Radiative capture of high-energy electrons*

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A simple theoretical method for calculating radiative capture cross sections is proposed. Applying the quantum defect theory, the radiative capture process and the tip bremsstrahlung process are treated together on the same footing. An application to radiative capture of 50-keV electrons by Au^{+49} ions is presented.

INTRODUCTION

Radiative capture of electrons by atomic ions is one of the processes important in plasmas. Such radiative two-body recombination may be expressed symbolically as

$$A^{+Z_i} + e^- \rightarrow A(n)^{+(Z_i-1)} + h\nu_n \qquad (1.1)$$

$$\searrow (A^{+(Z_i-1)})^{**} \rightarrow A(n)^{+(Z_i-1)} + h\nu_n , \qquad (1.2)$$

where $Z_i \geq 1$ is the charge of the atomic ion (to be distinguished from the charge $Z \geq Z_i$ of the atomic nucleus). The process (1.2) passing through intermediate quasibound states, i.e., autoionizing states may be important locally, when electron kinetic energies are close to resonance energies. These resonance energies are usually of an order of excitation energies of atomic ions. For electrons with kinetic energy larger than about 1 keV, we consider here only the process (1.1), i.e., the direct radiative capture process. The captured electron is treated as moving in an averaged central potential, i.e., Hartree-Slater potential.[1] The electron may be captured into one of the infinite number of unoccupied bound states which form Rydberg series of the "electron + atomic ion" system. Thus, it may be a formidable task to calculate all the cross sections for capture into each bound state and the sum of the cross sections.

In Sec. II we propose a simple method, based on the one-channel quantum defect theory[2] for nonrelativistic wave functions. Further, extended multichannel quantum defect theory has been applied to various atomic and molecular photoabsorption processes,[3] namely, to analyze *discrete*, *autoionization*, and *continuous* photoabsorption spectrum on the same footing. This theory is based on the fact that at atomic distances the behavior of bound and continuum wave functions of energies close to the ionization threshold varies slowly with the degree of excitation or ionization. Thus, the quantum-defect parameter μ_k and the cross-section density $d\sigma_k/d(k/Z_i^2\alpha^4)$ for each partial-wave channel KJL vary smoothly across the ionization threshold, namely from the radiative capture region to the bremsstrahlung tip region. (Here, J is the total angular momentum of the partial wave and L is orbital angular momentum of the large component of the partial wave; K is the quantum number which combines total angular momentum J and parity, e.g., $K = -1, 1, -2, 2, -3, \ldots$ corresponding to $S_{1/2}$, $P_{1/2}$, $P_{3/2}$, $d_{3/2}$, $d_{5/2}\ldots$, respectively.) The cross section $\sigma_{K,n}$ for each state is then calculated as defined in Eq. (2.22): $\sigma_{K,n} = N_{K,n}^2 \, d\sigma_k/d(k/Z_i^2\alpha^4)$, with the state density $N_{K,n}^2$ defined in Eq. (2.17). We expect this present method will give a fairly reliable estimate of the sum of the capture cross sections $\sum_k \sum_n \sigma_{k,n}$.

Section III presents an application to direct radiative capture of 50-keV electrons by Au ions with charge $+49e$ (Zn isoelectric). The validity of the theoretical method is also discussed.

THEORETICAL METHOD

The differential cross section for an electron $\vec{p}$ to radiate a photon $\vec{k}$ and then to be captured into a bound state (n, K, J, L, M) is

$$d\sigma = (2\pi)^{-2} p^{-1} E \, |H_{\rm int}|^2 \, d^3k \, \delta(E - k - \epsilon_{K,n}) , \qquad (2.1)$$

where

$$H_{\rm int} = -e(2\pi/k)^{1/2} \int d^3r \, \Psi_f^*(nKJLM) \, \vec{\alpha} \cdot \hat{e}^* e^{-i\vec{k}\cdot\vec{r}} \Psi_i . \qquad (2.2)$$

Here, we will adopt natural units throughout (i.e., $\hbar = c = m = 1$, $e^2 = \alpha = 1/137.04$). $E = (1 + p^2)^{1/2}$ is the total energy of the incident electron $\vec{p}$ and $\epsilon_{K,n}$ is the energy of a bound state $(nKJLM)$. The final state has its conventional bound-state normalization and the initial state is normalized to a unit volume. Thus, the total cross section for capture into the bound states $(nKJL)$ is

$$\sigma_{K,n} = (2\pi)^{-2} p^{-1} E \sum_M \int d^3k \, |H_{\rm int}|^2 \delta(E - k - \epsilon_{K,n}) . \qquad (2.3)$$

