Radiative capture and recombination in electron-atom collisions*

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A comprehensive theory of electron scattering from atoms and ions at high energies is formulated, incorporating the coupling of the scattering system to the radiation field. In particular, the photocapture process is discussed in detail, which can proceed either by a direct radiative capture or by dielectronic recombination following a radiationless capture into excited states. The latter process involves a collisional excitation of the inner-shell electrons of the target, followed by radiative decay of that excited state. The required sum over excitation probabilities to all the allowed bound states is estimated using the semiclassical projection operators and the single-particle model for the target system. A preliminary estimate of the cross sections for these modes of capture is obtained for the case of a hot-electron plasma interacting with highly ionized impurity ions.

I. INTRODUCTION

When high-energy electrons collide with ions of asymptotic charge Z_I, many reaction channels are open for the final state of the system, such as the elastic, inelastic and the ionization channels. In particular, the coupling of the system to the radiation field produces one or more photons in the final state; thus

$$e + A(Z_C, Z_I) \rightarrow e' + A(Z_C, Z_I) + \gamma \quad (1.1)$$

$$\rightarrow A(Z_C, Z_I - 1) + \gamma \quad (1.2)$$

$$\rightarrow A^*(Z_C, Z_I - 1) \rightarrow A(Z_C, Z_I - 1) + \gamma \quad (1.3a)$$

$$\rightarrow A(Z_C, Z_I) + e\ , \quad (1.3b)$$

where Z_I is the degree of ionization of the target A and Z_C is by definition the core charge. The process (1.1) is termed bremsstrahlung for a composite target and has been the subject of many studies.[1,2] It is distinguishable from the other processes by the presence of a continuum electron and a photon in the final state, while the target atom may or may not stay in its ground state. Direct radiative capture[3] is represented by (1.2), and dielectronic recombination[4] by (1.3a) which competes[5] with Auger emission (1.3b). Again, the atom in the final state need not be in the ground state, and all possible excited states have to be summed incoherently in the estimate of the reaction cross sections.

The radiative processes (1.1)–(1.3a) are of special interest here, because they are important mechanisms for energy loss in a hot-electron plasma.[6] For example, electrons of high velocity in a fusion device are spatially confined by a strong magnetic field. However, photons produced by these electrons through the processes described above have a much longer mean free path to escape from the confinement area, thus continuously cooling the plasma itself. The rate of cooling depends critically on the relative cross sections for these reactions, in addition to other factors such as the density of the electrons and impurity ions. It is the purpose of this paper to formulate a comprehensive reaction theory which includes these channels, thus providing a systematic framework for more detailed future calculations of these cross sections.

The general formalism for the reactions (1.2) and (1.3) is presented in Sec. II in the case when typical radiation widths involved are rather small, so that the target system is not affected by the radiation field in the lowest order. The bremsstrahlung (1.1), and other processes which are higher order in the coupling to the radiation field, are considered in Sec. V.

The cross section for direct radiative capture is considered in detail in Sec. III. The target system is represented by a simple single-particle model of Green *et al.*,[7] while the sum over many available excited (bound) states is carried out using the semiclassical projection operators[8] developed earlier. This is followed by a detailed discussion of the two-step process, dielectronic recombination, in Sec. IV. Obviously, for complex atomic targets, specific autoionization levels are not well known except in some special cases, and perhaps it is not even possible to single out a subset of these states. Thus, we have considered both the isolated and overlapping resonance states. The earlier work[9] on multiple ionization of atoms and ions by high-energy electron impact is modified slightly to obtain estimates of this effect in the nonresonant situation (with the actual numerical estimate given in Sec. VI).

Refinements and extensions of the theory presented in Sec. II are considered in Sec. V, where higher-order effects in the radiation coupling are presented, including those corrections to the simple bremsstrahlung process. Throughout the formal discussion, however, the nonradiative part of the interaction is treated exactly to all orders.

Finally, a crude estimate of the dielectronic recombination cross section is presented in Sec. VI and the results compared with the value for direct capture. Although the calculation presented here is useful in clarifying the physical picture of what is going on with the system, the present paper puts emphasis on a formal and unified development of the theory and on collecting some of the methods which are useful in actually carrying out the more detailed calculations.

II. THEORY OF RADIATIVE CAPTURE AND RECOMBINATION

We consider the collision process in which an electron of energy E_i collides with ions of core charge Z_C and degree of ionization Z_I. We are interested in the capture of the electron with emission of a photon. That is,

$$e + A(Z_C, Z_I) \rightarrow B(Z_C, Z_I - 1) + \gamma \ . \tag{2.1}$$

The matrix element for this process to first order in the coupling with the radiation field is given by

$$M_{mk} = \langle \Psi_{Bm} | D_\epsilon | \Psi_{ik} \rangle \ , \tag{2.2}$$

where D_ϵ is the electromagnetic coupling operator, which, in the long-wavelength nonretardation limit, is given by

$$D_\epsilon \approx -e \sum_{i=0}^{Z_A} \vec{\epsilon} \cdot \vec{r}_i \, \alpha_\omega \quad (Z_A = Z_C - Z_I) \ . \tag{2.3}$$

Throughout the paper, we omit the explicit photon state indices from the wave functions and also the photon operators from D_ϵ to simplify notations. The correct normalization for the photon-electron coupling is given by α_ω. In (2.2), Ψ_{ik} is the initial wave function, with full interactions between the e^- and A taken into account, and Ψ_{Bm} is for the final (bound) state. Thus, Ψ_{ik} satisfies

$$(H - E)\Psi_{ik} = 0 \ , \tag{2.4a}$$

where

$$H = H_A(\vec{r}_1, \ldots, \vec{r}_A) + T_{\vec{r}_0} + V(\vec{r}_0, \vec{r}) + H_{\rm rad}$$

and similarly

$$(H - E_{Bm})\Psi_{Bm} = 0 \ . \tag{2.4b}$$

The effect of the coupling to the radiation field is neglected in (2.4a) and (2.4b); the modifications necessary to include the higher-order effect in D_ϵ are immediate, as e.g., with $H_{\rm tot} = H + D_\epsilon$,

$$\Psi_{ik}^{\rm tot} = \Psi_{ik} + GD_\epsilon \Psi_{ik} + (GD_\epsilon)^2 \Psi_{ik} + \cdots \ , \tag{2.5}$$

where

$$G = (E + i\eta - H)^{-1} \quad (\eta \rightarrow 0^+) \ .$$

The form (2.5) will be considered further in Sec. V.

The above formulation presupposes that the effect of the radiation field on the atomic structure is small so that Ψ_{ik} and Ψ_{Bm} are determined in the absence of the coupling to the radiation field. Now, consider the solution of (2.4) for Ψ_{ik}, which we simply denote without the subscripts. It is purely a scattering problem, for which we follow the usual reaction theory formulation.[10] Thus,

$$\Psi(\vec{r}_0, \vec{r}) = P\Psi + Q\Psi \ (\equiv \Psi_{ik}) \tag{2.6}$$

with

$$P = \psi_0(\vec{r}) \rangle \langle \psi_0^*(\vec{r}'), \quad Q = 1_{\vec{r}} - P \ , \tag{2.7}$$

and

$$\vec{r} \equiv (\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \ ,$$

$$H_A(\vec{r})\psi_n(\vec{r}) = e_n \psi_n(\vec{r}) \ .$$

The ψ_n's are properly antisymmetrized for all the target electrons. The scattering equation (2.4) is then written as

