic recombination to be complete until the ion (Z, N) has been stabilized by deexcitation to a level lying below the ionization limit m_0 . For all cases of interest here, collisional deexcitation rates are negligible at electron densities of 10^{14} cm^{-3} , and the only process of importance is radiative decay (usually of the inner of the two excited

electrons) to some lower level k , at the rate A_r^{jk} given by (A.14). The probability that decay will be via a radiative transition to a specific lower level k is given by the branching ratio

$$B^{jk} = \frac{A_r^{jk}}{\sum_{m'} A_a^{jm'} + \sum_{k'} A_r^{jk'}}, \quad (B.8)$$

where the summation over m' here extends over all possible levels of the ion $(Z, N-1)$ that lie below j , and the summation over k' extends over all levels of (Z, N) that lie below j . The summation over m' represents re-autoionization transitions, or (in another vocabulary) single-electron Auger transitions.

The rate of emission of photons in the spectrum line $j \rightarrow k$, per unit volume, is

$$R(j \rightarrow k) = n_e \left[\sum_m n_{N-1}^m \alpha_d^{mj} (T_e) \right] B^{jk}, \quad (B.9)$$

where the summation is over the states of the ion $(Z, N-1)$. The total net dielectronic recombination rate is

$$R_d = \sum_{jk} R(j \rightarrow k) = n_e \sum_j \left[\sum_m n_{N-1}^m \alpha_d^{mj} (T_e) \right] \sum_k B^{jk}. \quad (B.10)$$

It is here assumed that all levels k involved in the summation either lie below the ionization limit m_0 so that further autoionization is not possible, or that they make small contributions to the sum and/or that further transitions are mainly by radiative decay to nonautoionizing levels.

B-3. CALCULATION OF A_a^{ji}

As shown by Fano,²⁵ autoionization transition probabilities may be calculated from the first-order perturbation theory expression

$$\begin{aligned} A_a^{ji} &= \frac{2\pi}{\hbar} |(j|H|i)|^2 \\ &= \frac{2\pi}{\hbar} \left| \sum_{bb'} \langle j|b \rangle \langle b|H|b' \rangle \langle b'|i \rangle \right|^2. \end{aligned} \quad (B.11)$$

The basis functions b' needed for expansion of the continuum state i are formed in exactly the same way as are basis functions for bound states such as j and k , except that one of the N radial functions is a continuum function $P_{\epsilon\ell}(r)$ for a free electron of kinetic energy $\epsilon = E_{\ell}^m$. This continuum function is obtained from a differential equation like (A.2), except that ϵ is known ahead of time instead of being an eigenvalue to be determined by satisfying a boundary condition at $r = \infty$. For the central-field potential, we use a function of the mathematical form

$$V_{\epsilon\ell}(r) = \lim_{n \rightarrow \infty} V_{n\ell}(r) \quad (B.12)$$

This function is such that $P_{\epsilon\ell}$ depends on the self-consistent-field radial functions for the ion-core state m (including an exchange term), but this ion core is completely unaffected by the free electron. The function $P_{\epsilon\ell}$ is obtained by numerically integrating outward from $r = 0$ on a suitably fine integration mesh (of 2201 mesh points, total) until $P_{\epsilon\ell}$ reaches essentially its asymptotic amplitude. P is then normalized to have an asymptotic amplitude of

$$\frac{1}{\pi \cdot \epsilon^{1/2}}$$

where ϵ is in rydbergs; with this normalization, the squared matrix element in (B.11) has units of rydbergs (if H is also in rydbergs), and $\hbar$ is then to be measured in Ry-sec.

The basis-function matrix elements $H_{bb'}$ in (B.11) are evaluated just as for any other configuration-interaction problem. The radial integrals involve one continuum function, but this produces no complications because the integration is effectively cut off at a finite radius by a bound function that goes exponentially to zero; the angular factors are evaluated automatically by the computer program previously mentioned.²¹ The expansion coefficients $\langle j|b \rangle$ and $\langle b'|i \rangle$ are obtained in the usual way by the matrix diagonalization that follows evaluation of the Hamiltonian matrix in the basis representation. [In the perturbation-

theory expression (B.11), the states j and i are assumed to be pure discrete and continuum states, respectively. Mixing of these two states in the course of the matrix diagonalization can be effectively prevented by artificially shifting the centers of gravity of continuum configurations by large negative amounts; this simultaneously provides the computer program with an easy means of distinguishing continuum states from discrete states by means of the large negative eigenvalues of the former.]

B-4. ACCURACY

The accuracy of computed autoionization transition probabilities and of dielectronic recombination rates is uncertain because there exist no experimental data whatever for highly ionized atoms. Results calculated by the methods outlined above can, however, be compared with Gabriel's values²⁶ for the Fe XXIV/XXV intensity ratios I_s/I , which are proportional to dielectronic recombination rates. Agreement is rather poor (e.g., our $\sum I_s/I$ is 0.24 compared with Gabriel's 0.44), but is much better when compared with the revised calculations of Bhalja, Gabriel, and Presnyakov,²⁷ both in detail and in total ($\sum I_s/I = 0.30$). We estimate our calculations to be accurate to ± 25 to 50%, except for the relatively unimportant weaker transitions.

The perturbation formula (B.11) does not take into account possible interference effects between overlapping, closely spaced autoionizing levels. This should be of little consequence in the ions of interest here: Autoionization transition probabilities A_a are no greater than 10^{13} to 10^{14} sec^{-1} , which implies level widths $2\Gamma = \hbar A_a$ of 0.006 to 0.06 eV (50 to 500 cm^{-1})--values that are one or two orders of magnitude smaller than typical mean separations between levels of the same J .

The small autoionization widths imply that (possibilities of overlap aside) a first-order perturbation calculation of A_a is basically adequate--indeed, radiative transition probabilities are comparable in magnitude, and perturbation calculation of A_r is the universally used method. Nonetheless, it is interesting to consider a calculational method in which the detailed mixing of discrete and continuum states (with associated interference effects)

is computed explicitly, and in which autoionization line shapes are obtained in detail;²⁸ the interference between overlapping neighboring autoionizing states could be handled in this way if desired.

The method consists of breaking up an appropriate section of the continuum into a sequence of small segments of width $\Delta\epsilon$, and then representing each of these segments by a pseudodiscrete configuration. It is necessary only that all radial integrals representing configuration interactions between the discrete (autoionizing) basis state and the pseudodiscrete continuum basis states be given an appropriate weighting factor proportional to $\sqrt{\Delta\epsilon}$ for the pertinent continuum segment; the same is true of radial dipole integrals associated with electric dipole transitions between some discrete configuration and the discretized continuum configurations. The numerical problem then becomes identical with the numerical matrix diagonalization problem described in Appendix A for a system of purely discrete configurations. Only the interpretation of the results is slightly modified: The square of an eigenvector component corresponding to the m^{th} pseudodiscrete configuration represents the integrated contribution to the (mixed) quantum state of the m^{th} continuum segment. Similarly, the strength of the spectrum "line" corresponding to a transition between a discrete state and the m^{th} pseudodiscrete state represents the photoionization cross section integrated over the width $\Delta\epsilon$ of the m^{th} continuum segment.

As an illustration of the application of this method to the calculation of the Beutler-Fano line shape for radiative absorption from a discrete state to an autoionizing (mixed discrete + continuum) state, we consider the case

The autoionization half-width at half maximum computed via the perturbation formula (B.11) is

$$\Gamma_a = \frac{1}{2} A_a = \frac{1}{2} \cdot (8.94 \cdot 10^{12} \text{ sec}^{-1}) = 23.7 \text{ cm}^{-1} .$$

(This takes account of the fact that the intermediate-coupled $2s2p^2 10s \text{ } ^3D_3$ level is computed to

be only 92.9% pure 3D_3 and 7.1% pure 5P_3 .) The value of the Fano parameter q , computed as the square root of the ratio of the line strength for the unperturbed discrete spectrum line to the integrated line strength for absorption to a band width $\pi\Gamma_a$ of the unperturbed continuum,²⁵ is -74. (Again, this includes the effect of the intermediate-coupling mixing of 3D_3 and 5P_3 .) In order to obtain a more appropriate illustrative example, we have arbitrarily reduced the discrete line strength by a factor 400, thus giving a value $q = -74/\sqrt{400} = -3.70$. The result of the numerical discretized-continuum calculation, using 48 continuum segments each of width $\Delta\epsilon = 20 \text{ cm}^{-1}$, is indicated by the circles in Fig. B-2 (the ordinates representing the ratios of the various perturbed pseudodiscrete line strengths to the integrated "line" strength for a width $\Delta\epsilon$ of unperturbed continuum). The solid curve in the figure is Fano's analytical result²⁵

$$\frac{(n+q)^2}{1+n^2} , \quad n = \frac{\epsilon - \epsilon_d}{\Gamma_a} , \quad (\text{B.13})$$

using $\Gamma_a = 23.7 \text{ cm}^{-1}$ and $q = -3.70$. (The energy ϵ_d is the effective perturbed position²⁵ of the discrete autoionizing level; this is identical with the unperturbed position in the present case of a constant-strength continuum.)

The discrepancy between the circles and the Fano curve at large $|n|$ is partly due to an inherent inaccuracy²⁵ in the formula (B.13), but is mainly due to end effects resulting from use of a finite section of the continuum; this is shown by the fact that the discrepancy becomes greater when five segments are discarded from each end of the continuum section. The close agreement between the two curves at small $|n|$ shows that if the circles were parametrically fit by an expression of the form (B.13) over the range $|n| \leq 3$, say, then the value of Γ_a thereby obtained would not differ by more than a few percent from the result given by the perturbation expression (B.11).

It should not be forgotten that the low- q Fano profile shown in the figure was chosen only for clarity of illustration. Typical profiles for highly ionized iron atoms correspond to much higher

Fig. B-2. Beutler-Fano autoionization profile for an absorption transition with $\Gamma_a = 23.7 \text{ cm}^{-1}$ and $q = -3.70$, as calculated (circles) via the numerical pseudodiscrete configuration-interaction method and (solid curve) from the Fano formula (B.13). The horizontal dashed line represents the unperturbed continuum; the unperturbed discrete spectrum line would be a very narrow line at $\eta = 0$ with total area equal to that of the unperturbed continuum for $|\eta| \leq 4\pi q^2 = 21.5$. (Note: For clarity, a nonlinear ordinate scale has been used--specifically, the logarithm of the dependent variable plus 0.1.)

values of q , so that the peak of the profile lies very much higher--at $q^2 + 1 = 74^2 + 1 = 5477$ for the Fe XXI example, rather than at $3.7^2 + 1 = 14.7$ for the plotted modification.