Expanding the initial wave function into various partial-wave components κjl, the total cross section can be rewritten as

$$\sigma_{K,n}=\lambda_0\sum_{\kappa}\sum_{M=1/2}^{J}\left[\left|R_\kappa^+(M)\right|^2+\left|R_\kappa^-(M)\right|^2\right], \tag{2.4}$$

where we utilize the same symbols and expressions as in Ref. 4:

$$\lambda_0=16\pi kE\,\alpha/p\,, \tag{2.5}$$

$$R_\kappa^\pm(M)=\sum_{n=1}^{2}Q_n^\pm(M)\sum_{\lambda}{}'P_n^\pm(M)S_n\,. \tag{2.6}$$

The index λ runs from $|l'-L|$ to $l'+L$ in steps of 2 for $n=1$, and from $|l-L'|$ to $l+L'$ in steps of 2 for $n=2$:

$$L'=L+\eta_K,\quad \eta_K=-K/|K|\,, \tag{2.7}$$

$$l'=l+\eta_\kappa,\quad \eta_\kappa=-\kappa/|\kappa|\,, \tag{2.8}$$

$$Q_1^\pm(M)=\eta_\kappa(-)^{L-l'+M\mp1/2}[(2L+1)(2J+1)(2l'+1)(2j+1)]^{1/2}\begin{pmatrix} l' & \frac12 & j\\ M\pm\frac12 & \pm\frac12 & -M\mp1\end{pmatrix}\begin{pmatrix} L & \frac12 & J\\ M\pm\frac12 & \mp\frac12 & -M\end{pmatrix}, \tag{2.9}$$

$$Q_2^\pm(M)=-\eta_\kappa(-)^{L'-l+M\mp1/2}[2(L'+1)(2J+1)(2l+1)(2j+1)]^{1/2}\begin{pmatrix} l & \frac12 & j\\ M\pm\frac12 & \pm\frac12 & -M\mp1\end{pmatrix}\begin{pmatrix} L' & \frac12 & J\\ M\pm\frac12 & \mp\frac12 & -M\end{pmatrix}, \tag{2.10}$$

$$P_1^\pm(M)=(-)^{(l'+L-\lambda)/2}(2\lambda+1)\begin{pmatrix} l' & L & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l' & L & \lambda\\ -M\mp\frac12 & M\pm\frac12 & 0\end{pmatrix}, \tag{2.11}$$

$$P_2^\pm(M)=(-)^{(l'+L-\lambda)/2}(2\lambda+1)\begin{pmatrix} l & L' & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l & L' & \lambda\\ -M\mp\frac12 & M\pm\frac12 & 0\end{pmatrix}, \tag{2.12}$$

$$S_1=\int dr\, j_\lambda(kr)G_K f_\kappa\,, \tag{2.13}$$

$$S_2=\int dr\, j_\lambda(kr)F_K g_\kappa\,. \tag{2.14}$$

The G_K and F_K are, respectively, large and small components of a relativistic radial wave function of a bound state $(nKJL)$; correspondingly, the g_κ and f_κ refer to a continuous state $(E\kappa jl)$. The G_K, F_K, g_κ, and f_κ are obtained by solving radial Dirac equations numerically.[4] The integrals S are then calculated by numerical integrations. For each partial-wave channel KJL, there exist an infinite number of bound states which form a Rydberg series. Thus, it is not attractive to calculate by brute force with Eq. (2.4) all cross sections $\sigma_{K,n}$.

Before discussing a useful way to calculate each $\sigma_{K,n}$ and the sum $\sum_k\sum_n\sigma_{k,n}$, let us first examine the behavior of the final-state wave functions $\Psi_f(nKJL)$. For those Rydberg states which are unoccupied, it may be reasonable to consider only the large components of the wave functions, i.e., to take a nonrelativistic limit. Now it is well known that at atomic distances a Rydberg-state wave function resembles the wave function of a low-energy continuum electron in the corresponding partial-wave channel KJL. Such behavior has been formulated mathematically in the quantum defect theory.[2] For each partial-wave channel KJL, one can construct a radial wave function $R_K(\epsilon,r)$ such that the following conditions hold.

(1) The wave function $R_K(\epsilon,r)$ is a smooth function of energy ϵ at atomic distances (continuous states for $\epsilon\geq1$ and bound states for $\epsilon<1$).

(2) The logarithmic derivative of $R_K(\epsilon,r)$ at the edge $r=r_0$ of the atomic ion is a smooth function of energy ϵ.

