DIELECTRONIC RECOMBINATION

I. THEORY

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CONTENTS

Abstract

Dielectronic recombination (inverse autoionization) is treated as a special example of a resonance collision process; quantum scattering theory is used to parameterize the appropriate cross-section for resonance capture, with particular attention to overlapping levels, degeneracy, and the complete specification of angular momentum structure.

I. INTRODUCTION

The dilute plasmas that are found in the solar corona, in gaseous nebulae, and in interstellar space differ substantially from a plasma in local thermodynamic equilibrium (LTE). In these astrophysical plasmas, populations of energy levels and ionization stages cease to be governed by the Boltzmann-Saha equation and instead must be determined by balancing rates of excitation and ionization against countervailing rates of deexcitation and electron capture. For a plasma composed entirely of hydrogen (neutral and ionized), rate calculations involve the use of hydrogen wavefunctions, the properties of which are well established. When atoms other than hydrogen are considered, application of hydrogenic formulas may lead to gross inaccuracies. For example, Burgess (1964) pointed out that the electron-capture rate is substantially enhanced by the mechanism which Bates dubbed "dielectronic recombination". This mechanism, to be discussed below, contributes to the capture rate whenever the electron and ion can form a doubly-excited quasi-bound state (i.e., an autoionizing state). Burgess (1964), Goldberg (1966), and Goldberg and Dupree (1967) have drawn attention to several significant

astrophysical consequences of dielectronic recombination, and future study of non-LTE phenomena is likely to disclose additional consequences.

Although Burgess' simplified calculations (Burgess 1964, 1965, 1966) sufficed to indicate the importance of dielectronic recombination, questions remain concerning details of calculation. Recently Trefftz (1967) has discussed refinements based on the Mott and Massey (1965) treatment of electron-scattering resonances, and she has noted the inadequacy of earlier discussions of degeneracy and overlapping levels. Tucker and Gould (1966) have estimated dielectronic recombination rates, but because of their unjustified degeneracy assumptions, their results cannot be considered correct.

The present paper derives and examines the rate coefficient for dielectronic recombination, using results from the quantum theory of resonance collision processes, with particular attention to the complete specification of angular momentum structure and degeneracy. Several formulas, susceptible of straightforward computation, are presented. Subsequent papers will give the results of specific computations.

II. BASIC FORMULA

Electron capture occurs when a free electron of energy ϵ encounters an ion in state i and forms an atom in a stabilized state s (ordinarily an excited state). As Figure 1 illustrates schematically, the final stabilized state s can arise either by direct radiative capture, in which a single electron changes from a continuum to a bound orbital, or through formation of a doubly-excited state d, followed by a stabilizing radiative decay to the singly-excited bound state s. This latter process is dielectronic recombination.

The rate per unit volume at which capture occurs into state s, both direct capture and dielectronic-recombination, is written

$$R\ (s) = \sum_i N_e\ N(i)\ \alpha\ (i \rightarrow s), \qquad (2.1)$$

where N_e is the electron density and N(i) the density of ions in state i. Equation (2.1) defines the rate coefficient $\alpha\ (i \rightarrow s)$.

Similarly, the total rate of capture to all stabilized levels is written

$$R\ (\mathrm{tot}) = \sum_{s} R\ (s) = \sum_{i} N_e\ N(i)\ \alpha\ (i;\mathrm{tot}), \tag{2.2}$$

so that the total recombination coefficient is

$$\alpha\ (i;\mathrm{tot}) = \sum_{s} \alpha\ (i \rightarrow s). \tag{2.3}$$

The connection between these rate coefficients and the quantum theory of collisions is made manifest by introducing the cross-section $\sigma(\epsilon)$ for capture of an electron of energy $\epsilon = mv^2/2$ onto an ion state i to yield a stabilized state s plus a photon γ:

$$\sigma(\epsilon) \equiv \sigma(i\epsilon \rightarrow s\gamma). \tag{2.4}$$

That is, we view electron capture as a particular example of a rearrangement collision, A + a → B + b, in which the initial system A + a is an ion plus an electron and the final system B + b is an atom plus a photon.