In principle, the detailed configuration-interaction method has the advantages that it can straightforwardly handle multiple nonconstant continua, and very wide overlapping multiple autoionizing levels. In practice, limitations of computer time and storage restrict applications to problems involving only one or two autoionizing levels at a time, in relatively simple configurations.

B-5. LOW-DENSITY, HIGH-TEMPERATURE PLASMAS

For the highly ionized atoms present in high-temperature plasmas, the energy levels within a configuration tend to lie close together compared with kT (e.g., the energy spreads within the ground configurations $1s^2 2s^2 2p^w$ and within excited configurations such as $1s^2 2s 2p^{w+1}$, $1s^2 2s^2 2p^{w-1} 3d$, and

$1s 2s^2 2p^{w+1}$ of Fe XXI to XVIII are all less than $1000 \text{ kK} \approx 0.1 \text{ keV}$). Consequently, for a set of levels j belonging to a specific configuration of the ion (Z, N) and a set of levels m belonging to the ground configuration of the ion $(Z, N-1)$, we can, at temperatures $T \gtrsim 0.8 \text{ keV}$, consider $E_{jm} \approx E_s =$ constant in (B.5). In the low electron-density limit, collisional excitation rates and dielectronic recombination rates will be negligible compared with radiative decay rates, and so essentially all ions will exist in the ground level m_0 ; (B.9) and (B.10) may then be written

$$R(j \rightarrow k) = n_e n_{N-1} \frac{4\pi^{3/2} a^3}{T_e^{3/2}} e^{-E_s/T_e} F_{m_0}^{jk} \quad (\text{B.14})$$

$$R_d = n_e n_{N-1} \frac{4\pi^{3/2} a^3}{T_e^{3/2}} e^{-E_s/T_e} F_{m_0}^t, \quad (\text{B.15})$$

where T_e and E_s are in rydbergs,

$$n_{N-1} = \sum_m n_{N-1}^m = g_{m_0} n_{N-1}^{m_0} \quad (\text{B.16})$$

is the total density of ions $(Z, N-1)$ in all states (of the ground level m_0),

$$F_m^{jk} = \frac{g_j A_a^{jm}}{g_m} B^{jk} = \frac{g_j A_a^{jm}}{g_m} \cdot \frac{A_r^{jk}}{\sum_{m'} A_a^{jm'} + \sum_{k'} A_r^{jk'}} \quad (\text{B.17})$$

and

$$F_m^t = \sum_{jk} F_m^{jk}, \quad (\text{B.18})$$

the summation over j being carried over all levels j of the configuration in question.

At nonzero electron densities, ions in excited levels will be present in appreciable numbers only if excitation rates are comparable with

radiative decay rates. For all levels of excited configurations (except for a few large-J levels of $2p^{W-1}3d$, where electric-dipole decay to $2p^W$ is prevented by the $\Delta J = 0, \pm 1$ selection rule), decay rates in iron ions are of the order 10^7 to 10^{14} sec^{-1} (Table B-1); these rates are much greater than excitation rates and so these levels will not be appreciably populated for $n_e \approx 10^{14} \text{ cm}^{-3}$.

Levels of the ground configuration, on the other hand, can decay only by magnetic-dipole radiation ($A \approx 10^3$ to 10^5 sec^{-1}) or by electric-quadrupole radiation ($A \approx 10^{-1}$ to 10^2 sec^{-1}). At $n_e = 10^{14}$ and $T_e = 1 \text{ keV}$, dielectronic recombination rates are less than 10^2 sec^{-1} , and so are negligible compared with $A \approx 10^3$. Strictly speaking, collisional excitation rates within the ground configuration cannot be estimated via the optical approximation (40), which applies only to electric-dipole-allowed transitions. It is, however, known that in neutral one- and two-electron atoms excitation rates for optically forbidden transitions are usually only a factor 3 or so smaller than for allowed transitions. For lack of any better theoretical method, we shall estimate excitation rates within the ground configuration by means of the following modification of the optical approximation: We calculate an effective oscillator strength "f" by replacing the radial electric-dipole integral

$$\int_0^\infty P_{n\ell}(r) r P_{n'\ell'}(r) dr \quad (\ell' = \ell \pm 1)$$

by

$$\int_0^\infty P_{n\ell}(r) r P_{n\ell}(r) dr = \langle r \rangle_{n\ell}$$

and by ignoring the corresponding angular factor (which is zero for the case at hand, and of the order unity for optically allowed transitions). For $2p^W$ configurations in Fe ions we find $\langle r \rangle_{2p} \approx 0.2$, and hence from (A.12)

$$g''f'' = 3 \cdot 10^{-6} \text{ So}$$

$$= 3 \cdot 10^{-6} (0.2)^2 \sigma = 1.2 \cdot 10^{-7} \sigma$$

[For transitions within these configurations, $\sigma \approx 0.4 \cdot 10^5$ to $3 \cdot 10^5 \text{ cm}^{-1}$, and hence $f'' \approx 0.01$.] Using the Van Regemorter formula (40) for $T_e = 1 \text{ keV} = 74 \text{ Ry}$, $E_o = \sigma / 1.1 \cdot 10^5 = 0.4$ to 3 Ry , $P \approx 1$, and $n_e = 10^{14} \text{ cm}^{-3}$, and adding a factor 1/3 for the ratio of optically forbidden to optically allowed cross sections, we find

$$n_{e\alpha x} = \frac{1}{3} n_e \cdot 3 \cdot 10^{-7} \frac{f P}{E_o T_e^2} e^{-E_o/T_e}$$

$$= \frac{1}{3} \cdot 3 \cdot 10^7 \frac{1.2 \cdot 10^{-7} \sigma \cdot 1}{(10^{-5} \sigma) \cdot 8.6}$$

$$= 1.4 \cdot 10^4 \text{ sec}^{-1}$$

This is quite comparable with the magnetic-dipole decay rates of excited ground-configuration levels (10^3 to 10^5 sec^{-1}).

It seems likely, therefore, that at electron densities of 10^{14} cm^{-3} all levels of the ground configuration will be fairly strongly populated. For simplicity, we assume the population to be more or less a Boltzmann-equilibrium one. Because $E^m - E^m_o \leq 0.1 \text{ keV} \ll T_e$, we shall assume more precisely that all states are equally populated. We then have in place of (B.14) and (B.15)

$$R(j \rightarrow k) = n_e n_{N-1} \frac{4\pi^{3/2} a_o^3}{T_e^{3/2}} e^{-E_s/T_e} \bar{F}^{jk} \quad (\text{B.19})$$

$$R_d = n_e n_{N-1} \frac{4\pi^{3/2} a_o^3}{T_e^{3/2}} e^{-E_s/T_e} \bar{F}^t \quad (\text{B.20})$$

where

TABLE B-I

MEAN RADIATIVE TRANSITION PROBABILITIES IN Fe XXI AND Fe XXV

Path ^a	Transition	$\bar{\sigma}$ (MK)	p^2	wt. ^b	$\bar{A} \cdot 10^{-12}$ (sec ⁻¹)
c	$1s^2 2s^2 2p^2 - 1s 2s^2 2p^3$	52.8	0.00236	1/2	352
c	$1s^2 2s^2 2p n\ell - 1s 2s^2 2p^2 n\ell \quad (n > 2)$	53.0	0.00239	1/3	241
d	$1s^2 2s^2 2p^2 - 1s 2s^2 2p^2 3p$	60.8	0.00037	1/6	28
e	$1s 2s^2 2p^2 3s - "$	0.2	0.314	1/3	0.002
d	$1s^2 2s^2 2p^2 - 1s 2s^2 2p^2 4p$	63.4	0.00013	1/6	11
e	$1s 2s^2 2p^2 3s - "$	2.8	0.0445	1/3	0.67
e	$4s - "$	0.1	1.08	1/3	0.001
f	$1s 2s^2 2p^3 - 1s 2s^2 2p^2 3s$	7.9	0.00222	2/3	1.47
f	$1s 2s^2 2p^3 - 1s 2s^2 2p^2 4s$	10.6	0.00035	2/3	0.56
g	$1s 2s^2 2p^2 3p - "$	2.5	0.0169	1	0.54
f	$1s 2s^2 2p^3 - 1s 2s^2 2p^2 3d$	8.3	0.0740	2/15	11.4
g	$1s 2s^2 2p^2 3p - "$	0.3	0.436	1/5	0.003
c	$1s 3p - 2p 3p$	56.1	0.00246	1/3	293
d	$1s 2p - 2p 3p$	65.8	0.00039	1/3	75
e	$2s 2p - 2p 3p$	10.1	0.0139	1/3	9.7
	$2s 3p - 2p 3p$	0.1	0.0402	1/3	$3 \cdot 10^{-5}$

^aSee Fig. B-3.^bThe factor in (A.21) that involves w_i , l_i , etc.

$$\bar{F}^{jk} = \frac{\sum_m g_m F_m^{jk}}{\sum_m g_m}$$

$$= \frac{g_j \sum_m A_a^{jm}}{\sum_m g_m} B^{jk}$$

$$= g_j \frac{\sum_m A_a^{jm}}{\sum_m g_m} \cdot \frac{A_r^{jk}}{\sum_{m'} A_a^{jm'} + \sum_{k'} A_r^{jk'}}$$

(B.21)

and

$$\bar{F}^t = \frac{\sum_m g_m F_m^t}{\sum_m g_m} = \sum_{jk} \bar{F}^{jk}$$

$$= \frac{1}{\sum_m g_m} \sum_j g_j \sum_m A_a^{jm} \frac{\sum_k A_r^{jk}}{\sum_{m'} A_a^{jm'} + \sum_{k'} A_r^{jk'}}$$

(B.22)

All summations over m are over the levels (not states) of the ground configuration of the ion

(Z,N-1); summations over m' and k' are (as before) over all levels of (Z,N-1) and (Z,N), respectively, that lie below the level j. If a total recombination rate R_d is desired (not just an apparent recombination rate R_d that gives rise to radiative decay in a specific transition array), then the summation over k extends over the same levels as does k' (rather than only over levels of a single configuration) and (B.20) must be summed over all possible upper configurations.