$$P(H - E)P\Psi = -PH\Psi \ , \tag{2.8}$$

$$Q(H - E)Q\Psi = -QHP\Psi \ . \tag{2.9}$$

We remark here on the problem of antisymmetrization between the projectile electron and those electrons in the target atom. Since the electron energy is quite high ($E_i \gtrsim 1000$ eV), we may be able to neglect the antisymmetrization when Z_C is small. On the other hand, when $Z_C \gtrsim 10$, the inner-shell electrons are bound with the energies of the same order as E_i and thus the scattering is no longer in the "high energy" regime. (However, when we introduce the single-particle model for the target states ψ_n, the problem may be less critical.) In so far as the formal theory of this section is concerned, this approximation is not needed, as we will simply *assume* that a proper form of P, different from that given in (2.7), exists.[11] This question will be discussed more fully in Secs. III and IV, however. The set of equations (2.8) and (2.9) may be solved formally using the Green's functions

$$G^P = [P(E + i\eta - H)P]^{-1} \tag{2.10}$$

and

$$G^Q = [Q(E + i\eta - H)Q]^{-1} \ . \tag{2.11}$$

The inelastic channel Green's function G^Q can in

turn be represented in terms of the eigenstates of QHQ, defined by

$$Q[H-\mathcal{E}_n]Q\Phi_n=0\ , \tag{2.12}$$

where $Q\Phi_n$ describes a multiply excited (autoionization) state. As will be seen in Sec. IV, an isolated state $Q\Phi_r$ with the energy $\mathcal{E}_r \approx E$ assumes a dominant role in G^Q. In such cases, we may conveniently split G^Q into two parts as

$$G^Q = G_S^Q + Q\Phi_r)(E-\mathcal{E}_r)^{-1}(Q\Phi_r\ , \tag{2.13}$$

where G_S^Q represents the "smooth" background contribution. The effective optical potential for the elastic channel may be defined in the usual way[10] as

$$U \equiv PHG^QHP = U_s + U_r\ , \tag{2.14}$$

where U_r is the resonant part of U involving the $Q\Phi_r$ state. As it is in general extremely difficult to estimate U or U_s, we introduce an approximate phenomenological potential U_T which simulates U in the elastic channel and the scattering equation

$$P[H-E+U_T]P\Psi^T=0 \tag{2.15}$$

with

$$P\Psi^T \equiv \psi_0(\vec{r})u_0^T(\vec{r}_0)\ . \tag{2.16}$$

The function $P\Psi^T$ may be compared with $P\Psi^{Ps}$ defined in terms of U_s as

$$P[H+U_s-E]P\Psi^{Ps}=0 \tag{2.17}$$

and the corresponding Green's function defined by

$$P[H+U_s-E]PG^{Ps}P=-P\ . \tag{2.18}$$

Since both these functions have to be introduced phenomenologically in actual calculations, we will use them interchangeably, $P\Psi^T \approx P\Psi^{Ps}$.

The collision amplitude M_{fi} for the transition $i(=ik) \to f(=Bm)$ is given to first order in D_ϵ by

$$M_{fi} \cong \langle \Psi_f | D_\epsilon | \Psi_i \rangle\ , \tag{2.19}$$

which may be conveniently written in the form

$$\begin{aligned} M_{fi} &\approx \langle \Psi_f | D_\epsilon | P\Psi_i \rangle + \langle \Psi_f | D_\epsilon G^Q H | P\Psi_i \rangle \\ &= M_{fi}^P + M_{fi}^Q\ , \end{aligned} \tag{2.20}$$

where

$$\begin{aligned} M_{fi}^P &\approx \langle \Psi_f | D_\epsilon | P\Psi_i^T \rangle\ , \\ M_{fi}^Q &\approx \langle \Psi_f | D_\epsilon G^Q H | P\Psi_i^T \rangle\ . \end{aligned} \tag{2.21}$$

Here we have neglected the following effects: (i) Radiative capture to excited states, followed by a cascade down with γ emissions and with the target still in the ground state. This process will be included in the direct radiative capture amplitude by summing over all the allowed excited-state transitions (i.e., sum over f). (ii) As electrons approach the target, they can radiate by the bremsstrahlung process, i.e., continuum $\to$ continuum transitions (real transitions). This will be dealt with separately in Sec. V, and is related to the sum over f discussed in (i). (iii) The effect of the radiation field on the atomic scattering system. This is neglected throughout.

Now we explicitly consider all the kinematic factors which are needed to obtain cross sections from the matrix elements we have defined above. To begin with, the transition probability for the process $i \to f$ is given, to first order in the electromagnetic coupling, by

$$W_{if} = (2\pi/\hbar)\rho_f |\tilde{M}_{fi}|^2\ , \tag{2.22}$$

where

$$\tilde{M}_{fi} = \int \Psi_f^* \mathcal{H}' \Psi_i\, d\tau \tag{2.23}$$

and

$$\mathcal{H}' = \mathcal{H}_e' + \mathcal{H}_m' \tag{2.24}$$

for the electric and magnetic couplings

$$\begin{aligned} \mathcal{H}_e' &= \sum_{i=0}^{Z_A} \left(-\frac{e}{m}\right)\left(\frac{2\pi\hbar}{\omega}\right)^{1/2} \vec{\epsilon}\cdot\vec{p}_i\, e^{-i\vec{k}_\omega\cdot\vec{r}_i} + \text{H.c.}, \\ \mathcal{H}_m' &= \pm \sum_{i=0}^{Z_A} \left(\frac{ie\hbar}{2m}\right)\left(\frac{2\pi\hbar}{\omega}\right)^{1/2} \vec{\epsilon}\times\vec{k}_\omega\cdot\vec{\mu}_i\, e^{-\vec{k}_\omega\cdot\vec{r}_i} + \text{H.c.} \end{aligned} \tag{2.25}$$

The differential cross section is then given by

$$\sigma_{fi}\, d\Omega \equiv W_{if}/F_i = (2\pi/\hbar)|\tilde{M}_{fi}|^2(\rho_f/F_i)\ . \tag{2.26}$$

The explicit forms for the final-state density ρ_f and the initial-state flux F_i depend on the normalization of Ψ_i and Ψ_f in the matrix element $\tilde{M}_{fi}$.

For the photocapture process of interest here, we have

$$\rho_f = \frac{1}{(2\pi\hbar)^3}\,\frac{\hbar^2\omega^2}{c^3}\,d\Omega \quad \text{and} \quad F_i = \frac{p}{m}\ , \tag{2.27}$$

for the case in which Ψ_i and Ψ_f are normalized, for example, as

$$\begin{aligned} &\Psi_i = e^{i\vec{p}\cdot\vec{r}_0/\hbar}\psi_0(\vec{r})\ , \\ &\Psi_f = \Psi_{Bm}, \quad \int |\Psi_{Bm}|^2\, d\vec{r} = 1\ . \end{aligned} \tag{2.28}$$

In the absence of retardation and in the electric-dipole approximation, $\mathcal{H}'$ reduces to a form,

$$\mathcal{H}' \approx \mathcal{H}_e' \to D_\epsilon, \quad \alpha_\omega = (2\pi\hbar\omega)^{1/2}\ , \tag{2.29}$$

where D_ϵ is defined by (2.3) and we have used in (2.29) the usual replacement $\vec{p}_i \to im\omega\vec{r}_i$ without making a distinction between ω and the fre-

quency obtained by the projection of $\vec{p}_i$ on the polarization axis. Inserting (2.27) into (2.26), we obtain the capture cross section, in the same approximation,

$$\sigma_{\rm cap} \approx \frac{1}{2\pi}\frac{e^2}{\hbar c}\left(\frac{\omega}{c}\right)^3 \frac{mc}{p}\langle \vec{\epsilon}\cdot\vec{r}\rangle^2_{mp} . \qquad (2.30)$$

By detailed balance, the photodisintegration cross section is related to the above by

$$\frac{\sigma_{\rm cap}}{\sigma_{\rm dis}} = \frac{g_c \rho_c F_d\, d\Omega_d}{g_d \rho_d F_c\, d\Omega_c} = \frac{\omega^2\hbar^2 g_c}{p^2 c^2 g_d} , \qquad (2.31)$$

where g_c and g_d are the appropriate statistical weighting factors for the capture and disintegration processes.