(3) Outside the edge of the atomic ion, $r\geq r_0$, $R_K(\epsilon,R)$ is expressed as a linear combination of regular and irregular Coulomb wave functions, $\mathfrak{f}(\epsilon,L,r)\cos\pi\mu_K(\epsilon)-\mathfrak{g}(\epsilon,L,r)\sin\pi\mu_K(\epsilon)$, where $\mathfrak{f}$ and $\mathfrak{g}$ are nonrelativistic regular and irregular Coulomb wave functions,[2] respectively, and are continuous functions of energy ϵ. The parameter μ_K, which is determined by matching the inner form and the outer form of the wave function, is a smooth function of energy. Thus, we have

$$\begin{aligned}R_K(\epsilon,r)&=(\text{a smooth function of energy}),\quad \text{for } r<r_0\\ &=\mathfrak{f}(\epsilon,L,r)\cos\pi\mu_K-\mathfrak{g}(\epsilon,L,r)\sin\pi\mu_K,\\ &\qquad\text{for } r\geq r_0\,.\end{aligned} \tag{2.15}$$

The wave function $R_K(\epsilon, r)$ is normalized to unit energy in $Z_i^2\alpha^4$. For each bound state $nKJL$ with an energy $\epsilon_{K,n} = 1 - \frac{1}{2}Z_i^2\alpha^4/\nu_{K,n}^2 < 1$, the radial wave function G_K is

$$G_K = N_{K,n}^{-1} R_K(\epsilon, r) . \tag{2.16}$$

The normalization factor $N_{K,n}$ is determined by the bound-state boundary condition at $r = \infty$ and conventional bound-state normalization[2,5]:

$$N_{K,n}^2 = \left(\nu_{K,n}^3 + \frac{d\mu_K}{d(\epsilon/Z_i^2\alpha^4)}\right)\delta_{\epsilon,\epsilon_{K,n}} \tag{2.17}$$

with

$$\begin{aligned} \epsilon_{K,n} &= 1 - \tfrac{1}{2}Z_i^2\alpha^4/\nu_{K,n}^2 , \\ \nu_{K,n} &= n - \mu_K . \end{aligned} \tag{2.18}$$

Here n is the principal quantum number of the bound state. For a low-energy continuous state with energy $\epsilon = 1 + \frac{1}{2}p_2^2 \geq 1$, the wave function normalized to unit volume is then

$$\begin{aligned} G_K &= \frac{\pi Z_i^2\alpha^4}{2\epsilon p_2} R_K(\epsilon, r) \\ &\overset{r\to\infty}{\sim} \frac{1}{p_2}\left(p_2 r - \frac{L}{2}\pi + \frac{Z\alpha_i}{p_2}\ln 2p_2 r + \sigma_L + \pi\mu_K\right) . \end{aligned} \tag{2.19}$$

Here, $\pi\mu_K$ is the short-range phase shift and the σ_L is the Coulomb phase shift[6] corresponding to charge Z_i.

Taking the nonrelativistic limit of the final-state wave function, the reduced matrix elements, S in Eq. (2.13) and (2.14) can be rewritten as

$$\begin{aligned} S_1 &= \int dr\, j_\lambda(kr) f_\kappa G_K , \\ S_1 &= \frac{1}{2}\int dr\, j_\lambda(kr) g_\kappa\left(\frac{d}{dr} + \frac{K}{2}\right) G_K . \end{aligned} \tag{2.20}$$

Substituting Eq. (2.16) into Eq. (2.20), we then have

$$\begin{aligned} S_1 &= N_{K,n}^{-1}\bar{S}_1 = N_{K,n}^{-1}\int dr\, j_\lambda(kr) f_\kappa R_K(\epsilon, r) , \\ S_2 &= N_{K,n}^{-1}\bar{S}_2 = N_{K,n}^{-1}\int dr\, j_\lambda(kr) g_\kappa\left(\frac{1}{2}\frac{d}{dr} + \frac{1}{2}\frac{K}{2}\right) R_K(\epsilon, r) . \end{aligned} \tag{2.21}$$