Then using the electron-velocity distribution $d\varphi(v)$, a Maxwellian distribution in the cases of interest,

$$d\varphi(v) = \left(\frac{d\varphi}{dv}\right)\frac{d\epsilon}{v} = \frac{4\pi v^2}{(2\pi kT)^{3/2}}\exp(-\epsilon/kT)\, d\epsilon, \tag{2.5}$$

we can write the capture rate as

$$R(s) = \sum_i N_e\, N(i) \int d\varphi(v) \cdot v \cdot \sigma(\epsilon). \tag{2.6}$$

(I use atomic units, $e = m = \hbar = 1$.) Thus the recombination coefficient is

$$\alpha(i \to s) = \int d\epsilon \left(\frac{d\varphi}{dv}\right) \sigma(i\epsilon \to s\gamma). \tag{2.7}$$

In practice, our interest centers on recombination to a particular configuration or a particular term (SL). We then wish to sum the rate over a set of quantum numbers, say J. The required rate then has the form

$$R(s) = \sum_{J_s} R\,(sJ_s) = \sum_{J_s} \sum_{iJ_i} N_e\, N(iJ_i)\, \alpha(iJ_i \to sJ_s), \tag{2.8}$$

where

$$N(i) = \sum_{J_i} N(iJ_i). \tag{2.9}$$

The rate coefficient is then

$$\alpha(i \rightarrow s) = \sum_{J_i} \frac{N(iJ_i)}{N(i)} \sum_{J_s} \int d\epsilon \left(\frac{d\varphi}{dv}\right) \sigma\ (iJ_i\epsilon \rightarrow sJ_s\ \gamma). \tag{2.10}$$

If, as is ordinarily assumed, the initial ion states are populated according to their statistical weight, so that

$$N(iJ_i) = \frac{(2J_i+1)}{\varpi_i} N(i), \tag{2.11}$$

where

$$\varpi_i \equiv \sum_{J_i} (2J_i+1), \tag{2.12}$$

then the rate coefficient is

$$\alpha(i \rightarrow s) = \sum_{J_i} \frac{(2J_i+1)}{\varpi_i} \sum_{J_s} \int d\epsilon \left(\frac{d\varphi}{dv}\right) \sigma(iJ_i\epsilon \rightarrow sJ_s\ \gamma). \tag{2.13}$$

That is, equation (2.7) requires the cross-section

$$\sigma(i\epsilon \to s\gamma) = \sum_{J_i} \frac{(2J_i+1)}{\varpi_i} \sum_{J_s} \sigma(iJ_i\ \epsilon \to sJ_s\ \gamma)$$

$$= \frac{1}{\varpi_i} \sum_{(is)} \sigma(i\epsilon \to s\gamma) \qquad (2.14)$$

where $\sum_{(is)}$ denotes a summation (or integration) over all unspecified quantum numbers of initial and final systems.

According to the quantum theory of collision processes, the cross-section for capture of an electron of energy $\epsilon = v^2/2$ resulting in a photon of energy $\omega = \alpha k$ is (Shore 1967):

$$\sigma(i\epsilon \to s\gamma) = \frac{1}{\varpi_i \varpi_e} \frac{4\pi^3}{v^2} \sum_{(is)} |\langle s\gamma|T|i\epsilon\rangle|^2 \qquad (2.15)$$

$$= \frac{1}{\varpi_i \varpi_e} \frac{2\pi^2}{v^2} \left(\frac{4}{3} k^3\right) \sum_{(is)} \left|\langle s|D|i\epsilon\rangle + \sum_{d} \frac{\langle s|D|d\rangle\langle d|V|i\epsilon\rangle}{\epsilon + E_i - E_d + i\frac{1}{2}\Gamma(d)}\right|^2,$$

where ϖ_i and ϖ_e denote the intrinsic statistical weights of target ion i and electron projectile.

The scattering amplitude $\langle s\gamma|T|i\epsilon\rangle$ comprises two parts. The first part, the dipole-moment matrix element $\langle s|D|i\epsilon\rangle$, expresses direct capture of an electron (inverse photoionization). This part varies slowly with electron energy ϵ and is

most important for small ϵ. The second part, the sum $\sum_d$, shows rapid variation with energy ϵ near discrete energies E_d of resonances, and expresses the effect of dielectronic recombination (inverse autoionization). That is, each resonance is attributable to the formation of a quasi-bound resonance state which subsequently decays by emitting an electron or photon. The resonance states d that influence electron capture are doubly excited autoionizing states.

The resonance width $\Gamma(d)$ is the sum of two parts: an autoionizing width $\Gamma^{auto}(d)$ and a radiative width $\Gamma^{rad}(d)$. These partial widths express the respective probabilities for decay of state d by autoionization and by radiative transitions:

$$\Gamma^{auto}(d) = \sum_i A^{auto}(d \to i\epsilon) \equiv \sum_i 2\pi |\langle d|V|i\epsilon\rangle|^2 \qquad (2.16)$$

$$\Gamma^{rad}(d) = \sum_s A^{rad}(d \to s) \equiv \sum_s \tfrac{4}{3} k^3 \, |\langle d|D|s\rangle|^2 \qquad (2.17)$$

$$\Gamma(d) = \Gamma^{auto}(d) + \Gamma^{rad}(d). \qquad (2.18)$$

Although each individual resonance may make only a slight contribution to the cross-section, the cumulative effect of