The difference between (B.14)-(B.15) and (B.19)-(B.20) is nil for hydrogen-like through beryllium-like ions because in each case there is only one level in the ground configuration, and is negligible for boron-like ions because there are only two levels of a single LS term (2P) and A_d depends only on LS and not on J. However, differences can be quite large for higher N ions. An extreme case is the recombination

where (B.20) is 6.7 times larger than (B.15); this is because the ground level of $2p^3$ is fairly pure $^4S_{3/2}$ and can thus to a first approximation give rise only to 3,5S and 3,5D continuum states, which cannot recombine (via Coulomb forces) with $1s 2s^2 2p^5 \ ^1,3P$. Although the ratio of (B.20) to (B.15) is only 3.2 and 1.3 for the analogous cases in Fe XVIII and Fe XX, respectively, it is evidently in general rather important to know just how the ions are distributed among the levels of the ground configuration, and the dependence on n_e of R_d/n_e may be quite strong in the vicinity of $n_e = 10^{14} \text{ cm}^{-3}$. Nevertheless, for the lack of any better information on excitation rates within the ground configuration, we shall always assume all states of the ground configuration to be equally populated, and shall use only (B.19)-(B.22).

B-6. APPLICATION TO K_α RADIATION FROM Fe IONS

We now discuss some of the details of dielectronic recombination processes leading to the emission of K_α radiation. As a specific example of the various possible terms that must be considered in (B.6) and in (B.22), we take the case of an electron recombining with an Fe XXII ion to form an Fe XXI

ion having a 1s hole, so that $2p \rightarrow 1s$ radiative decay is possible. The ground configuration m of Fe XXII is $1s^2 2s^2 2p$, and the possible recombination processes $i \rightarrow j$ are

$$1s^2 2s^2 2p \epsilon l' \longrightarrow \begin{cases} 1s 2s^2 2p^3, \\ 1s 2s^2 2p^2 n l', & n > 2, \\ 1s 2s^2 2p n' l' n l', & n \geq n' > 2. \end{cases} \quad (\text{B.24})$$

All values of l' must be considered that give configurations i having the same parity as, and LS terms in common with, the configuration j under consideration; all configurations on the right-hand side of (B.24) must in principle be examined. Initially, we consider the second path in (B.24), which includes the first path as the special case $n l' = 2p$; parity and angular-momentum selection rules for the Coulomb interaction are such that l' can only be $l \pm 1$. The various possible decay paths $j \rightarrow i'$ (and m') and $j \rightarrow k'$ that must be considered in (B.22) are summarized in Fig. B-3.

We consider first the re-ionization processes. Path a leaves the ion back in the ground configuration again; paths b of course result in an excited ion configuration. The energetics are such that many additional resultant configurations besides a and b are possible, for example

$$\begin{aligned} a' &: 1s^2 2s^2 n' l' \epsilon' l', \\ b' &: 1s^2 2s n' l' n' l' \epsilon' l', \\ b'' &: 1s^2 2s n' l' l' \epsilon' l' \epsilon' l', \\ b''' &: 1s^2 2p^3 \epsilon' l'. \end{aligned} \quad (\text{B.25})$$

(Path b'' represents ejection of two Auger electrons; all other paths listed are single-Auger-electron transitions.) However, none of these paths is allowed in first order because each differs from $1s 2s^2 2p^2 n l'$ by more than two electrons, and the Coulomb interaction is only a two-electron operator. Such resultants are possible in higher order, but only by virtue of configuration-interaction mixing with either a or b--for example, interaction of $1s^2 2p^3$ with $1s^2 2s^2 2p$. The second-order transition probabilities A_a allowed by such mixings are stolen

Fig. B-3. Possible autoionization and radiative decay paths, following the dielectronic recombination of an electron with a ground-configuration, 5-electron ion to produce a 6-electron ion in an autoionizing state j of the configuration $1s 2s^2 2p^2 n\ell$.

from those for the paths a and b and do not alter the total significantly; hence we shall consider only the five first-order paths.

So far as radiative decay is concerned, path c in Fig. B-3 is the only one that contributes to the $1s$ - $2p$ region of the spectrum. It is also the most probable mode of decay, as is shown by the sample calculations of Table B-I, made with the aid of the approximate expression (A.21). It is evident that compared with $j \rightarrow k$ decays ($2p \rightarrow 1s$, path c), the only $j \rightarrow k'$ decays of more than 10% importance are $3p \rightarrow 1s$ transitions (path d for $n\ell = 3p$). Even this latter we shall neglect throughout, for the following reason: Sample calculations show that recombination for $n\ell = 3p$ is unimportant compared with $n\ell = 2p$ except for Fe XVIII and XIX (where the configuration with $n\ell = 2p$ has an unusually low statistical weight $\sum g_j$), and in these ions the calculations are very uncertain anyway, as discussed following (B.23) above.

Returning to the re-ionization possibilities $j \rightarrow m'1'$ (via the autoionization paths b in Fig. B-3), we shall neglect these completely in all cases except $n\ell = 2p$, for the same reason given in the paragraph above. [The values of $\sum g_j A_a^{jm'}$ for the paths b are comparable to those for path a (or even much larger, because of the high statistical weights of the configurations b); however, the effect on $\bar{F}$ of including these terms is only about a 25% reduction,

because the radiative decay terms in the denominator of (B.22) tend to be large compared with the autoionization terms.]

Neglecting the decay paths other than a and c ($n\ell > 2p$) thus introduces an error of only 35% or so in contributions that tend to be small compared with the case $n\ell = 2p$. In addition, this error tends to compensate errors introduced by neglecting completely cases for large n .

Finally, we have yet to consider the third recombination path in (B.24). This will tend to be more important than the second path because of the greater statistical weight $\sum g_j$, but will tend to be less important because of the smaller values of A_a^{jm} . The only test case that we have calculated in detail is*

$$\text{Fe XVIII } 1s^2 2s^2 2p^4 \text{ } 500.s, d \rightarrow 1s 2s^2 2p^4 3p^2 \quad (B.26)$$

Compared with

$$\text{Fe XVIII } 1s^2 2s^2 2p^4 \text{ } 435.s, d \rightarrow 1s 2s^2 2p^5 3p \quad (B.27)$$

$\sum g_j$ is greater by a factor $450/72 = 6.25$ but the

*The values 500., 435., etc., are the values of the free-electron kinetic energy, E_s , in rydbergs.

A_a 's are smaller by about a factor 0.19; $\bar{F}^t$ is smaller by a factor 0.32 (the statistical-weight ratio 6.25 being nowhere near fully effective because of autoionization selection rules and low stabilizing transition probabilities A_r for many upper levels). The only other case examined (by the approximate method described in Sec. B-7) is

$$\text{Fe XVIII } 1s^2 2s^2 2p^4 \rightarrow 503.p, f \rightarrow 1s^2 2s^2 2p^4 3p3d \quad (B.28)$$

Here the statistical weight is a factor 4 larger even than for (B.26), but the A_a 's again are smaller by about a factor 0.19; thus $\bar{F}^t$ is probably an order of magnitude smaller than for (B.27). The importance of these cases is decreased further by the exponential factor in (B.20): The only ions for which even the second-type path in (B.24) is not small compared with the first are Fe XVIII - XX, and these are of consequence only for $T_e \lesssim 1.2 \text{ keV} = 88 \text{ Ry}$; the exponential thus reduces the importance of (B.26) or (B.28) relative to (B.27) by a further factor $\lesssim e^{-(500-435)/88} = 0.43$. In addition, there is for these ions the inherent uncertainty by factors of 1.3 to 6.7 discussed at the end of Sec. B-5. For these reasons, we shall in all cases neglect the third-type path in (B.24).

By way of summary, all cases considered are listed in Table B-II. For each set of configurations, the value of $\bar{F}^t$ is given as obtained by detailed computer evaluation of the expression (B.22), using the computer-calculated values of the individual transition probabilities (A.14) and (B.7), (B.11). Also given are values of the array-averaged transition probabilities

$$\bar{A}_{at} \equiv \frac{\sum_j g_j \sum_m A_a^{jm}}{\sum_j g_j} \quad (B.29)$$

$$\bar{A}_{rt} \equiv \frac{\sum_j g_j \sum_k A_r^{jk}}{\sum_j g_j} \quad (B.30)$$

and of the mean branching ratio

$$\bar{B} = \frac{\sum_m g_m \bar{F}^t}{\sum_j g_j \bar{A}_{at}} \quad (B.31)$$

These values are the ones used in the x-ray diagnostic calculations described in Sec. VI.

For comparison, the table also includes approximate values calculated as described in the following section.

B-7. APPROXIMATE CALCULATION OF DIELECTRONIC RECOMBINATION RATES

For rough calculations not requiring knowledge of the spectral distribution function $\bar{F}^{jk}$, an approximate expression for $\bar{F}^t$ can be obtained in the following way.

For simplicity, we neglect (as in most cases considered in Table B-II) those terms in the summations over m' and k' that are not included in the summations over m and k . The expression (B.22) then reduces to

$$\bar{F}^t = \frac{1}{\sum_m g_m} \sum_j g_j A_{at}^j \frac{A_{rt}^j}{A_{at}^j + A_{rt}^j} \quad (B.32)$$

where the subscripts t indicate total transition probabilities from the level j (summed over m or k).