Finally, we note that the dipole approximation without retardation, (2.29), may have to be improved eventually as higher-energy electrons are involved with subsequent emission of high-energy photons. However, for inner electrons of the target ions, the interaction size $\bar{a}$ is rather small, and the relevant $k\bar{a}$ factor may still be considerably smaller than the unity, if the photon energy is not too high.

III. DIRECT RADIATIVE CAPTURE

In this section, we derive the amplitude for the direct capture of electrons by ions of core charge Z_C and the degree of ionization Z_I. The amplitude is given by (2.21) in the dipole approximation

$$M^P_{fi} \approx \langle \Psi_f | D_\epsilon | P \Psi^T \rangle , \qquad (3.1)$$

where, again omitting the photon state function for simplicity, we have

$$\Psi_f = \Psi_{Bm} , \qquad (3.2)$$

the final bound state specified by the quantum number m. The approximation (2.29) in the original matrix element is not necessary here, but used for convenience of notation. When m corresponds to the lowest unoccupied state, M^P_{fi} describes the one-step capture process. On the other hand, for m corresponding to any of the higher excited bound states, M^P_{fi} implies a radiative capture followed by further cascade transitions with additional photon emissions. This latter category of processes should eventually be included in the energy-loss estimate. (The only process which is not explicitly included here is then the bremsstrahlung corresponding to the continuum → continuum transitions. This will be considered in Sec. V.)

The simplest case described by (3.1) would be the capture by a completely stripped ion, with $Z_I = Z_C$. In this case, the dipole matrix element can be calculated exactly analytically, as given, e.g., by Bethe-Salpeter[1] for the capture to the $1s$ state from the p-wave continuum; for the polarization of the emitted photon in the z direction, we have

$$|M'_{0k}|^2 = \left| \int u^*_w \left(\sum_i z_i \right) u_b \, d\tau \right|^2$$

$$= \frac{2^8 Z_C^6}{3(Z_C^2 + k^2)^5} \cdot \frac{\exp[-4(Z_C/k)\arctan(k/Z_C)]}{1-\exp(-2\pi Z_C/k)}$$

$$= \frac{2^8}{3Z_C^4}\left(\frac{n'^2}{1+n'^2}\right)^5 \frac{\exp(-4n'\,\mathrm{arccot} n')}{1-\exp(-2\pi n')} , \qquad (3.3)$$

where

$$k = \sqrt{E_k} \equiv \sqrt{2W} ,$$

with

$$W = E_k/2 \text{ (a.u.)} \quad \text{and} \quad n' = Z_C/k .$$

To compare the expression (3.3) with that in (3.1), we have to adjust the normalization of the continuum wave function. In (3.1), we have used the function u_w, which behaves at large r as

$$u_{kl_i}(\vec{r}) \to \sin(kr - \tfrac{1}{2} l_i \pi + \delta_{l_i} + \sigma_{l_i} - \alpha \ln 2kr) \times Y_{l_i 0}(\theta, \varphi)/kr , \qquad (3.4)$$

where

$$\alpha = -Z_A/ka_0 , \quad Z_A \equiv Z_I + 1 \text{ or } Z_I ,$$

$$\sigma_{l_i} = \arg\Gamma(l_i + 1 + i\alpha) .$$

The function u_w which appears in (3.3) is normalized as[1]

$$u_w = u_{kl_i}(2/\pi k)^{1/2}$$

and thus

$$|M_{0k}|^2 = \tfrac{1}{2}\pi k |M'_{0k}|^2 . \qquad (3.5)$$

Of course this difference in the normalization is compensated by the change in the expression for the incident flux.

A slightly different form for the capture cross section is also given by Bond, Watson, and Welch.[12] This form will be discussed in Sec. VI.

For $Z_C \neq Z_I$, we have one or more electrons attached to the target ion in addition to the incoming electron. The effective potential that the incoming particle sees is then no longer pure Coulombic, although, for Z_C large and $Z_I \lesssim Z_C$, the Coulomb approximation is still effective. We may take the screening effect into account by a simple single-particle model[7] defined by the potential

$$V = (1/r)[(Z_C - Z_I - 1)Y(r) - Z_C] \qquad (3.6)$$

with

$$Y(r) = 1 - \Omega(r) ,$$

$$\Omega(r)=[H(e^{r/d}-1)+1]^{-1},$$
$$H=\tilde{\alpha}(Z_C-Z_I-1)^{\nu}d,$$

where

$$\nu=0.4, \quad \tilde{\alpha}=1.00,$$

and the parameter d is tabulated in Ref. 7, with the value, for example,

$$d=0.500, \quad Z_C=10$$
$$d=1.154, \quad Z_C=20, \quad \text{etc.}$$

Thus, the radial parts of u_{nl_i} and u_{nl_f} are given by

$$\left(-\frac{d^2}{dr^2}+\frac{l_i(l_i+1)}{r^2}+2V-k^2\right)R_{kl_i}(r)=0,$$
$$\left(-\frac{d^2}{dr^2}+\frac{l_f(l_f+1)}{r^2}+2V+e_{nl_f}\right)R_{nl_f}(r)=0. \tag{3.7}$$

As Z_C gets large, it is more convenient to rescale[9] the variable r in the actual calculation of these radial functions; thus we set

$$r\to s=2\sqrt{e_{nl_f}}\,r,$$
$$V\to V(r\to s,\ d\to d'=2\sqrt{e_{nl_f}}\,d). \tag{3.8}$$

Equation (3.8) replaces (3.7) by

$$\left(-\frac{d^2}{ds^2}+\frac{2V(s)}{2\sqrt{e_{nl_f}}}+\frac{1}{4}\,\frac{(l_f+\frac{1}{2})^2-\frac{1}{4}}{s^2}\right)R_{nl_f}(s)=0,$$
$$\left(-\frac{d^2}{ds^2}+\frac{2V(s)}{2\sqrt{e_{nl_f}}}+\frac{(l_i+\frac{1}{2})^2-\frac{1}{4}}{s^2}-\frac{k^2}{4e_{nf}}\right)R_{kl_i}(s)=0. \tag{3.7a}$$

Therefore, we have

$$M_{mk}=\langle\Psi_{Bm}|D_\epsilon|\Psi_k(\vec{r})\rangle=\int u^*_{ml_f}Zu_{kl_i}(\vec{r})\,d\vec{r}$$
$$=C_{l_f l_i}\int_0^\infty r^3R^*_{ml_f}(r)R_{kl_i}\,dr, \tag{3.9}$$

where

$$C_{l_f l_i}=\int d\Omega\,Y^*_{l_f 0}\cos\theta\,Y_{l_i 0}$$
$$=\frac{l_f+1}{[(2l_f+1)(2l_i+1)]^{1/2}}, \quad l_i=l_f+1$$
$$=\frac{l_f}{[(2l_f+1)(2l_i+1)]^{1/2}}, \quad l_i=l_f-1.$$

The form (3.6) has recently been improved[7] to take into account the effect of screening for different subshells. However, we prefer the simpler form (3.6) for the simple reasons that our estimate will be only preliminary and further that the wave functions thus generated for a given (Z_C,Z_I) would be mutually orthogonal. For different shells, we could also use the effective charges for screening.[1]

The direct radiative capture cross section σ^P will be estimated for the cases $Z_C=20$ and 40, with various degrees of ionization Z_I. The calculation is crude, but gives a reference point with which we can compare the magnitude of the dielectronic recombination cross section. Whereever possible, the numerical integration result is compared with the exact form obtained from (3.3). The electron energy is taken to be 1 keV. The details of the numerical results are discussed in Sec. VI.