many such resonances can become quite large when the mean electron energy coincides with the limit of a Rydberg series of autoionizing levels. Thus it often suffices to neglect the direct capture amplitude $\langle s|D|i\epsilon\rangle$, and so to obtain from equations (2.7), (2.5), and (2.15), the dielectronic recombination rate:

$$\alpha(i \to s) \cong \alpha^{di}(i \to s)$$

$$= \frac{1}{\omega_i \omega_e} \int d\epsilon \left(\frac{d\varphi}{d\epsilon}\right) \frac{2\pi^2}{v^2} \left(\frac{4}{3}k^3\right)$$

$$\sum_{(is)} \left| \sum_{d} \frac{\langle s|D|d\rangle \langle d|V|i\epsilon\rangle}{\epsilon + E_i - E_d + \frac{1}{2}i\Gamma(d)} \right|^2 . \qquad (2.19)$$

The integral over ϵ would appear to introduce interference effects between overlapping levels, such as

$$2\pi \sum_{(is)} \sum_{d} \sum_{d'} \frac{\langle s|D|d\rangle \langle s|D|d'\rangle^* \langle d|V|i\epsilon\rangle \langle d|V|i\epsilon\rangle^* [\Gamma(d)+\Gamma(d')]}{[E_d - E_{d'}]^2 + \frac{1}{4}[\Gamma(d) + \Gamma(d')]^2} . \qquad (2.20)$$

However, as we will see in Section VIII, selection rules eliminate interference except between levels such that

$$2(E_d - E_{d'}) >> \Gamma(d) + \Gamma(d'), \qquad (2.21)$$

in which case interference may be neglected. Thus we obtain the basic formulas of dielectronic recombination:

$$\alpha^{di}(i \to s) = \left(\frac{2\pi}{kT}\right)^{3/2} \sum_{d} \exp(-\epsilon/kT) \; \frac{\varpi_d}{\varpi_i \varpi_e} \sum_{(is)} \frac{A^{rad}(d \to s) A^{auto}(d \to i\epsilon)}{\Gamma^{rad}(d) + \Gamma^{auto}(d)} \tag{2.22}$$

$$\alpha^{di}(i;tot) = \left(\frac{2\pi}{kT}\right)^{3/2} \sum_{d} \exp(-\epsilon/kT) \; \frac{\varpi_d}{\varpi_i \varpi_e} \sum_{(is)} \frac{\Gamma^{rad}(d \to s) A^{auto}(d \to i\epsilon)}{\Gamma^{rad}(d) + \Gamma^{auto}(d)} \; . \tag{2.23}$$

Here ϖ_d is the number of resonances having identical resonance parameters $A^{rad}(d \to s)$, $A^{auto}(d \to i\epsilon)$ and E_d, and $\sum_{(is)}$ denotes, as above, a summation over all unspecified quantum numbers of initial and final systems. With Γ and A expressed in atomic units, we require the value

$$\left(\frac{2\pi}{k}\right)^{3/2} = \left(\frac{2\pi\hbar^2}{mk}\right)^{3/2} \times \left(\frac{me^4}{\hbar^3}\right) = 17.1200 \text{ cm}^{-3} \text{ sec}^{-1} (^\circ\text{K})^{3/2} \; .$$

To illustrate the meaning of the symbol $\sum_{(is)}$, consider dielectronic recombination onto helium. Formula (2.22) might then read

$$\alpha^{di}(1s \rightarrow 1s,\ n\ell) = \left(\frac{2\pi}{kT}\right)^{3/2} \sum_{n_1\ell_1 n'\ell'} \exp(-\epsilon/kT)\ (2\ell_1+1)(2\ell'+1)$$

$$\times \sum_{\mu} \int d\Omega \sum_{LSJM} A^{rad}(n_1\ell_1, n'\ell'\ LSJM \rightarrow 1s, n\ell\ LSJM)$$

$$\times \frac{A^{auto}(n_1 p, n\ell\ LSJM \rightarrow 1s, \epsilon\ \Omega\mu)}{\Gamma(n_1\ell_1,\ n'\ell'\ LSJM)} \qquad (2.24)$$

where Ω and μ denote respectively the propagation direction and the spin projection of the captured electron. In subsequent sections we shall consider alternative specifications of quantum numbers.