Let us first consider cases (such as the Fe K_α problem) where radiative decay tends to be much more probable than autoionization. If departures from pure coupling conditions are large so that no radiative selection rules are effective except for $\Delta J = 0, \pm 1$, then $A_{rt}^j \gg A_{at}^j$ and the branching ratio in (B.32) is unity for essentially all j , and we obtain

$$\bar{F}^t \approx \frac{1}{\sum_m g_m} \sum_j g_j A_{at}^j = \frac{G_j}{G_m} \bar{A}_{at} \quad (B.33)$$

where $\bar{A}_{at}$ is the weighted average value (B.29) of A_{at}^j (averaged over all levels j of the configuration in question), and

$$G_j \equiv \sum_j g_j, \quad G_m \equiv \sum_m g_m \quad (B.34)$$

TABLE B-II

DIELECTRONIC RECOMBINATION PROCESSES FOR 1s-2p EXCITATION IN IRON IONS
($\epsilon = E_s$ IN Ry; $\bar{\sigma}$ IN MK = 10^6 cm $^{-1}$; $\bar{A}_{at}$, $\bar{A}_{rt}$, AND $\bar{F}^t$ IN UNITS OF 10^{11} sec $^{-1}$)

Ion	I		I'		J	K	Detailed								Approximate ^a				Rough		
	m	$\epsilon l'$	m'	$\epsilon l'$			G_m	G_i	$\bar{A}_{at}$	$\bar{A}_{rt}$	$\bar{B}$	$\bar{F}^t$	G_a^{LS}	G_r^{LS}	G_{ar}^{LS}	$\bar{G}$	$\bar{A}_{at}$	$\bar{A}_{rt}$	r	r	
Fe XXV	1s	349p			2s2p	1s2s	2	12	428	2880	0.74	1900	12	12	12	55.9	348	2880	0.98	0.98	
		351s,d			2p ²	1s2p		15	909	5720	0.81	5540	6	12	6	55.9	582	5720	0.63	0.72	
Fe XXIV	1s ²	339p			1s2s2p	1s ² 2s	1	24	200	1300	0.32	1531	12	6	6	53.7	163	1290	1.43	2.27	
		343s,d			1s2p ²	1s ² 2p		30	429	2570	0.76	9740	12	18	12	53.6	550	2560	1.28	1.39	
		425p			1s2p3s	1s ² 3s		24	41	1330	0.66	648	12	6	6	53.9	30	1320	0.55	1.09	
		426s,d			3p	3p		72	85	1320	0.75	4610	24	16	12	53.9	118	1320	0.86	1.69	
		427p,f			3d	3d		120	15	1320	0.98	1710	40	30	20	53.9	29	1310	1.00	1.99	
		455s,d			4p	4p		72	33	1330	0.65	1580	24	18	12	53.9	48	1320	1.07	2.11	
		468s,d			5p	5p		72	17	1330	0.65	773	24	18	12	53.9	24	1320	1.10	2.20	
Fe XXIII	1s ² 2s	343p	1s ² 2p	339s	1s2s ² 2p	1s ² 2s ²	2	12	385	1260	0.11	255	12	3	3	53.4	314	1260	1.62	2.87 ^b	
		347s,d	1s ² 2p	343p	1s2s2p ²	1s ² 2s2p		60	414	2500	0.69	8600	24	45	24	53.3	530	2490	1.28	1.44	
		426p			1s2s2p3s	1s ² 2s3s		48	39	1290	0.57	530	33	12	12	53.6	39	1280	0.64	1.71	
		428s,d			3p	3p		144	81	1290	0.63	3680	66	36	24	53.6	153	1280	1.02	2.67	
		429p,f			3d	3d		240	13	1290	0.98	1530	110	60	40	53.6	36	1280	1.01	2.75	
		455s,d			4p	4p		144	31	1300	0.68	1520	66	36	24	53.6	61	1290	1.02	2.76	
		467s,d			5p	5p		144	15	1300	0.71	792	66	36	24	53.6	30	1290	0.98	2.67	
Fe XXII	1s ² 2s ²	352s,d	$\left\{ \begin{array}{l} 1s^2 2s 2p \\ 1s^2 2p^2 \end{array} \right\}$	$\left\{ \begin{array}{l} 348p \\ 342s \end{array} \right\}$	1s2s ² 2p ²	1s ² 2s ² 2p	1	30	398	2430	0.53	6306	12	18	12	53.1	510	2420	1.74	1.81	
		428p			1s2s ² 2p3s	1s ² 2s ² 3s		24	37	1260	0.65	580	12	6	6	53.3	27	1250	0.55	1.09	
		429s,d			3p	3p		72	76	1260	0.76	4160	24	18	12	53.3	105	1250	0.85	1.68	
		431p,f			3d	3d		120	12	1260	0.98	1350	40	30	20	53.3	23	1250	1.01	2.01	
		455s,d			4p	4p		72	29	1260	0.65	1370	24	18	12	53.3	41	1250	1.05	2.09	
		466s,d			5p	5p		72	14	1260	0.64	662	24	18	12	53.4	20	1260	1.07	2.14	

TABLE B-II (cont)

Fe XXI	$1s^2 2s^2 2p$	$357s, d \left\{ \begin{array}{l} 1s^2 2s^2 2p^2 \\ 1s^2 2p^3 \end{array} \right. \begin{array}{l} 352p \\ 345s \end{array}$	$1s 2s^2 2p^3$	$1s^2 2s^2 2p^2$	6	40	1140	3520	0.53	4020	32	35	32	52.8	971	3510	1.17	1.18
		429p	$1s 2s^2 2p^2 3s$	$1s^2 2s^2 2p^3 s$	60	69	2420	0.80	552	45	36	36	53.0	36	2410	0.52	0.64	
		431s, d	3p	3p	180	140	2410	0.89	3730	128	104	104	53.0	205	2400	1.25	1.52	
		433p, f	3d	3d	300	19	2420	0.99	962	225	180	180	53.0	43	2410	1.76	2.20	
		455s, d	4p	4p	180	53	2430	0.91	1450	128	104	104	53.0	80	2410	1.31	1.60	
		465s, d	5p	5p	180	26	2430	0.94	738	126	104	104	53.1	40	2420	1.30	1.60	
Fe XX	$1s^2 2s^2 2p^2$	$363s, d \left\{ \begin{array}{l} 1s^2 2s^2 2p^3 \\ 1s^2 2p^4 \end{array} \right. \begin{array}{l} 356p \\ 348s \end{array}$	$1s 2s^2 2p^4$	$1s^2 2s^2 2p^3$	15	30	2150	4530	0.51	2200	30	30	30	52.5	1150	4520	0.79	0.79
		430p	$1s 2s^2 2p^3 3s$	$1s^2 2s^2 2p^2 3s$	80	97	3500	0.89	458	74	70	70	52.7	42	3490	0.46	0.48	
		433s, d	3p	3p	240	194	3490	0.91	2840	218	210	206	52.7	243	3490	1.21	1.28	
		435p, f	3d	3d	400	24	3500	0.99	647	370	350	350	52.7	45	3490	1.73	1.83	
		455s, d	4p	4p	240	74	3510	0.94	1110	218	210	206	52.7	94	3500	1.25	1.32	
		464s, d	5p	5p	240	36	3510	0.96	556	218	210	206	52.8	46	3510	1.24	1.31	
Fe XIX	$1s^2 2s^2 2p^3$	$368s, d \left\{ \begin{array}{l} 1s^2 2s^2 2p^4 \\ 1s^2 2p^5 \end{array} \right. \begin{array}{l} 360p \\ 351s \end{array}$	$1s 2s^2 2p^5$	$1s^2 2s^2 2p^4$	20	12	3400	5450	0.49	996	12	12	12	52.2	1090	5440	0.88	0.88
		431p	$1s 2s^2 2p^4 3s$	$1s^2 2s^2 2p^3 3s$	60	120	4500	0.96	345	60	60	60	52.4	41	4490	0.35	0.35	
		434s, d	3p	3p	180	239	4490	0.94	2020	165	180	165	52.4	225	4490	0.95	0.95	
		433p, f	3d	3d	300	27	4500	0.99	402	275	300	275	52.5	37	4490	1.37	1.37	
		455s, d	4p	4p	180	90	4510	0.98	790	165	180	165	52.5	86	4500	0.96	0.96	
		463s, d	5p	5p	180	44	4520	0.99	389	165	180	165	52.5	42	4510	0.96	0.96	
Fe XVIII	$1s^2 2s^2 2p^4$	$373s, d \left\{ \begin{array}{l} 1s^2 2s^2 2p^5 \\ 1s^2 2p^6 \end{array} \right. \begin{array}{l} 364p \\ 355s \end{array}$	$1s 2s^2 2p^6$	$1s^2 2s^2 2p^5$	15	2	4810	6300	0.47	301	2	2	2	51.9	1029	6300	0.38	0.38
		432p	$1s 2s^2 2p^5 3s$	$1s^2 2s^2 2p^4 3s$	24	139	5420	0.97	215	24	24	24	52.2	38	5420	0.28	0.28	
		435s, d	3p	3p	72	274	5410	0.95	1240	68	72	68	52.2	211	5410	0.78	0.79	
		438p, f	3d	3d	120	28	5420	0.99	219	120	120	120	52.2	33	5420	1.20	1.20	
		454s, d	4p	4p	72	102	5430	0.98	482	68	72	58	52.2	80	5430	0.78	0.79	
		462s, d	5p	5p	72	50	5440	0.99	236	68	72	68	52.2	39	5440	0.79	0.79	

^aThe tabulated value of $\bar{A}_{at}$ is for the configuration i only. The values of r were calculated including also values of $\bar{A}_{at}$ for i' , namely: Fe XXIII, 409 and 166; XXII, 211 and 98; XXI, 199 and 93; XX, 188 and 89; XIX, 177 and 85; XVIII, 166 and 80.

^bComputed by the approximate method, using $G_r = G_{ar} = 6$.

Similarly, for the limiting case $A_{rt}^j \ll A_{at}^j$ (all j),

$$\bar{F}^t \approx \frac{G_j}{G_m} \bar{A}_{rt} \quad (B.35)$$

These two limiting cases can be combined into the single expression

$$\bar{F}^t \approx \frac{G_j}{G_m} \bar{A}_{at} \frac{\bar{A}_{rt}}{\bar{A}_{at} + \bar{A}_{rt}} \quad (B.36)$$

Because of sum rules applicable to radiative line strengths [see (A.17)] and to autoionization transition probabilities, both $\bar{A}_{rt}$ and $\bar{A}_{at}$ are independent of coupling conditions and can be evaluated under the assumption of pure LS coupling.