As noted previously, the results given by (3.3) or by (3.9) do not include the possibility of capture to many of the allowed excited states, followed by cascades with additional photon emissions. Although the initial capture to outer shells is known to be less likely, it is of interest to take into account these processes as well by summing over all the allowed states. Thus, by carrying out an incoherent sum,

$$|M^P|^2\equiv\sum_{m\in B}|M^P_{mi}|^2$$
$$=\sum_m\langle P\Psi^T|D_\epsilon|\Psi_{Bm}\rangle\langle\Psi_{Bm}|D_\epsilon|P\Psi^T\rangle$$
$$=\langle P\Psi^T|D_\epsilon\Lambda_BD_\epsilon|P\Psi^T\rangle. \tag{3.10}$$

In (3.10), Λ_B is the appropriate projection operator. It is not always possible to obtain Λ_B in a simple and usable form. However, a semiclassical approximation to this operator is possible, as given by[8]

$$\Lambda_B\equiv(\vec{r}|\Lambda_B|\vec{r}')$$
$$\approx(2\pi^2/u^3)(\sin G_B-\sin G_A), \tag{3.11}$$

where

$$u=|\vec{r}-\vec{r}'|, \quad v=\tfrac{1}{2}|\vec{r}+\vec{r}'|,$$
$$G_B=uP_B(v)/\hbar, \quad G_A=uP_A(v)/\hbar,$$
$$P_B(v)=\{2m[E_B-V(v)]\}^{1/2},$$
$$P_A(v)=\{2m[E_A-V(v)]\}^{1/2}, \tag{3.12}$$

and where E_B and E_A are the upper and lower bounds of the spectrum projected on by Λ_B. A slightly more convenient form for Λ_B is that corresponding to a specific angular momentum projection of (3.11), given by[8]

$$\Lambda^{l\pm}_B(r,r')=\frac{1}{\pi rr'u}(\sin P^{l\pm}_Bu-\sin P^{l\pm}_Au), \tag{3.13}$$

where

$$u=|r-r'|, \quad l^\pm\equiv l\pm1,$$
$$v=\tfrac{1}{2}(r+r'), \quad L^2_\pm\equiv(l+\tfrac{1}{2}\pm1)^2, \tag{3.14}$$

and

$$P_B^{l\pm}=[\,2E_B-2V(\nu)-L_\pm^2\nu^{-2}]^{1/2},\quad \text{etc.}$$

In the evaluation of the cross section using (3.10), however, an additional frequency-dependent factor ω_m^3 in (2.30) has to be incorporated in an averaged form, $\omega_m\to\bar{\omega}$. To improve on this approximate procedure requires a modification of the projection operator Λ_B as

$$\bar{\omega}^3\Lambda_B\to\Pi_B^{(3)}\equiv\sum_{m\in B}|\,\Psi_{Bm}\rangle\,\omega_m^3\langle\Psi_{Bm}| \tag{3.15}$$

with the obvious notation $\Pi_B^{(0)}=\Lambda_B$. A semiclassical approximation to this operator is given by

$$\begin{aligned}(r|\,\Pi_B^{(3)\,l\pm}(b,a)|\,r')&\approx\frac{2}{\pi}\int_{P_a}^{P_b}dp\,p^2 j_{l\pm}(pr)j_{l\pm}(pr')(p_0^2-p^2)^3(2m)^{-3}\\&\approx\frac{2}{\pi rr'}(2m)^{-3}\int_{P_a}^{P_b}(p_0^2-p^2)^3\,\frac{\cos(pu)}{2}\ .\end{aligned} \tag{3.16}$$

IV. INDIRECT CAPTURE—DIELECTRONIC RECOMBINATION

We consider here the second part of the matrix element in the capture amplitude

$$M_{fi}^Q=\langle\Psi_f|\,D_\epsilon\,G^Q H|\,P\Psi^T\rangle\ . \tag{4.1}$$

With a simple model for the target atom and an approximate form for G^Q, (4.1) may be simplified. We first consider the case in which a single resonance state dominates, followed by the case in which many resonance levels overlap.

A. Resonant capture—isolated resonance states (for Z_C small, or $Z_C\gtrsim Z_I$)

From (2.21), the leading term among the singular amplitudes is[10]

$$M_{fi}^Q\approx\frac{\langle\Psi_f|\,D_\epsilon|\,Q\Phi_r\rangle\langle Q\Phi_r|\,H|\,P\Psi^{Ps}\rangle}{E-E_r^Q}\ , \tag{4.2}$$

with

$$E_r^Q=\epsilon_r+\langle Q\Phi_r|\,HG^{Ps}H|\,Q\Phi_r\rangle\ .$$

As in the direct capture, both $P\Psi^{Ps}$ and Ψ_f may be obtained from the single-particle model. On the other hand, $Q\Phi_r$ requires at least two electrons in the excited states, corresponding to the two-particle one-hole configurations, and thus we may have for example

$$Q\Phi_r\approx(1/\sqrt{2}\,)[\,\varphi_{ra}(\vec{1})\,\varphi_{rb}(\vec{0})\pm\varphi_{ra}(\vec{0})\varphi_{rb}(\vec{1})]\,\Psi_C\ , \tag{4.3}$$

where Ψ_C is the core wave function, with symbolically

$$e_1^-+e_0^-+C=A+e_0^-=B\ . \tag{4.4}$$

Similarly, denoting the highest occupied state of the ions A by φ_b, we let

$$P\Psi^T=(1/\sqrt{2}\,)[\varphi_b(\vec{1})u_b^T(\vec{0})\pm\varphi_b(\vec{0})u_b^T(\vec{1})]\,\Psi_C\ , \tag{4.5}$$

where the excitation of φ_b electrons is assumed to dominate the contribution in (4.2). Otherwise (4.5) should be modified to include electrons in higher excited states as well. u_b^T is the wave function for the incoming electron with the distortion by the elastic optical potential.

We also have

$$\Psi_f\approx(1/\sqrt{2}\,)[\,\varphi_{ra}(\vec{1})\,\varphi_{b''}(\vec{0})\pm\varphi_{ra}(\vec{0})\,\varphi_{b''}(\vec{1})]\,\Psi_c \tag{4.6a}$$

or

$$\Psi_f\approx(1/\sqrt{2}\,)[\varphi_{b'}(\vec{1})\varphi_{b''}(\vec{0})\pm\varphi_{b'}(\vec{0})\varphi_{b''}(\vec{1})]\,\Psi_c\ . \tag{4.6b}$$

The forms (4.6) are dictated by the single-particle nature of the operator D_ϵ. The evaluation of the integrals involved in (4.2) is straightforward.

Two remarks are appropriate here: (i) Except in a two-electron model for the system $B=A+e^-=C+2e^-$, the construction of the projection operator P with full exchange effect is difficult, because the projection operator for one channel does not commute with that for the other exchange channels when the target ions contain more than one electron. However, explicit forms for the projection operator can be constructed in the single-particle formulation of scattering.[11] (ii) Except in the helium isoelectronic sequences, the degeneracy in the angular momentum operator $\vec{L}$ is not present, and consequently, the presence of resonance states does not follow in general from the main term involving different l states for the same n.