Since the important domain in configuration space for reduced matrix elements is at atomic distances, the $\bar{S}_1$ and $\bar{S}_2$ are thus smooth functions of energy. The total cross section $\sigma_{K,n}$ in Eq. (2.4) is then rewritten as

$$\sigma_{K,n} = N_{K,n}^{-2}\frac{d\sigma(k_n)}{d(k/Z_i^2\alpha^4)} , \tag{2.22}$$

with the photon energy $k_n = E - \epsilon_{K,n}$. The cross-section density,

$$\frac{d\sigma_K(k)}{d(k/Z_i^2\alpha^4)} = \lambda_0 \sum_\kappa \sum_{M=1/2}^{J} \left|\bar{R}_\kappa^+(M)\right|^2 + \left|\bar{R}_\kappa^-(M)\right| , \tag{2.23}$$

is a smooth function of energy, where

$$\bar{R}_\kappa^\pm(M) = \sum_{n=1}^{2} Q_n^\pm(M) \sum_\lambda{}' p_n^\pm(M)\bar{S}_n . \tag{2.24}$$

As the final-state energy $\epsilon_{K,n}$ approaches 1, i.e., $k \to E$, the cross-section density $d\sigma_K/d(k/Z_i^2\alpha^4)$ will approach a limit corresponding to the partial-wave contribution (KJL) in the electron-ion bremsstrahlung cross section $d\sigma_K/d(k/Z_i^2\alpha^4)$ with $k = E$. Thus, for each partial-wave channel KJL, to calculate each $\sigma_{K,n}$ in Eq. (2.21) requires only the calculation of two smooth energy-varying quantities, μ_K and $d\sigma_K(k)/d(k/Z_i^2\alpha^4)$. In practice, such calculations can be carried out by calculating a few points and performing interpolations, as will be demonstrated in the next section.

APPLICATION

Calculations for direct radiative capture of 50-keV electrons by Au ions with charge $+49e$ are presented. First, the cross sections $\sigma_{K,n}$ defined in Eq. (2.4) for the low-lying Rydberg states are calculated numerically. These Rydberg states are the first unoccupied states for each partial-wave channel (e.g., $5s_{1/2}$, $4p_{1/2}$, $4p_{3/2}$, $4d_{3/2}$, $4d_{5/2}$, $4f_{7/2}$, etc.). Their quantum-defect parameters μ_K, defined in Eq. (2.18), are displayed in Fig. 1. We also display two other sets of quantum-defect parameters μ_K which are calculated from short-range phase shifts defined in Eq. (2.19) for two energies $\epsilon \geq 1$. Figure 1 shows that the quantum-defect parameters μ_K for each partial-wave

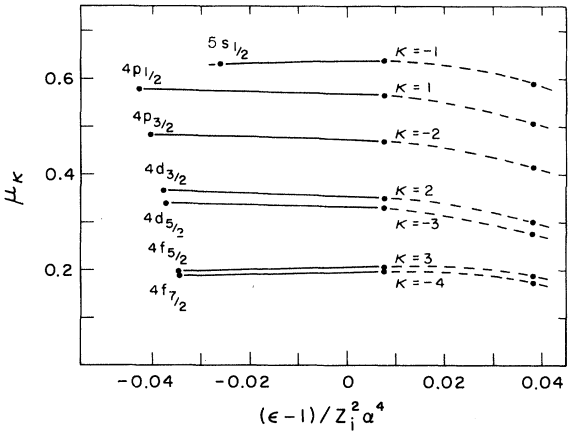

FIG. 1. Quantum defect μ_K vs energy $(\epsilon - 1)/Z_i^2\alpha^4$.

TABLE I. Quantum defect μ_K^α.

K	μ_K^0	μ_K^1
-1 $S_{1/2}$	0.636	0.204
1 $P_{1/2}$	0.564	−0.265
-2 $P_{3/2}$	0.470	−0.252
2 $d_{3/2}$	0.351	−0.339
-3 $d_{5/2}$	0.327	−0.325
3 $f_{5/2}$	0.205	0.297
-4 $f_{7/2}$	0.192	0.283

TABLE II. Cross-section density σ_K (10^{-24} cm^2/energy).

K	σ_K^0	σ_K^1
-1 $S_{1/2}$	93.94	33.17
1 $P_{1/2}$	61.12	52.28
-2 $P_{3/2}$	84.24	103.97
2 $d_{3/2}$	15.84	85.32
-3 $d_{5/2}$	18.61	101.84
3 $f_{5/2}$	1.27	23.32
-4 $f_{7/2}$	1.64	3.21

channel are indeed smooth functions of energy. Thus, each μ_K can be expanded as a power series in energy:

$$\mu_K = \mu_K^0 + \mu_K^1 \Delta \tag{3.1}$$

with

$$\Delta = (\epsilon - 1)/Z_i^2\alpha^4 . \tag{3.2}$$

The expansion coefficients μ_K^α are listed in Table I. With the quantum-defect parameters μ_K, we then obtain the normalization factors $N_{K,n}^2$ defined in Eq. (2.17) and the cross-section densities $d\sigma_K/d(k/Z_i^2\alpha^4)$ defined in Eq. (2.22), for these low-lying Rydberg states, which are displayed in Fig. 2. At two energies $\epsilon \geq 1$, the cross-section densities $d\sigma_K/d(k/Z_i^2\alpha^4)$ for each partial-wave channel KJL are calculated by partial-wave decomposition of the bremsstrahlung cross sections[7] for electrons scattered by Au ions with charge $+49e$. Again, Fig. 2 shows that the cross-section densities $d\sigma_K/d(k/Z_i^2\alpha^4)$ are smooth function of energy ϵ. Thus, each $d\sigma_K/d(k/Z_i^2\alpha^4)$ can be expanded as power series of Δ.

$$\frac{d\sigma_K}{d(k/Z_i^2\alpha^4)} = \sigma_K^0 + \sigma_K^1\Delta . \tag{3.3}$$

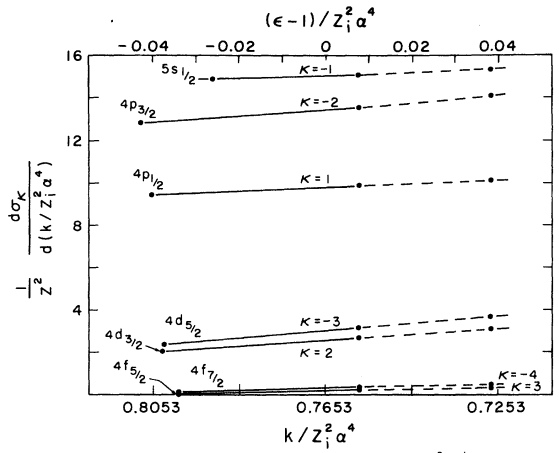

FIG. 2. Cross-section density $d\sigma_K/d(k/Z_i^2\alpha^4)$ vs photon energy $k/Z_i^2\alpha^4$.

The expansion coefficients σ_K^2 are listed in Table II. Figure 2 also shows something interesting: The cross sections for capture into the states with high orbital angular momentum $L \geq 5$ are negligible. With the quantum-defect parameters μ_K and the cross-section densities $d\sigma_K/d(k/Z_i^2\alpha^4)$ given in Tables I and II, respectively, each cross section $\sigma_{K,n}$ defined in Eq. (2.22) is easily calculated. The cross sections for capture into the first five Rydberg states in each partial-wave channel are presented in Table III. The sum of all cross sections $\sum_K \sum_n \sigma_{K,n}$ is 12.38 10^{-24} cm^2.

We would like to conclude with some comments. The present calculations are based on an independent electron approximation in the Hartree-Slater potential. For a highly stripped atomic ion, we expect that the calculations should give a fairly reliable estimate for the total radiative capture cross section $\sum_K \sum_n \sigma_{K,n}$, although the cross sections for the individual states may be redistributed owing to perturbations among the states due to

TABLE III. Cross section $\sigma_{K,n}$ (10^{-24} cm^2).

n	$nS_{1/2}$	$nP_{1/2}$	$nP_{3/2}$	$nd_{3/2}$	$nd_{5/2}$	$nf_{5/2}$	$nf_{7/2}$
4		1.48	1.85	0.27	0.30	0.008	0.010
5	1.11	0.69	0.89	0.14	0.16	0.007	0.008
6	0.60	0.38	0.49	0.08	0.09	0.005	0.005
7	0.36	0.23	0.30	0.03	0.04	0.003	0.004
8	0.23	0.15	0.20	0.02	0.03	0.002	0.003
9	0.16	0.10	0.14	0.017	0.02	0.001	0.002
10	0.11	0.07	0.10	0.013	0.015	0.001	0.001
•							
•							
•							
Sum	3.07	3.40	4.36	0.69	0.79	0.03	0.04

electron-electron correlations. To treat strong perturbations among various Rydberg series, it would be necessary to extend the one-channel quantum-defect treatment to a multichannel quantum-defect treatment.[3] In the present application, a ground state of Au ion with charge $+49e$ may have a closed-shell configuration $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$. Hence, a one-channel quantum-defect treatment may be adequate, except that a few states of a Rydberg series will be perturbed locally by states not belonging to the corresponding Rydberg series. For instance, a few states of the Rydberg series (core) $4s^2 ns, n \geq 5$, which are close to a state (core) $4s4p^2$ with $J = \frac{1}{2}$, will be perturbed. Thus, we expect that the corresponding cross sections $\sigma_{K,n}$ would deviate locally from the present calculations.

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