When radiative and autoionization decay rates are comparable, or when selection rules are important because of the existence of fairly pure coupling conditions, (B.36) may be only a very rough approximation. In an attempt to derive a better expression for $\bar{F}^t$, we take the following approach. In the summation over j in (B.32), we neglect all terms for which either A_{at}^j or A_{rt}^j is abnormally small. For the remaining levels j , we replace the actual transition probabilities by weighted averages similar to (B.29) and (B.30), except averaged over only these values of j . Thus,

$$\bar{F}^t \approx \frac{G_{ar}}{G_m} \bar{A}'_{at} \frac{\bar{A}'_{rt}}{\bar{A}'_{at} + \bar{A}'_{rt}} \quad (B.37)$$

where

$$\bar{A}'_{at} \approx \frac{G_j}{G_a} \bar{A}_{at} \quad (B.38)$$

$$\bar{A}'_{rt} \approx \frac{G_j}{G_r} \bar{A}_{rt} \quad (B.39)$$

Here G_a , G_r , and G_{ar} are total statistical weights for those levels of the configuration j for which, respectively, only A_{at}^j , only A_{rt}^j , and both are not abnormally small, under the coupling conditions actually present. Combining (B.37)-(B.39) we obtain

$$\bar{F}^t \approx \frac{G_j}{G_m} \bar{A}_{at} \bar{B} \quad (B.40)$$

where

$$\bar{B} \approx \frac{G_{ar} \bar{A}_{rt}}{G_r \bar{A}_{at} + G_a \bar{A}_{rt}} \quad (B.41)$$

is an approximate expression for the mean branching ratio (B.31). When departures from pure coupling are extreme, G_a , G_r , and G_{ar} will all be approximately equal to G_j ; (B.36) will then be valid even when autoionization and radiative decay rates are comparable. By and large, however, selection-rule effects are great enough that the more complicated expression (B.41) should be used. As an extreme example, for the case

we have $G_j = G_a = 12$, but the rigorous ΔJ selection rule $1 \rightarrow 0$ makes $G_r = G_{ar} = 6$; if $1s 2s^2 2p$ were closely LS coupled, then we would have $G_r = G_{ar} = 3$. Similarly, if in the case

the two bound configurations were closely LS coupled, then only the two 2P terms of $1s 2p 3s$ could autoionize, and only one of these could decay radiatively (one 2P would be based on $1s 2p^3 P$, and this could not decay to $1s^2 1s$); thus we would have $G_j = 24$, $G_a = 12$, $G_r = G_{ar} = 6$. Although such extreme LS selection rules are seldom valid for individual spectrum lines, sample calculations indicate that the array-averaged expressions (B.40)-(B.41) work best when these rules are assumed to apply rigorously.

A suitable expression for $\bar{A}_{rt}$ is given by (A.21), which requires knowledge only of the radial dipole integral P (in Bohr units) and the mean transition energy $\bar{\sigma}$ (in cm^{-1}). For $1s$ - $2p$ transitions in Fe ions, $\bar{\sigma} \approx 5.3 \cdot 10^7 \text{ cm}^{-1}$ and $P \approx 0.049$ for all ions so that

$$\bar{A}_{rt}(\text{Fe } 1s-2p) \cong 1.2 \cdot 10^{14} w_j (3 - w_i) \quad , \quad (\text{B.42})$$

where $w_i = 1$ for Fe XXV and $w_i = 2$ for all lower ionization stages.

For the quantity $\bar{A}_{at}$ we need, from (B.29) and (B.7), a value (averaged over all states j) of

$$\sum_m A_a^{jm} = \sum_m \left[\left(\sum_i A_a^{ji} \right)_{\text{fixed } m \text{ and } J_i} \right] \quad . \quad (\text{B.43})$$

Because this averaged sum is (essentially) independent of coupling conditions, we may assume j and i to be pure LS-coupled basis states. Then because of the Coulomb-operator selection rules

$L_i S_i J_i = L_j S_j J_j$, the summation over i in (B.43) reduces to a summation over ℓ' . In all cases of present interest, there are at most two possible values of ℓ' (Table B-II) and one of these (usually the larger of the two) is much more important than the other. We therefore limit the summation over i to this single term, and likewise approximate the summation over m by the largest term (there are usually only one or two terms anyway):

$$\begin{aligned} \bar{A}_{at} &\cong \left\langle \left(A_a^{ji} \right)_{\text{max}} \right\rangle_j \\ &= \frac{2\pi}{h} \left\langle \left(\sum_k r_k R^k \right)_{\text{max}}^2 \right\rangle_j \quad , \end{aligned}$$

where R^k is a standard two-electron Coulomb radial integral except that one of the four radial wavefunctions involved is a continuum function [see (B.46) below], and r_k is the corresponding angular integral. The summation is over those integral values of k allowed by the four one-electron orbital angular momenta involved, and in the cases of interest usually consists of only one or two terms; we again approximate the sum by the largest term, and have

$$\bar{A}_{at} \cong \frac{2\pi}{h} \left(\bar{r}_k R_{\text{max}}^k \right)^2 \quad . \quad (\text{B.44})$$

For pure LS coupling, and for LS terms for which autoionization is allowed, typical values of the mean $|r_k|$ are about 0.8 for $k = 0$ and 0.4 otherwise. Thus with R^k measured in $\text{Ry}^{1/2}$ (Sec. B-3),

$$\begin{aligned} \bar{A}_{at} &\cong \frac{G_a^{LS}}{G_j} \cdot \frac{2\pi \cdot 0.4^2}{1.055 \cdot 10^{-27} \text{ erg-sec} \cdot 4.59 \cdot 10^{10} \text{ Ry/erg}} \\ &\times \left[\max(R^k, 2R^0) \right]^2 \\ &\cong \frac{G_a^{LS}}{G_j} \cdot 2 \cdot 10^{16} \left[\max(R^k, 2R^0) \right]^2 \quad , \quad (\text{B.45}) \end{aligned}$$

where G_a^{LS} is the total statistical weight of those levels of the configuration j for which autoionization is allowed under pure-LS coupling conditions.

The expressions (B.20), (B.40)-(B.41), (A.21) [or (B.42) for Fe K_α radiation], and (B.45) provide a means of calculating approximate dielectronic recombination rates of highly ionized atoms. No detailed spectrum calculations are involved--only the RX radial-wavefunction calculations for the configurations i , j , and k that provide the various configuration-average energies E^m , E^j , and E^k (from which $\epsilon \equiv E_s \cong E^j - E^m$ and $\bar{\sigma} \cong E^j - E^k$ are obtained), the radial dipole integral P for the radiative transition $j \rightarrow k$, and the Coulomb radial integrals R^k for the autoionization transition $j \rightarrow i$.

Results calculated by these approximate formulae are compared in Tables B-II and B-III with those obtained by the detailed computer method of Sec. B-5. (The results for aluminum ions are of course not pertinent to the iron-seeded plasma discussed in this report, but are included to provide examples for a lower Z element.) The columns labeled "Approximate" give $\bar{A}_{at}$ as calculated from (B.45), $\bar{A}_{rt}$ as calculated from (A.21) [using the tabulated individual values of $\bar{\sigma} = E^j - E^k$ rather than the overall mean value employed for Fe in (B.42) in order to illustrate better the inherent accuracy of (A.21) for $\Delta n \neq 0$ transitions], and the ratio r of the approximate $\bar{F}^E$ (B.40)-(B.41) to the detailed value (B.22). The "Rough" values of r , calculated using the approximate $\bar{A}_{at}$ and $\bar{A}_{rt}$ in (B.36) instead of in (B.41), show that it is important to take the

TABLE B-III

MISCELLANEOUS DIELECTRONIC RECOMBINATION PROCESSES IN Fe AND Al IONS
 ($\epsilon = E_s$ IN Ry; $\bar{\sigma}$ IN MK = 10^6 cm^{-1} ; $\bar{A}_{at}$, $\bar{A}_{rt}$, and $\bar{F}^t$ IN UNITS OF 10^{11} sec^{-1})

	i		j	k	G _m	G _j	Detailed				Approximate				Rough			
	m	εl'					$\bar{A}_{at}$	$\bar{A}_{rt}$	$\bar{B}$	$\bar{F}^t$	G ^{LS} _a	G ^{LS} _r	G ^{LS} _{ar}	$\bar{\sigma}$		$\bar{A}_{at}$	$\bar{A}_{rt}$	r
Fe XXI	2s ² 2p	0.85s,d	2s2p ² 10p	2s ² 2p10p	6	180	41.1	0.144	0.0035	4.3	128	108	104	0.59	110.2	0.066	0.44	0.46
		0.90d,g	10f	10f		420	30.7	0.144	0.0046	9.8	315	252	252	0.59	57.6	0.066	0.47	0.47
		0.90i,l	10h	10k		900	8.8	0.144	0.0145	19.1	675	540	540	0.59	17.1	0.066	0.51	0.51
		3.4s,d	15p	15p		180	11.7	0.144	0.0120	4.2	128	108	104	0.59	31.7	0.066	0.45	0.47
		3.4d,g	15f	15f		420	8.7	0.144	0.0155	9.4	315	252	252	0.59	16.3	0.066	0.49	0.49
		3.4i,l	15k	15k		900	3.0	0.144	0.0401	17.8	675	540	540	0.59	5.7	0.066	0.55	0.55
Fe XXI	2s ² 2p	25p	2s2p3p3s	2s ² 2p3s	6	144	334	30.6	0.079	634	99	36	36	8.64	344	30.4	0.93	1.06
		27s,d	2s2p3p ²	3p		180	14.7	61.2	0.744	328	128	108	104	8.64	33.0	60.9	1.68	1.96
		28p,f	2s2p3p3d	3d		720	42.1	30.3	0.242	1222	495	180	180	8.62	317	30.1	2.4	2.70
		61s,d	5p	5p		432	2.0	31.6	0.819	116	297	108	108	8.73	6.2	31.4	1.30	3.20
		62d,g	5f	5f		1008	7.9	31.7	0.706	940	693	252	252	8.73	43.6	31.5	1.88	3.27
		62f,h	5g	5g		1296	1.6	31.6	0.920	320	891	324	324	8.74	6.5	31.5	1.49	3.65
Al XII	1s	88p	2s2p	1s2s	2	12	421	172	0.210	531	12	12	12	13.80	345	172	1.30	1.30
		89s,d	2p ²	1s2p		15	865	338	0.141	916	6	12	6	13.78	553	339	1.06	1.72
Al XI	1s ²	83p	1s2s2p	1s ² 2s	1	24	181	69.2	0.090	391	12	6	6	12.70	149	68.4	2.19	2.88
		85s,d	1s2p ²	1s ² 2p		30	379	136	0.132	1508	12	18	12	12.68	486	134	1.50	2.09
		102p	1s2s3p	1s ² 2s		24	49.5	17.3	0.220	262	12	6	6	14.76	40.7	17.2	0.85	1.11
		108p	1s2s4p	1s ² 2s		24	20.3	6.9	0.209	102	12	6	6	15.45	16.7	6.9	0.89	1.14
		103s,d	1s2p3p	1s ² 2p		72	77.6	17.0	0.109	608	24	18	12	14.69	107	17.0	1.11	1.74
		109s,d	1s2p4p	1s ² 2p		72	30.5	6.8	0.137	300	24	18	12	15.37	42.8	6.8	0.90	1.41
		122p	1s3s3p	1s ² 3s		24	10.6	18.2	0.357	90	12	6	6	14.97	8.6	18.1	0.92	1.55
		129p	1s3s4p	1s ² 3s		24	4.2	7.1	0.531	54	12	6	6	15.70	3.5	7.0	0.62	1.03
		123s,d	1s3p ²	1s ² 3p		30	22.1	36.3	0.508	338	12	18	12	14.96	27.9	36.3	1.15	1.40
		129s,d	1s3p4p	1s ² 3p		72	7.3	7.1	0.226	119	24	18	12	15.68	9.4	7.0	1.42	2.44

effects of selection rules into account, even though departures from pure coupling conditions are rather great.