Incidentally, the matrix elements involved in (4.2) may, in some cases, be obtained from the result of an earlier study on the fluorescence yield.[5] In particular, the matrix element involving the initial configuration

$$\langle Q\Phi_r|\,H|\,P\Psi^{Ps}\rangle$$

can be obtained from the Auger transition amplitude. In fact, it is the inverse Auger process, with both direct and exchange effects. Typically, in terms of the single-particle orbitals φ_n,

$$\langle Q\Phi_r|H|P\Psi^{Ps}\rangle \sim \int d\vec{r}_1\, d\vec{r}_0\, \varphi^*_{r'}(\vec{r}_1)\varphi^*_{r''}(\vec{r}_0)\frac{e^2}{|\vec{r}_1-\vec{r}_0|}\varphi_b(\vec{r}_1)u_b^{Ps}(\vec{r}_0)$$
$$\pm \int d\vec{r}_1\, d\vec{r}_0\, \varphi^*_{r'}(\vec{r}_1)\varphi^*_{r''}(\vec{r}_0)\frac{e^2}{|\vec{r}_1-\vec{r}_0|}\varphi_b(\vec{r}_0)u_b^{Ps}(\vec{r}_1)\,. \tag{4.7}$$

B. Overlapping resonances

In this case, it is not desirable from a practical point of view to construct individual resonances and to sum them all at the end. Instead, we treat the entire set of states $\{Q\Phi_\alpha\}$ as a "smooth" continuum. The matrix element is given by

$$M^Q_{fi} = \langle \Psi_f | D_\epsilon G^Q H | P\Psi^T\rangle$$
$$= \sum_\alpha \langle \Psi_f | D_\epsilon | Q\Phi_\alpha\rangle \frac{1}{E-\mathcal{E}_\alpha}\langle Q\Phi_\alpha | H | P\Psi^T\rangle\,. \tag{4.8}$$

First of all, we note that the particular configuration Ψ_f will limit the number of allowed single-particle states in $Q\Phi_\alpha$, because D_ϵ is a sum of single-particle operators. Thus, if we were to write, for example,

$$\Psi_f = \varphi_{n'}(\vec{1})\varphi_{n''}(\vec{0})\Psi_c \tag{4.9}$$

and

$$D_\epsilon = D_\epsilon(\vec{0})\,, \tag{4.10}$$

then, all the $Q\Phi_\alpha$ are of the form (neglecting the exchange term), with the same n',

$$Q\Phi_\alpha = \varphi_{n'}(\vec{1})\varphi_m(\vec{0})\Psi_C\,. \tag{4.11}$$

Now, with

$$H(\vec{0},\vec{1}) = H\,, \tag{4.12}$$

$$P\Psi^{PT} = \varphi_b(\vec{1})u_b^T(\vec{0})\Psi_C\,, \tag{4.13}$$

we have

$$M^Q_{fi} \approx \sum_m \langle \varphi_{n'}(\vec{1})\varphi_{n''}(\vec{0})|D_\epsilon(\vec{0})|\varphi_{n'}(\vec{1})\varphi_m(\vec{0})\rangle$$
$$\times \frac{1}{E-\mathcal{E}_{mn'}}\langle \varphi_{n'}\varphi_m|H|\varphi_b u_b^T\rangle$$
$$= \langle \varphi_{n''}(\vec{0})|D_\epsilon(\vec{0})g^Q_{n'}(\vec{0},\vec{0}')V_{n'b}(\vec{0}')|u_b^T(\vec{0}')\rangle\,, \tag{4.14}$$

where

$$g^Q_{n'}(\vec{0},\vec{0}') = [q_b(E+i\eta-e_{n'}-t_0-v_{n'})q_b]^{-1}\,,$$
$$q_b = 1-p_b,\quad p_b = \varphi_b\rangle\langle\varphi_b\,. \tag{4.15}$$

When M^Q_{fi} is summed over the final allowed states, $f=(n',n'')$, $n'\neq b$, then

$$|M^Q|^2 \equiv \sum_{n'n''}|M^Q_{fi}|^2$$
$$= \sum_{n'n''}\langle u_b^T|V_{bn'}g^Q_{n'}D_\epsilon|\varphi_{n''}\rangle\langle\varphi_{n''}|D_\epsilon g^Q_{n'}V_{n'b}|u_b^T\rangle\,. \tag{4.16}$$

Two alternative ways to evaluate $|M^Q_{fi}|^2$ will be considered below:

(a) As a first possibility, we recognize the fact that the first part of the amplitude in M^Q_{fi},

$$A \equiv \langle Q\Phi_\alpha|H|P\Psi^T\rangle\,, \tag{4.17}$$

is the same matrix element one evaluates in the Auger transition.[5] Thus, the result of a previous study, as in (4.7), may be used directly for this matrix element. On the other hand, the second part of M^Q_{fi},

$$R \equiv \langle \Psi_f|D_\epsilon|Q\Phi_\alpha\rangle\,, \tag{4.18}$$

with

$$Q\Phi_\alpha = \varphi_{n'}(\vec{1})\varphi_m(\vec{0})\,, \tag{4.19}$$

e.g., involves simply a single-particle radiative dipole decay of an excited atom, which is straightforward to evaluate.

The energy denominator in (4.8)

$$(E-\mathcal{E}_\alpha)^{-1}$$

may be evaluated approximately by the single-particle values, as

$$E-\mathcal{E}_\alpha \approx E-e_{n'}-e_m-V_{n'm;\,n'm}\,,$$

thus,

$$M^Q_{fi} \approx \sum_m \frac{R_{n'n'';n'm}A_{n'm;bk}}{E-e_{n'}-e_m-V_{n'm;\,n'm}}\,. \tag{4.20}$$

In our simple model above,

$$R_{n'n'';\,n',\,m} \equiv R_{n''m}$$
$$= \langle\varphi_{n''}|D_\epsilon|\varphi_m\rangle \quad \text{(independent of } n'\text{)}\,.$$

The amplitude (4.20) may also be used to estimate the amplitude for the two-step process, $e^- + A \to e^{-'} + A^* \to e^{-'} + A + \gamma$, by taking the state n' to be in the continuum. Aside from the sum over the intermediate states m, the problem has been considered in some detail earlier.[13]

(b) The second alternative possibility is to follow the previous work on the multiple impact ioniza-

tion. That is, in the plane-wave approximation for the incoming electron at high energies, the Auger ionization cross section is given by

$$\sigma^A = \sum_\alpha \sigma_\alpha^A ,$$

where

$$\sigma_\alpha^A = (\pi a_0^2)\frac{4Z_\alpha}{(k_\alpha a_0)^2}\ln\left(\frac{4\epsilon_\alpha}{\Delta_\alpha^B}\right)\overline{M}_D^\alpha W_\alpha , \tag{4.21}$$

with k_α the momentum of the initial state electron, ϵ_α the initial kinetic energy, Δ_α^B the ionization energy, $Z_\alpha \equiv Z_{nl} = 2(2l+1)$, $W_\alpha = 1 - Y_\alpha$, Y_α the fluorescence yield, and

$$\overline{M}_D^\alpha = [3(2l+1)]^{-1}[(l+1)M_D^{nl+} + lM_D^{nl-}] , \tag{4.22}$$

$$M_D^{nl\pm} = \langle nl|\,\vec{r}\cdot\Lambda_D^{l\pm}\vec{r}'\,|nl\rangle , \tag{4.23}$$

which is chosen such that $E_a = E_D < E_b = 0$ for the projection between E_a and E_b.

Three modifications of (4.21) are needed; first, the incoming electron energy is low (except for very low Z_C) such that the Coulomb distortion should be incorporated. Second, W_α is to be replaced by Y_α. Third, we should have the Coulomb-distorted (continuum or) bound-state function for the final state of the (incoming) electron. Thus, we have[9]

$$\sigma_{\rm cap}^Q \approx \sum_\alpha \sigma_\alpha^Q ,$$

where

$$\sigma_\alpha^Q = (\pi a_0^2)\frac{4Z_\alpha}{(k_\alpha a_0)^2}F(Z_I, E)\ln\left(\frac{4\epsilon_\alpha}{\Delta_\alpha^B}\right)\overline{M}_D^\alpha Y_\alpha \tag{4.24}$$

with $F(Z_I, E) \to 1$ as $Z_I \to 0$ being the Coulomb correction factor for the incoming electron both in the initial and final states. The present approach with (4.24) is roughly equivalent[13] to taking in the M_{fi}^Q,

$$(G^Q)^2 \approx -i\pi\delta(Q[E-H]Q)/(i\Gamma/2) , \tag{4.25}$$

where

$$\Gamma \equiv 2\pi\langle Q\Psi|V\delta(P[E-H_{\rm tot}|P)V|Q\Psi\rangle ;$$

that is, the on-shell probability amplitude for the excitation to the Q space in the matrix S is singled out. Thus, in this approximation, the dispersive effect is neglected in the G^Q propagator. With

$$\delta(Q[E-H]Q) \to \Lambda_D ,$$

we essentially recover (4.22).