The accuracy of the approximation (A.21) for $\bar{A}_{rt}$ is quite high for $\Delta n \neq 0$ transitions (usually better than 1% in highly ionized atoms). However, the accuracy of this approximation may be very low for $\Delta n = 0$ transitions (Table B-III). This is because the energy-level spread within a configuration is comparable to the distance $E^j - E^k$ between centers of gravity of the two configurations, and because the strong spectrum lines tend to be the high-energy lines of the array. The accuracy can be improved by using $\bar{O} = c(E^j - E^k)$ with $c = 1.2$ to 1.4 (thereby increasing $\bar{A}_{rt}$ by a factor of 1.7 to 2.7). The accuracy of the approximation (B.45) for $\bar{A}_{at}$ is generally poor. Even so, (B.40)-(B.41) usually gives results good to about a factor 2.

B-8. ASYMPTOTIC DEPENDENCE ON $n\ell$ OF AUTOIONIZATION TRANSITION PROBABILITIES

With increasing n or ℓ of the (most highly) excited electron in the recombined atom (B.24), $\bar{A}_a$ decreases rapidly but $\bar{A}_r$ remains essentially constant. It follows from (B.40)-(B.41) that (for sufficiently large $n\ell$) dielectronic recombination rates are proportional to $\bar{A}_a$ and hence from (B.44) to the square of the largest of the configuration-interaction radial integrals

$$R^k = \int_0^\infty \frac{2r_1^k}{r_1^{k+1}} P_{n_1 \ell_1}(r_1) P_{n\ell}(r_1) P_{n_2 \ell_2}(r_2) P_{n_2 \ell_2}(r_a) P_{\epsilon \ell}(r_b) dr_1 dr_2, \quad (B.46)$$

where $r_a = r_1$ and $r_b = r_2$ for the direct Coulomb interaction, and $r_a = r_2$ and $r_b = r_1$ for the exchange interaction. For large $n\ell$, ϵ is essentially constant and the only variable function is $P_{n\ell}(r_2)$. The value of this function is unimportant at large r_2 because of the denominator r_2^{k+1} , and because of the oscillatory form of $P_{\epsilon \ell}(r_2)$ [direct integral] or the exponential cutoff of $P_{n_2 \ell_2}(r_2)$ [exchange integral].

At small r_2 , the shape of $P_{n\ell}(r_2)$ is independent of n and merely decreases in amplitude like $n^{-3/2}$, so that $\bar{A}_a \propto n^{-3}$.

The dependence on ℓ cannot be described simply, but will depend on the shape of the effective radial potential

$$V(r) = -\frac{2Z^*}{r} + \frac{\ell(\ell+1)}{r^2}.$$

This is positive [and hence $P_{n\ell}(r_2)$ will have very small amplitude] out to a critical radius

$$r_c = \frac{\ell(\ell+1)}{2Z^*} \propto \ell^2.$$

Hence, exchange integrals rapidly become negligibly small with increasing ℓ because of the exponential cutoff of $P_{n_2 \ell_2}(r_2)$. Direct integrals are not cut off in this fashion by the continuum function, but should decrease at least as fast as $1/r_c^{k+1} \propto 1/\ell^{2k+2}$.

Thus, asymptotic behavior of the dielectronic recombination rate R_d should be something like

$$\bar{A}_a \propto \frac{1}{n^3 \ell^{2k+2}}, \quad (k = k_{\min}) \quad (B.47)$$

For recombinations in which the second excited electron corresponds to an electric-dipole-allowed excitation ($k_{\min} = |\ell_1 - \ell_2| = 1$),

$$\bar{A}_a \propto \frac{1}{n^3 \ell^4}. \quad (B.48)$$

Some examples for Fe XXI, calculated by the detailed method described in Sec. B-5, are shown in Fig. B-4. Note that as $\ell \rightarrow n-1$, the dependence on ℓ becomes much stronger than the above rough estimate.

Fig. B-4. Dependence on nl of the mean autoionization transition probability (B.29) for two cases in Fe XXI. Note that the minimum energetically-allowed value of n is much greater for $\Delta n' = 0$ excitation of the inner electron (right) than for $\Delta n' \neq 0$ (left), and that the branching ratio (B.41) is small for many more $\Delta n' = 0$ than $\Delta n' \neq 0$ cases.

APPENDIX C

ACCURACY OF THE BURGESS FORMULA

Dielectronic recombination rate coefficients for use in the ionization-equilibrium and power-loss calculations were obtained from the Burgess formula (25) for $\Delta n = 0$ excitations. In view of the large uncertainties in other important rate coefficients (particularly for collisional ionization), it did not seem appropriate to expend the effort required to calculate accurate values for all the ions involved, and we limited ourselves to making a rough

modification to the Burgess formula for $\Delta n \neq 0$ excitations. This modification was arrived at by making a least squares fit to some results of Shore²⁹ and results of our own early crude calculations; it consisted (page 8) of replacing the function $A(x)$ by a modified function $A'(x)$, which reduced the value of α_d by a factor of 2 to 4 below that given by Burgess' original formula (which was primarily intended for application to $\Delta n = 0$ cases).

We later developed much more refined methods of computing α_d , which are however very time consuming and so have as yet been applied only to a number of specific cases in Fe ions. Preliminary indications are that the above $\Delta n \neq 0$ modification was in the right direction, but only roughly correct in magnitude. In addition, there appear to be some $\Delta n = 0$ cases (involving especially simple configurations) for which the Burgess formula gives values that are appreciably too large. For illustrative purposes, we consider in some detail the following four cases:

$$\text{Fe XXI } 1s^2 2s^2 2p \ell \ell' \rightarrow 1s^2 2s 2p^2 n \ell + 1s^2 2s^2 2p n \ell, \quad n \geq 10,$$

$$\text{Fe XXII } 1s^2 2s^2 \ell \ell' \rightarrow 1s^2 2s 2p n \ell + 1s^2 2s^2 n^2, \quad n \geq 11,$$

$$\text{Fe XXI } 1s^2 2s^2 2p \ell \ell' \rightarrow 1s^2 2s 2p 3p n \ell + 1s^2 2s^2 2p n \ell, \quad n \geq 3,$$

$$\text{Fe XXI } 1s^2 2s^2 2p \ell \ell' \rightarrow 1s 2s^2 2p^2 n \ell + 1s^2 2s^2 2p n \ell, \quad n \geq 2.$$

Basically, each term of the Burgess formula (25) is an analytical fit to our approximate expression (21)-(22): $G_{j_0} A_{r,m}^{j_0} / G_m$ has been replaced with the aid of (A.14) by $0.667 \bar{f} \sigma^2$, where $\bar{f}$ is the averaged array absorption oscillator strength defined in (A.19); $\bar{E} = E_s^\infty / a$ represents an effective mean value of $E_s \equiv E_s^{n\ell}$, averaged over all $n\ell$; and the product $B(z) A(x)$ represents an analytical fit to $\sigma^2 \sum B_n(\infty)$, assuming all $C^{n\ell} = 1$. [Note that σ^2 is approximately equal to $(109737 E_s^\infty)^2$ only for $\Delta n \neq 0$ transitions, for reasons discussed on page 41.]

In Table C-I, we compare values of $\alpha_d(j_0)$ given by the Burgess formula with those (horizontal line labeled $\bar{A}_{at}$) given by numerical evaluation of (21)-(24), using values of $A_a^{n\ell} \equiv \bar{A}_{at}$ and $A_r^{j_0} \equiv \bar{A}_{rt}$ obtained from (B.29)-(B.30) and detailed spectral calculations of the individual transition probabilities A_a^{jm} and A_r^{jk} . The agreement is quite good for the $\Delta n = 0$ excitations, especially considering that we have lost about 10% by truncating the summation in (22) at $\ell = 8$. For the $\Delta n \neq 0$ excitations, the Burgess formula gives results too large by factors of 2 to 3 or more. (Shore²⁹ has noted this point also; a factor 5 for $1s-2p$ excitation in recombination to O VII can be inferred from Table 1 of his

paper.) Our modification $A'(x)$ provides considerable improvement for Fe XXI $2s-3p$; it overcorrects for $1s-2p$, but this excitation contributes little to the total dielectronic recombination rate.

We wish to emphasize that the above discussion relates only to the accuracy with which the Burgess formula represents the expression (21)-(22). This latter involves several approximations, which have been made in practically all treatments of dielectronic recombination in the literature. In many cases these approximations are highly suspect. They have been discussed at some length in connection with Eqs. (B.14)-(B.36), with emphasis on the $1s-n'\ell'$ excitations relevant to the K_α diagnostic problem. Here we repeat some of this discussion, with emphasis on the $2s-n'\ell'$ and $2p-n'\ell'$ excitations important for the calculation of α_d .

There are first of all the fundamental approximations inherent in the use of the one-electron central-field model and (in most cases) the single-configuration approximation. The resulting errors are difficult to estimate. They may be quite large in some individual values of A_a^{jm} and A_r^{jk} , or even fairly large in the averaged array-total values $\bar{A}_{at}$ and $\bar{A}_{rt}$ for a few isolated cases. However, by the time we have summed over all $n\ell$ and j_0 to obtain the total rate coefficient α_d , it is doubtful that errors arising from this source are greater than about $\pm 20\%$ for highly ionized atoms. Other sources of error which are much easier to estimate quantitatively, are the following:

(a) We have assumed (page 31) that, before recombining, all atoms of any given ionization stage are statistically distributed among the levels of the ground configuration. This will certainly be a poor approximation at low electron density for ground configurations involving more than one LS term. However, extreme cases like that of (B.23) will not occur for L-shell excitations in the ions of interest here, because the analogous case $1s^2 2s^2 2p^3 \ell \ell' \rightarrow 1s^2 2s 2p^5$ is not energetically allowed. By the time we have summed over $n\ell$ and j_0 , and at the densities of interest here, the error arising from this assumption should be small--of about the same magnitude as that arising from the following:

(b) The approximation (B.36) involving $\bar{A}_{at}$ and $\bar{A}_{rt}$ has been employed in Eq. (22), in place of the

TABLE C-1

COMPARISON OF NUMERICAL CALCULATIONS OF $\alpha_d(j_o)$ WITH THE BURGESS FORMULA FOR $T_e = 1$ keV

	Fe XXI 2s-2p	Fe XXII 2s-2p	Fe XXI 2s-3p	Fe XXI 1s-2p
<u>Input Data</u>				
Statistical weight, G_m	6	1	6	6
Statistical weight, G_{j_o}	30	12	72	30
C_F^{3p} or C_g^{2p}	----	----	144/432 ^a	40/180 ^b
C_r^{3p} or C_r^{2p}	----	----	2 ^a	3/2 ^b
E_S^∞ (Ry)	5.4	4.1	80	483
$A_r^{j_o}$ (sec^{-1})	$1.44 \cdot 10^{10}$	$4.61 \cdot 10^9$	$3.16 \cdot 10^{12}$	$2.42 \cdot 10^{14}$
f	0.183	0.187	0.745	0.645
<u>$\alpha_d(j_o)$ (cm^3/sec)</u>				
Burgess, $A(x)$	$3.1 \cdot 10^{-12}$	$3.0 \cdot 10^{-12}$	$14.3 \cdot 10^{-12}$	$6.4 \cdot 10^{-14}$
$A^+(x)$	----	----	$5.2 \cdot 10^{-12}$	$1.7 \cdot 10^{-14}$
Numerical, $\bar{A}_{at}$	$2.8 \cdot 10^{-12}$	$2.7 \cdot 10^{-12}$	$4.1 \cdot 10^{-12}$	$3.3 \cdot 10^{-14}$
$\bar{A}_{at}^{\text{eff}}$	$2.5 \cdot 10^{-12}$	$1.7 \cdot 10^{-12}$	$3.1 \cdot 10^{-12}$	$3.1 \cdot 10^{-14}$

^aSee Table B-III; a more accurate value of C_r^{3p} is 61.2/31.6.^bSee Table B-II; a more accurate value of C_r^{2p} is 3520/2430.

detailed sum (B.32) involving the individual A_a^{jm} and A_r^{jk} . An indication of the magnitude of the resulting error is given in Table C-II. As discussed in Sec. B-7, the error is particularly serious when $\bar{A}_{at} \approx \bar{A}_{rt}$, and also (ratios as low as 0.3) when conditions in the ion lie close to pure LS coupling or involve especially simple configurations so that selection-rule restrictions become especially important. Fortunately, conditions in the iron ions of interest here usually lie far from pure LS coupling; also, the number of terms in the summation over $n\ell$ in Eq. (20) for which $\bar{A}_{at} \approx \bar{A}_{rt}$ is not great, and so the approximation (21)-(22) is not too severe. Nevertheless, the error is not negligible. In order to remove this approximation, but still be able to use the formalism provided by (22), we define an effective value $\bar{A}_{at}^{eff}$ that, when used in (B.36) in place of $\bar{A}_{at}$, will give the detailed result (B.32)--namely,

$$\frac{\bar{A}_{at}^{eff} \bar{A}_{rt}}{\bar{A}_{at}^{eff} + \bar{A}_{rt}} = \frac{1}{G_j} \sum_j R_j \frac{A_{at}^j A_{rt}^j}{A_{at}^j + A_{rt}^j} \equiv y, \quad (C.1)$$

or

$$\bar{A}_{at}^{eff} = \left[\frac{1}{y} - \frac{1}{\bar{A}_{rt}} \right]^{-1}. \quad (C.1)$$

By using this quantity in (22) in place of A_a^{nk} , we obtain the corrected value of $\alpha_d(j_o)$. [Note that Eq. (23) has to be somewhat modified because $\bar{A}_{at}^{eff}$ varies as n^{-3} only at very large n .] Values obtained in this manner are given in the final line of Table C-I. The effect of removing the approximation is greatest (a 35% decrease) for

$$\text{Fe XXII } 1s^2 2s^2 2p^2 \ell' \rightarrow 1s^2 2s^2 2p n \ell + 1s^2 2s^2 n \ell, \quad$$

where particularly simple configurations are involved; for more complex ions it would appear to produce only a 10-20% decrease.

(c) In obtaining (B.36) from (B.22), we have truncated the summations over k and k' to include only decay of the inner excited electron. It is generally assumed^{7-9,29} that the truncation is not

TABLE C-II

RATIO OF THE DETAILED SUM (B.32)
TO THE ARRAY-AVERAGE EXPRESSION (B.36)

Final Ion	Excitation	$n\ell$	$\bar{A}_{at}$	$\bar{A}_{rt}$	Ratio ^a
Fe XXI	2s-2p	10g	$3.27 \cdot 10^{12}$	$1.44 \cdot 10^{10}$	0.98
		40g	$4.71 \cdot 10^{10}$	$1.44 \cdot 10^{10}$	0.84
		150g	$8.94 \cdot 10^8$	$1.44 \cdot 10^{10}$	0.96
Fe XXII	2s-2p	11d	$1.00 \cdot 10^{12}$	$4.61 \cdot 10^9$	0.90
		25d	$7.79 \cdot 10^{10}$	$4.61 \cdot 10^9$	0.75
		60d	$5.64 \cdot 10^9$	$4.61 \cdot 10^9$	0.55
		150d	$3.62 \cdot 10^8$	$4.61 \cdot 10^9$	0.78
Fe XXI	2s-3p	3s	$3.34 \cdot 10^{13}$	$3.06 \cdot 10^{12}$	0.94
		6s	$1.48 \cdot 10^{12}$	$3.17 \cdot 10^{12}$	0.59
		25s	$1.53 \cdot 10^{10}$	$3.18 \cdot 10^{12}$	0.79

^aOther values of this ratio can be obtained from the "detailed" entries in Tables B-II and B-III, and the relation $\text{Ratio} = \bar{B}(\bar{A}_{at} + \bar{A}_{rt})/\bar{A}_{rt}$. For the 1s-2p excitations in Fe XXIII to XVIII, the additional $\bar{A}_{at}$ given in the table footnote must be included, and the resulting ratios then include also the effects of the alternate autoionization paths discussed in the text [approximation (e)].

serious, and this is probably true so far as calculation of the total α_d is concerned; however, the truncation can be a very crude approximation in certain terms contributing to the total. In Fe XXI $2s^2 2p \ell' - 2s 2p^2 10d$, for example, we calculate that inclusion of decay of the 10d electron to $2p, 3p, 4p, 4f \dots$ increases the radiative decay rate by a factor of about 25 over the value given by the $2p \rightarrow 2s$ decay. This means that C_r^{10d} in Eq. (22) is equal to 25, and (because A_a^{10d} is very large--see Fig. B-4) that the $\ell = 2$ contribution to B_{10} in Eq. (22) is increased by almost this same factor. The effect is smaller for larger ℓ of the highly excited electron (10f can decay only to states with $n' \geq 3$, 10g to states with $n' \geq 4$, etc),* so that the value of B_{10}

*This is not inconsistent with the statement on page 5 that $\bar{A}_{rt}$ is independent of ℓ , because the present effect is important only at small n , whereas the collisional redistribution (as we shall see shortly) is important only at large n .

is increased by a factor of only 5 over that plotted in Fig. 1. Also, the effect falls off very rapidly with increasing n , becoming unimportant by about $n = 25$. We estimate the total effect on $\alpha_d(j_0)$ to be only about 30% for Fe XXI 2s-2p, and about 15% for Fe XXI 2s-3p.

(d) It is important to realize that in the usual application of the Burgess formula (including the manner in which we have used it), the summations kk' have not only been restricted to include decay of only the inner excited electron, but also this decay has been assumed to be the inverse of the original excitation; i.e., the decay has been assumed to be a return to the ground configuration of the ion core. This is evident from the fact that in Eq. (25) the oscillator strength f_{im} corresponding to the radiative decay is for the same transition as the excitation energy $\bar{E}$, and it implies that only dipole-allowed excitations are to be considered. However, dipole-forbidden excitations such as 2s-3s, 2s-3d, 2p-3p are in no way forbidden under the Coulomb forces involved in dielectronic recombination; in fact, for the one case we have checked (Fe XXI 2s-3d), the values of $\bar{A}_{at}$ are essentially the same as for the dipole-allowed excitation 2s-3p. Radiative stabilization can take place not only by decay of the outer electron, as discussed under (c), but usually (at least for $\Delta n \neq 0$ excitations) also by decay of the inner electron; e.g., for the excitation 2s-3d, stabilization can take place via the very strong decay 3d-2p. The total contribution to α_d of all dipole-forbidden excitations is probably between 50 and 100% as large as the total from dipole-allowed $\Delta n \neq 0$ excitations.

(e) In obtaining (B.36) from (B.22), we have truncated the summation over m' to include reionization only to levels m of the ground configuration of the ion. This involves no approximation whatever for minimum excitation of the recombining ion (2s-2p), but for $\Delta n \neq 0$ excitations the effect can be very large. For example, in Fe XXI 2s²2p²l'-2s2p3p3d, we calculate inclusion of reionization to 2s2p²l' to increase the total autoionization rate by a factor 22; this practically eliminates the contribution of the term $n\bar{l} = 3d$ to $\alpha_d(2s-3p)$. For other $n\bar{l}$, a more typical increase in the total $\bar{A}_{at}$

is a factor of about 4 rather than 22. Assuming this value for all $n\bar{l}$ except 3d produces an overall decrease in $\alpha_d(2s-3p)$ of only about 40%, the importance of the effect being reduced by the presence of the term $\bar{A}_{rt}$ in the denominator of (B.36). If we assume such a decrease for all $\Delta n \neq 0$ excitations (which comprise about 70% of the total), the reduction in the total α_d would be about 30%.