On the other hand, the Green's functions such as $g_{n'}^Q$ in (4.14) may be obtained approximately using the semiclassical method, as noted earlier in Ref. 8; in this way, the drastic approximations on G^Q, as in (4.25), may be avoided.

V. BREMSSTRAHLUNG AND HIGHER-ORDER PROCESSES

The matrix elements considered in Sec. II, and in more detail in Secs. III and IV, are linear in the electromagnetic coupling D_ϵ, except for the fact that the final states Ψ_{Bm} are summed over m incoherently so that any further decays of these states by additional photon emissions are approximately included. To make the formal part of the analysis more complete, we consider here all the matrix elements which are quadratically dependent on the coupling D_ϵ.

In place of (2.4) we now consider

$$(H_{\rm tot} - E)\Psi_{ik}^{\rm tot} = 0 , \tag{5.1}$$

where

$$H_{\rm tot} \equiv H + D_\epsilon \tag{5.2}$$

with H defined in Sec. II. Obviously,

$$\Psi_{ik}^{\rm tot} = \Psi_{ik} + GD_\epsilon\Psi_{ik}^{\rm tot} \approx \Psi_{ik} + GD_\epsilon\Psi_{ik} , \tag{5.3}$$

where

$$G = (E + i\eta - H)^{-1} \quad (\eta > 0) . \tag{5.4}$$

The exact amplitude is then given by

$$\overline{M}_{mk} = \langle\Psi_{Bm}|D_\epsilon|\Psi_{ik}^{\rm tot}\rangle , \tag{5.5}$$

which, to second order in D_ϵ, can be written out explicitly in the form

$$\begin{aligned}\overline{M}_{mk} \approx {} & \langle\Psi_{Bm}|D_\epsilon|P\Psi_{ik}\rangle + \langle\Psi_{Bm}|D_\epsilon G^Q V|P\Psi_i\rangle + \langle\Psi_{Bm}|D_\epsilon G^P D_\epsilon|P\Psi_{ik}\rangle + \langle\Psi_{Bm}|D_\epsilon G^Q D_\epsilon|P\Psi_{ik}\rangle + \langle\Psi_{Bm}|D_\epsilon G^P V G^Q D_\epsilon|P\Psi_{ik}\rangle \\ & + \langle\Psi_{Bm}|D_\epsilon G^Q V G^P D_\epsilon|P\Psi_{ik}\rangle + \langle\Psi_{Bm}|D_\epsilon G^P D_\epsilon G^Q V|P\Psi_{ik}\rangle + \langle\Psi_{Bm}|D_\epsilon G^Q D_\epsilon G^Q V|P\Psi_{ik}\rangle .\end{aligned} \tag{5.6}$$

As noted earlier, for Ψ_{Bm} which are limited to the bound-state configurations only, the first and the third terms may be combined simply by summing over m incoherently. However, if we extend the sum over m to include the continuum as well, the bremsstrahlung process and its correction are also contained in the resulting terms. The second term of (5.6) involves excited target states and possible resonance states, as described in detail in Sec. IV.

The fourth term is thus the first leading correction which contains D_ϵ twice. However, the nature

of the operator D_ϵ implies that the $P \to Q$ transition there describes a photoexcitation of the target by absorption of a photon, which is unlikely at the photon density of interest here. Therefore, we expect this term to be very small (unless the electron correlation is very strong). Now, we expand the Q-space Green's function as

$$G^Q = G_0^Q + G_0^Q V G_0^Q + \cdots , \tag{5.7}$$

where

$$G_0^Q = \{Q[E + i\eta - H_A - T_{\vec{r}_0} - H_{\rm rad}]Q\}^{-1} ,$$

and obtain

$$\langle \Psi_{Bm} | D_\epsilon G^Q D_\epsilon | P\Psi_{ik} \rangle \approx \langle \Psi_{Bm} | D_\epsilon G_0^Q D_\epsilon | P\Psi_{ik} \rangle + \langle \Psi_{Bm} | D_\epsilon G_0^Q V G_0^Q D_\epsilon | P\Psi_{ik} \rangle . \tag{5.8}$$

The second term on the right-hand side of (5.8) is, in principle, of the same order as the last four terms in (5.6). In fact the fifth term is very much of the same form as above. The sixth term in (5.6) is also a correction to the bremsstrahlung process in that the incoming particle emits a photon, followed by a dielectronic recombination similar to the second term. Finally, the seventh and the eighth terms are the two-photon corrections to the second term, and, as with the third term combined with the first, we can include these terms in the second by extending the sum over m. Therefore, by performing an incoherent sum over m of the final states Ψ_{Bm} with different energies, we can effectively include all the higher-order terms (in power of D_ϵ) in an approximate way. In addition to these corrections, the relativistic effect should be taken into account as Z_C increases. This effect is known to be important for $Z_C \gtrsim 40$, although the energy for the incoming electron will be taken to be in the region of ~1–10 keV.

The result presented here and in Sec. IV may be compared with the discussion given in Ref. 13 of the process $e^- + A \to e^{-\prime} + A^* \to e^{-\prime} + A + \gamma$. The problem is formulated there in terms of the noninteracting states generated by $H_0 = T_{\vec{r}_0} + H_A + H_{\rm rad}$. This is not so convenient for the capture process, however, because the interaction V plays a crucial role in (2.20) in generating the final state Ψ_f.

VI. NUMERICAL RESULTS

As a preliminary to a series of more detailed calculations of the radiative capture process to be reported on subsequently, we present here a rather crude estimate of the relative contribution of the two amplitudes considered in Secs. III and IV, in particular, those given by (3.9) and (4.24).

(1) The direct radiative capture amplitude is calculated numerically using the single-particle radial wave functions defined by (3.7a) for the potential (3.6). For the nuclear core charge $Z_C = 20$ and 40, we have a pure Coulomb field when the degree of ionization Z_I is

$$Z_I = Z_C ; \tag{6.1}$$

for this case, the exact amplitude (3.3) is available for checking the numerical accuracy, with the appropriate scaling factor given in (3.5). We have calculated first the single-particle energies by an iteration method[9] for different degrees of ionization. The result is summarized in Table I. The incident kinetic energy of the electron being captured is taken to be $E_k = 1$ keV, which corresponds more or less to the value attainable at presently available plasma confinement devices, although it may be far too low for the fusion threshold.

The matrix elements $|M_{mk}|^2$ are collected in Table II for some of the typical transitions, for the case $E_k = 1$ keV; that is, for $\langle \vec{\epsilon} \cdot \vec{r} \rangle_a^2$, where

$$\langle \vec{\epsilon} \cdot \vec{r} \rangle^2 \equiv \langle \vec{\epsilon} \cdot \vec{r} \rangle_a^2 \sin^2\Theta . \tag{6.2}$$

They decrease quite rapidly as E_k increases, and the values at $E_k = 10$ keV are compared in Table III. The cross sections are then estimated using the expression (2.3). For convenience we may write the σ^P in the form

$$\begin{aligned} \sigma^P &= \frac{1}{2\pi} \frac{e^2}{\hbar c} \left(\frac{\omega}{c}\right)^3 \frac{mc}{p} \langle \vec{\epsilon} \cdot \vec{r} \rangle^2 g_c \ \text{(a.u.)} \\ &= \frac{1}{2\pi^2} \frac{1}{\sqrt{2}\,\alpha^2} \left(\frac{\hbar\omega}{mc^2}\right)^3 \left(\frac{mc^2}{E_k}\right)^{1/2} \langle \vec{\epsilon} \cdot \vec{r} \rangle g_c \ \text{(in } \pi a_0^2\text{)} \\ &= (1.53 \times 10^4) \left(\frac{\hbar\omega}{mc^2}\right)^3 \langle \vec{\epsilon} \cdot \vec{r} \rangle^2 g_c \ (\pi a_0^2) , \end{aligned} \tag{6.3}$$

where E_k is the incident energy and the factor g_c is the degeneracy of the states involved. The result of this calculation for different sets defined

TABLE I. The single-particle energy is calculated for the nuclear charge $Z_C = 20$ and 40, and for different degrees of ionization Z_I. The single-particle states are denoted by (n, l) and the energy is given in rydberg units. The single-particle potential used is given by Eq. (3.6).