(f) The remarks under the headings (b) to (e) apply to the low-electron-density limit. At higher densities there are additional complications. There is firstly the cutoff (18) at the principal quantum number n_t , which from Eq. (19) occurs at $n_t \approx 65$ for $n_e = 10^{16} \text{ cm}^{-3}$. From Fig. 2, the effect is seen to be important only for the 2s-2p excitation, where it reduces the contribution $\alpha_d(2s-2p)$ by 25%; the reduction in the total α_d is only about 0.3 of this, or 8%--as stated on page 7. Lowering of the ionization limit by the sea of free electrons also introduces a finite maximum possible value of n , but at our density this occurs far above n_t . There is, however, a second important density effect of a different sort--namely, collisional redistribution of ions with outer excited electron $n\bar{l}$ from small l (the states for which recombination is most likely) to large l (the states carrying most of the statistical weight). Since (for large n) most of the statistical weight lies at $l \approx 9$, where the reionization rate A_a is small (Fig. B-4), the redistribution reduces the mean effective autoionization rate, as discussed on pages 4-5.* In order to obtain a rough estimate of this effect, we replace $A_a^{n\bar{l}}$ in the denominator of Eq. (22) by an effective rate

$$A_a^{n\bar{l}} N_c/N, \quad (C.2)$$

where N_c/N is the fraction of ions having l values for which $\bar{A}_{at}$ is relatively large (e.g., $l \leq l_1 \approx 7$). We estimate N_c from

* Since typing that portion of the report, we have become aware of a recent paper by Weiss ³⁰ that also discusses this point.

$$\frac{N_c}{N} \approx 1 - \frac{N_c}{N} = 1 - \frac{G_c}{G} \left(\frac{R_c}{\bar{A}_{at} + R_c} \right)$$

$$= \frac{\bar{A}_{at} + R_c G_c/G}{\bar{A}_{at} + R_c} \quad (C.3)$$

where R_c is the redistribution rate, and where (for any given $n > 2_1$) $G_c/G = (i_1 + 1)^2/n^2$ is the ratio of the statistical weight for $i_1 \pm 2_1$ to that for all i . The redistribution is caused mainly by heavy-particle collisions, rather than by electron collisions, and an appropriate expression for the rate coefficient is quoted by Weisheit.³⁰ At a proton density of about 10^{14} cm^{-3} , the redistribution effect is important only for $\Delta n = 0$ excitations, and then only for $n \lesssim 25$. Rough calculations indicate the effect to be an increase in $\alpha_d(2s-2p)$ of about 30% if only proton collisions are considered, and of about 80% if collisions with other Fe ions ($n_{Fe} = 10^{12} \text{ cm}^{-3}$) are also considered; even using the latter figure, the increase in the total α_d is only about 25%.

In summary, the combined effect on $\alpha(j_0)$ of deleting the kk' and m' truncations is about a +30% correction for $\Delta n = 0$ excitations, and about -25% for $\Delta n \neq 0$. Applying these corrections to the α_{at}^{eff} values in Table C-I, we conclude (as stated earlier) that the Burgess formula seems to give good results for $\Delta n = 0$ excitations except perhaps for ions involving especially simple electron configurations; however, even with the A' modification it gives results accurate only within about a factor 2 for $\Delta n \neq 0$ excitations. This latter error is serious because the $\Delta n \neq 0$ excitations contribute 70 to 80% of the total α_d .

Inclusion of dipole-forbidden $\Delta n \neq 0$ excitations would increase the total $\Delta n \neq 0$ contribution by 50 to 100%, and at the densities of interest here collisional effects would appear to increase the $\Delta n = 0$ contribution to α_d by about 50%. Overall, we judge that our use of the dipole-allowed, zero-density modified Burgess formula to calculate α_d for our finite-density plasma has given dielectronic recombination rates that are fairly close to correct. However, this result (if true) is rather fortuitous.

In view of the large number of rather sizeable corrections, it is quite possible that the values of α_d that we used were in error by as much as a factor two.

It must be emphasized that all of the above quantitative discussion is based on investigation of only a few special cases in Fe XXI and XXII. Approximations that appear to be satisfactory in these cases may be much poorer for other ions and elements. Because of the anticipated future importance of C, O, Fe, Mo, W, etc., plasma impurities, it would appear desirable that additional detailed calculations be made to clarify the overall picture as to the accuracy of the Burgess formula. In particular, a more careful investigation should be made of the importance of dipole-forbidden excitations, and of the applicability to these cases of the Burgess formula (using $\bar{E}$ and $A(x)$ for the forbidden excitation, and f_{im} for the dipole-allowed radiative decay).

REFERENCES

1. W. Lotz, "An Empirical Formula for the Electron-Impact Ionization Cross Section," *Z. Physik* **206**, 205-211 (1967).
2. W. Lotz, "Electron-Impact Ionization Cross Sections and Ionization Rate Coefficients for Atoms and Ions from Hydrogen to Calcium," *Z. Physik* **216**, 241-247 (1968).
3. H. Van Regemorter, "Rate of Collisional Excitation in Stellar Atmospheres," *Astrophys. J.* **136**, 906-915 (1962).
4. O. Bely, "Excitation of Lithium-Like Ions by Electron Impacts," *Proc. Phys. Soc. (London)* **88**, 587-595 (1966).
5. H. Brysk and C. D. Zerby, "Photoelectric Cross Sections in the keV Range," *Phys. Rev.* **171**, 292-298 (1968).
6. W. D. Barfield, G. D. Koontz, and W. F. Huebner, "Fits to New Calculations of Photoionization Cross Sections for Low-Z Elements," *J. Quant. Spectrosc. Radiat. Transfer* **12**, 1409-1433 (1972).
7. A. Burgess, "Dielectronic Recombination and the Temperature of the Solar Corona," *Astrophys. J.* **139**, 776-780 (1964).
8. A. Burgess, "Dielectronic Recombination in the Corona," *Ann. D'Astrophys.* **2E**, 774-778 (1965).
9. A. Burgess, "A General Formula for the Estimation of Dielectronic Recombination Coefficients in Low-Density Plasmas," *Astrophys. J.* **151**, 1588-1590 (1965).

10. A. Burgess and H. P. Summers, "The Effects of Electron and Radiation Density on Dielectronic Recombination," *Astrophys. J.* **157**, 1007-1021 (1969).
11. H. P. Summers, "The Density Dependent Ionization Balance of Carbon, Oxygen, and Neon in the Solar Atmosphere," *Mon. Not. R. astr. Soc.* **158**, 255-275 (1972).
12. D. R. Bates, A. E. Kingston, and R. W. P. McWhirter, "Recombination between Electrons and Atomic Ions I. Optically Thin Plasmas," *Proc. Roy. Soc. A267*, 297-312 (1962).
13. R. Bellman, Introduction to Matrix Analysis (McGraw-Hill Book Co., Inc., New York, 2nd ed., 1970), Chaps. 11, 14, 15.
14. R. Wilson, "The Spectroscopy of Non-Thermal Plasmas," *J. Quant. Spectrosc. Radiat. Transfer* **2**, 477-490 (1962).
15. H. R. Griem, Plasma Spectroscopy (McGraw-Hill Book Co., Inc., New York, 1964).
16. Ya. B. Zel'dovich and Yu. P. Raizer, Physics of Shock Waves and High Temperature Hydrodynamic Phenomena (Academic Press, New York, 1966), p. 406.
17. C. Jordan, "The Ionization Equilibrium of Elements between Carbon and Nickel," *Mon. Not. R. astr. Soc.* **152**, 501-521 (1969); "Ionization Equilibria for High Ions of Fe and Ni," *Mon. Not. R. astr. Soc.* **158**, 17-23 (1970).
18. W. Lotz, "Ionization Potentials of Atoms and Ions from Hydrogen to Zinc," *J. Opt. Soc. Am.* **57**, 873-878 (1967).
19. N. Bretz, D. Dimock, A. Greenberger, E. Hinnov, E. Meservey, W. Stodiek, and S. von Goeler, "Radiation from Plasmas in the ST Tokamak," in Plasma Physics and Controlled Nuclear Fusion Research 1974, Proc. 5th Intern. Conf., Tokyo, Nov. 11-15, 1974 (International Atomic Energy Agency, Vienna, 1975), Vol. I, p. 55.
20. R. D. Cowan, "Atomic Self-Consistent-Field Calculations Using Statistical Approximations for Exchange and Correlation," *Phys. Rev.* **161**, 54-61 (1967).
21. R. D. Cowan, "Theoretical Calculation of Atomic Spectra Using Digital Computers," *J. Opt. Soc. Am.* **58**, 808-818 (1968). The computer program described therein has since been expanded to make possible calculations with multi-configuration basis sets ("configuration-interaction calculations"), as well as calculations of auto-ionization transition probabilities and electric-dipole-forbidden radiative transition probabilities.
22. B. C. Fawcett, N. J. Peacock, and R. D. Cowan, "Classification and Oscillator Strengths of Lines in the Far Vacuum Ultra-Violet Spectrum of the Iron-Period Elements," *J. Phys. B* **1**, 295-306 (1968); G. A. Doschek, U. Feldman, R. D. Cowan, and L. Cohen, "Transitions $2s^2 2p^k - 2s 2p^{k+1}$ of the F I, O I, and N I Isoelectronic Sequences," *Astrophys. J.* **188**, 417-422 (1974).
23. Ref. 16, pp. 296 and 300.
24. A. H. Gabriel and T. M. Paget, "Measurement and Interpretation of Dielectronic Recombination Satellite Line Intensities," *J. Phys. B* **5**, 673-685 (1972).
25. U. Fano, "Effects of Configuration Interaction on Intensities and Phase Shifts," *Phys. Rev.* **124**, 1866-1878 (1961).
26. A. H. Gabriel, "Dielectronic Satellite Spectra for Highly-Charged Helium-Like Ion Lines," *Mon. Not. Roy. astr. Soc.* **160**, 99-119 (1972), Table X.
27. C. P. Bhalla, A. H. Gabriel, and L. P. Presnyakov, "Dielectronic Satellite Spectra for Highly-Charged Helium-Like Ions--II. Improved Calculations," *Mon. Not. Roy. astr. Soc.* **172**, 359-375 (1973).
28. R. D. Cowan, unpublished calculations (1971). R. D. Cowan, L. J. Radziemski, Jr., and V. Koufman, "Effect of Continuum Configuration Interaction on the Position of sp^6 in Neutral Chlorine and Other Halogens," *J. Opt. Soc. Am.* **64**, 1474-1478 (1974).
29. B. W. Shore, "Dielectronic Recombination," *Astrophys. J.* **158**, 1205-1218 (1969).
30. J. C. Weisheit, "Recombination in Dense Plasmas," *J. Phys. B* **8**, 2556-2564 (1975). [Note that the factor T^2 in Eq. (11) should read $T^{-1/2}$.]