Z_C	Z_I	1s	2s	2p	3s	3p	3d
20	18	398.0					
	16	391.4	92.84				
	10	362.0	72.25	70.70			
40	38	1598					
	36	1591	391.3				
	30	1559	365.2	364.6			
	28	1547	355.1	354.0	142.8		
	22	1503	322.1	319.2	119.5	117.2	
	12	1419	261.1	254.5	79.0	76.0	70.0

TABLE II. The dipole matrix element $\langle \vec{\epsilon} \cdot \vec{r} \rangle_a^2$ in the no-retardation approximation for the transition, continuum $(E_k, l_k) \rightarrow$ bound (n, l), with $E_k = 1$ keV. The Coulomb distortions are included. The values for $\langle \vec{\epsilon} \cdot \vec{r} \rangle_a^2$ are given in atomic units ($e^2 = \hbar = m = c = 1$), scaled up by 10^5.

Z_C	Z_I	(n, l)	l_k	$\langle \vec{\epsilon} \cdot \vec{r} \rangle_a^2 \times 10^5$
20	19	$1s$	p	3.63
	10	$1s$	p	4.8
		$2s$	p	16.8
		$2p$	s	0.4
		$2p$	d	20.5
40	39	$1s$	p	0.36
	12	$1s$	p	0.5
		$2s$	p	5.9
		$2p$	s	0.2
		$2p$	d	12.6
		$3s$	p	16.0
		$3p$	s	0.9
		$3p$	d	33.0
		$3d$	p	0.6
		$3d$	f	40.0

by (Z_C, Z_I, nl, kl_k) is given in Table IV. The values given in Table IV do not contain the factor $8\pi/3$ which comes from the integration over the photon angular distribution. The σ_{tot}^P should include this factor.

Obviously, there are many points in the above calculation which have to be improved. First of all, the dipole no-retardation approximation should be modified as the photon energy increases. Second, the single-particle nature of the bound states used in M_{mk} may be an oversimplification; this has a direct bearing on the correction terms discussed in Sec. V. Third, the major drawback of the present estimate neglects the possible contribution of captures to all the excited states, followed by additional cascade decays, as described by (3.10). Some attempts have been made to evaluate the relevant matrix elements using the semiclassical projection operators. However, due to inherent uncertainty in such operators in the region close to the classical turning point and

TABLE III. The energy dependence of the integral $\langle \vec{\epsilon} \cdot \vec{r} \rangle_a^2$ for $E_k = 1$ keV and $E_k = 10$ keV. The nuclear core charge $Z_C = 20$.

Z_I	(n, l)	l_k	$E_k = 1$ keV $\langle \vec{\epsilon} \cdot \vec{r} \rangle_a^2 \times 10^5$	$E_k = 10$ keV $\langle \vec{\epsilon} \cdot \vec{r} \rangle_a^2 \times 10^5$
19	$1s$	p	3.6	0.041
10	$1s$	p	4.8	0.046
	$2s$	p	16.8	0.014
	$2p$	s	0.4	0.000
	$2p$	d	20.5	0.030

TABLE IV. The direct radiative capture cross section σ^P is estimated from the matrix elements given in Table II, at $E_k = 1$ keV. ($\Theta = \pi/2$.)

Z_C	Z_I	(n, l)	l_k	σ^P (πa_0^2)
20	10	$2s, 2p$	s, p, d	3.0×10^{-7}
40	12	$3d$	p, f	2.3×10^{-7}
70	24	$4d$	p, f	$\sim 2 \times 10^{-7}$

apparent sensitivity of the integral M^P of (3.10) around that point, we were not able to obtain an estimate to the desired accuracy. The problem is further aggravated by rapid oscillations and subsequent cancellations within the integrals involved.

In connection with the direct capture discussed above, we also note the semiclassical formula considered by Bond, Watson, and Welch.[12] The classical result obtained earlier by Kramer[2] is modified to take into account the quantum mechanical effect by introducing the Gaunt factor g_{bf}. Thus, we have

$$\sigma_{\text{cap}} \approx \frac{Z^4 g_{bf} Z_n}{[n^5 (E_k + I_n) E_k]} \quad (\pi a_0^2 10^{-4}) , \tag{6.4}$$

where E_k and I_n are the energy of the incoming electron being captured and the ionization energy of the bound electron in the nth shell, respectively, and are given in the rydberg units. The multiplicity factor Z_n is approximately given by $Z_n \approx (n-1)2(2l+1) \approx 4n^2$, while g_{bf} is of the order unity.

(2) The dielectronic recombination cross section is estimated using the simple form (4.24), neglecting the possibility of isolated-resonance contributions. Although the formula is less likely to be effective at $E_k = 1$ keV than at the higher electron energies, we expect that the estimate should be a reasonable indication of the importance of this process in comparing with the direct capture cross section σ^P. In evaluating the cross section σ^Q, we have neglected the Coulomb correction factor F for both the initial and final states, and set

$$F(Z_I, E) \approx 1,$$

where the statistical weighting factor Z_α is chosen to be

$$Z_\alpha = 2(2l_i + 1) . \tag{6.5}$$

The required transition amplitudes $\overline{M}_D^\alpha$ have been calculated for $Z_C = 20$ and 40, and for different states of ionization Z_I. The result is given in Table V.

The evaluation of the cross section σ^Q requires an estimate of the fluorescence yield Y_α, which provides the probability of the autoionization state

TABLE V. The dielectronic recombination matrix elements are summed over all allowed bound states to which the incident electron can be captured without radiation emission, thus forming an autoionization state. $\bar{M}_D^\alpha$, as defined by (4.23) is given for $Z_C = 20$ and 40. The arrows indicate that the transitions involve $l_k = l+1$ (↑) or $l_k = l-1$ (↓), where l is the orbital angular momentum of the bound target electron.

Z_C	Z_I	Trans.	1s	2s	2p	3s	3p	3d
20	19	↑	0.0057					
	18	↑	0.0057					
	16	↑	0.0019	0.0029				
	10	↑	0.0014	0.0950	0.0707			
		↓			0.0427			
40	39	↑	0.0014					
	38	↑	0.0014					
	36	↑	0.0014	0.0258				
	30	↑	0.0004	0.0222	0.0022			
		↓			0.0094			
	28	↑	0.0004	0.0224	0.0024	0.0862		
		↓			0.0003			
	22	↑	0.0001	0.0023	0.0037	0.1039	0.0895	
		↓			0.0003		0.0652	
	12	↑	0.0001	0.0022	0.0047	0.1251	0.1279	0.0983
		↓			0.0004		0.0818	0.0502

being decayed by radiative transitions. To simplify the estimate, we take the result of the previous calculations as summarized by Bambynek *et al.*[5] The parameter Δ_α^B in (4.24) is taken to be the ionization energy of the last electron for a given ion (Z_C, Z_I); in the case of impurity ions in the hot plasma in quasiequilibrium,

$$\Delta_\alpha^B \approx 1 \text{ keV} . \tag{6.6}$$

Thus, (4.24) becomes, with $E_k = 1$ keV and in the units (πa_0^2),

$$\sigma_\alpha^Q \approx [4Z_\alpha/(k_\alpha a_0)^2]\ln(4)\bar{M}_D^\alpha Y_\alpha$$

$$\approx (7.6\times10^{-2})Z_\alpha \bar{M}_D^\alpha Y_\alpha . \tag{6.7}$$

The result for σ^Q is summarized in Table VI; only the terms with (a) are included in the cross section estimate. The result may be compared with the values in Table IV. It should be emphasized in examining the result in Table VI that the poor accuracy in Y_α for the higher shells makes it difficult to estimate the corresponding contributions. The M_D, on the other hand, increases rapidly for higher shells, which indicates that, although Y_α gets very small for outer shells, the corresponding σ^Q may still be appreciable and that the values for Y_α given in Table VI may be grossly inaccurate. We have sketched the Y_α in Fig. 1.

Now we compare the result of Table IV for the direct radiative capture with that for the dielectronic recombination given in Table VI. Obviously, σ^P is much smaller than σ^Q, by a factor of 10^2 or more for most cases. As noted above, however, the contribution to σ^P may have been underestimated due to the neglect of captures to all the available excited states. Many of the deficiencies in the derivation of (6.7) have already been discussed earlier; in particular, we should stress the fact that (6.7) is based on the nonresonant picture of the two-step capture process. The Coulomb distortion effect and the dipole approximation introduced in the calculation of M_D^α should

TABLE VI. The cross sections for the dielectronic recombination are estimated using the result of Table V, for $E_k = 1$ keV, and $Z_C = 20$, 40, and 70. The radiationless part of transitions and subsequent radiative decays are estimated using (4.24) or (6.7).

Z_C	Z_I	(n,l)	$\bar{M}_D^\alpha$	Z_α	Y_α	$\bar{M}_D^\alpha Z_\alpha Y_\alpha (\times 10^4)$
			$\sigma^Q = 2.8\times10^{-5}\ \pi a_0^2$			
20	10	1s	0.0005	2	0.15	1.5
		2s	0.032	2	0.002	1.3 [a]
		2p	0.020	6	0.002	2.4 [a]
			$\sigma^Q = 1.3\times10^{-5}\ \pi a_0^2$			
40	12	1s	0.000 03	2	0.75	0.45
		2s	0.0007	2	0.025	0.35
		2p	0.0011	6	0.025	1.65
		3s	0.042	2	0.0003	0.25 [a]
		3p	0.038	6	0.0003	0.69 [a]
		3d	0.026	10	0.0003	0.78 [a]
			$\sigma^Q = 0.6\times10^{-5}\ \pi a_0^2$			
70	24					

[a] Only these values are included in the σ^Q estimates.

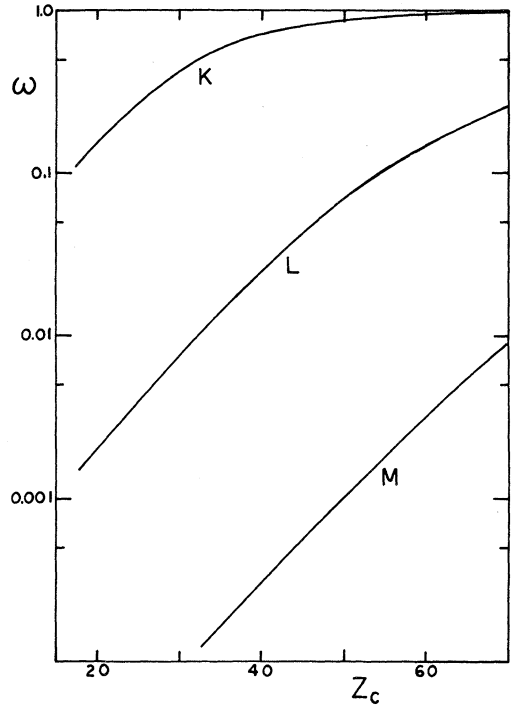

FIG. 1. Average fluorescence yields ω for the K, L, and M shells are given as functions of the atomic core charge Z_C. These values are extracted from Ref. 5, and used here in the evaluation of the dielectronic recombination cross section σ^Q.

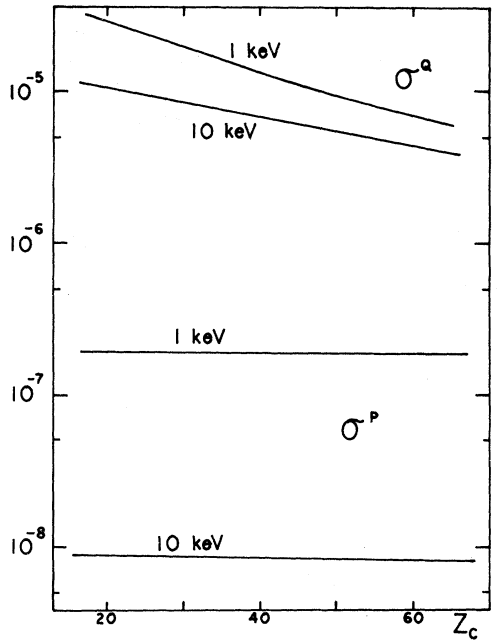

FIG. 2. Direct radiative capture cross section σ^P and the dielectronic recombination cross section σ^Q are given as functions of the atomic core charge Z_C. The equilibrium temperature is set at $kT=1$ keV, while the incident electron energy E_k is taken to be 1 keV and 10 keV. The cross sections are given in units of πa_0^2.

further be improved before a more reliable estimate for σ^Q can be made. We also note that the logarithmic factor in (4.24) and in (6.7) was obtained[9] from the Bethe integral involving two continuum functions without regard to inelastic energy loss by the projectile electron. For incident energies comparable to the typical excitation energies, the final-state wave function should be modified to represent correctly the reduction in the projectile energy.

In view of these approximations and the crudeness of the calculation, the result presented in Tables IV and VI and Fig. 2 for σ^P and σ^Q can only suggest roughly the relative magnitude of these quantities and could easily be off by a factor of 10. Incidentally, the value for σ^Q estimated earlier by Burgess[4] for the case $Z_C=26$ and $Z_I=15$, compares favorably with the interpolated value from Table VI, i.e.,

$$\sigma^Q \approx 6\times10^{-5}\ \pi a_0^2 \quad \text{(Burgess)},$$

$$\approx 3\times10^{-5}\ \pi a_0^2 \quad \text{(from Table VI)},$$

for the case of incident electron energy $E_k=1$ keV.

VII. DISCUSSION

The general theoretical formulation we have presented in Secs. II–V is reasonably complete, in which the electronic interactions are fully taken into account, while the coupling between the particles and the radiation field has been treated by perturbation theory. The theory will be the basis for further consideration of many of the details which should be worked out separately for each individual case.

The estimate we have obtained in Sec. VI is, of course, very crude and may not be totally reliable. On the other hand, it has served its purpose in suggesting future directions for improvements. Any serious comparison of the data calculated here with measurements is thus entirely *premature*. The following areas seem to require more careful study: (i) An improved estimate of the incoherent contribution to the direct capture cross section σ^P, resulting in cascade transitions. This contribution, which includes the bremsstrahlung, seems to be consistently small. (ii) The validity of the dipole and no-retardation approximations as the photon energy increases. (iii) The Coulomb dis-

tortion of the incoming electron wave functions both in the initial and final states as they appear in the dielectronic recombination amplitude. This may seriously affect the present estimate. (iv) Some isolated resonance contributions may be large, although we have neglected this possibility in our estimate of σ^Q. (v) Even for the approach based on (4.24) for σ^Q, better values of Y_α for higher subshells may improve the estimate, rather than the crude approximation used in Table VI. (vi) Many of the higher-order corrections to the amplitudes we have formulated should be estimated approximately to ascertain their effect. The general discussion given in Sec. V should be useful for this purpose.

Additional work along the lines suggested above is in progress.

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