III. ALTERNATIVE FORMULAS

Previous workers have used several alternative forms for the basic equations (2.22) - (2.23). If we introduce a "capture cross-section" σ^{cap} by writing

$$\int d\epsilon\ \sigma(\epsilon) = \sum_d \sigma^{cap}(i \to d)\ \frac{A^{rad}(d \to s)}{\Gamma(d)}\ , \tag{3.1}$$

then σ^{cap} is given by the expression

$$\sigma^{cap}(i \to d) = \frac{2\pi^2}{v^2}\ \frac{\varpi_d}{\varpi_e \varpi_i}\ A^{auto}(d \to i). \tag{3.2}$$

Using σ^{cap} we can write the rate coefficient (2.22) in the form used by Burgess:

$$\alpha^{di}(i;tot) = \sum_d \frac{4\pi v^2}{(2\pi kT)^{3/2}}\ \exp(-\epsilon/kT) \times \int_{(is)} \frac{\Gamma^{rad}(d)\ x\ \sigma^{cap}(i \to d)}{\Gamma^{rad}(d) + \sum_i \frac{v^2}{2\pi^2}\ \frac{\varpi_e \varpi_i}{\varpi_d}\ \sigma^{cap}(i \to d)}. \tag{3.3}$$

Alternatively, if autoionization from d occurs only to

the continuum of ion state i, equation (2.16) reads

$$\Gamma^{auto}(d) = A^{auto}\ (d \rightarrow i). \tag{3.5}$$

We can then introduce "partial lifetimes", defined by the equations

$$\tau^{auto}\ (d) = 1/\Gamma^{auto}\ (d) \tag{3.6a}$$

$$\tau^{rad}\ (d) = 1/\Gamma^{rad}\ (d), \tag{3.6b}$$

and write, as did Bates and Dalgarno (1962):

$$\alpha^{di}(i;tot) = \sum_{d} \left(\frac{2\pi}{kT}\right)^{3/2} \exp(-\epsilon/kT)\ \frac{\varpi_d}{\varpi_e \varpi_i}\ [\tau^{rad}(d)+\tau^{auto}(d)]^{-1}. \tag{3.7}$$

Here, with Γ expressed in seconds, we require the value

$$\frac{1}{2}\left(\frac{2\pi}{k}\right)^{3/2} = \frac{1}{2}\left(\frac{2\pi\hbar^2}{mk}\right)^{3/2} = 2.0706 \times 10^{-16}\ cm^{-3}\ (^\circ K)^{3/2}.$$

As another alternative, we can introduce equilibrium

populations N^*, defined by the equation

$$\frac{N^*(d)}{N_e N^*(i)} = \frac{\varpi_d}{\varpi_e \varpi_i} \frac{h^3}{(2\pi mkT)^{3/2}} \exp(-\epsilon/kT). \tag{3.8}$$

We can then write equation (2.22) as

$$\alpha^{di}\ (i \to s) = \sum_d \frac{N^*(d)}{N_e N^*(i)} \sum_{(is)} A^{rad}(d \to s)\ b(d) \tag{3.9}$$

and equation (2.8) as

$$R^{di}(s) = \sum_i \frac{N(i)}{N^*(i)} \sum_d N^*(d)\ b(d) \sum_{(s)} A^{rad}(d \to s) \tag{3.10}$$

where

$$b(d) = \frac{1}{\varpi_d} \sum_{(id)} \frac{A^{auto}(d \to i)}{\Gamma^{rad}(d) + \Gamma auto(d)}. \tag{3.11}$$

With A^{rad} expressed in atomic units, we require the atomic unit of rate,

$$\left(\frac{me^4}{\hbar^3}\right) = 4.13413 \times 10^{16}\ \text{sec}^{-1}.$$

Previous derivations of the rate coefficients balanced the rate of capture into state d with the rate of decay from

state d, $\Gamma(d)xN(d)$, and equated this capture rate with the equilibrium rate of autoionization, $\Gamma^{auto}(d)xN^{*}(d)$. The derivation from scattering theory, as done here, may seem unnecessarily roundabout compared with a derivation based on detailed balancing of radiative decay against the inverse of autoionization. I submit a twofold justification: first, to clarify the treatment of degeneracy and overlapping levels; and second, to provide a prescription for perturbation-theory calculations of the resonance parameters Γ, Γ^{auto}, Γ^{rad}, etc., which removes concern over treating short-lived resonance states on the same footing as the more familiar singly-excited states.

IV. AUTOIONIZING PROBABILITIES

In the cases of interest here, autoionization occurs because the inter-electron Coulomb repulsion,

$$V = -\sum_{i<j} \frac{1}{r_{ij}} , \tag{4.1}$$

mixes bound and continuum configurations (see Fano 1961). The autoionizing probability of equation (2.16) is not yet completely specified; quantum numbers which do not appear explicitly are to be summed over. Because one ordinarily employs angular-momentum states to describe free atoms, it is convenient to describe the continuum electron in an angular momentum representation. (Alternatively, one could use distorted plane-waves, with integration over propagation directions.) Then the continuum orbital,

$$\varphi(\epsilon \ell m \mu | \underset{\sim}{r}\ \underset{\sim}{s}) = P_{\epsilon \ell}(r)\ Y_{\ell m}(\theta \phi)\ \chi_{\mu}(\underset{\sim}{s}), \tag{4.2}$$

differs from a bound orbital only in the radial factor $P_{\epsilon \ell}(r)$. This assumption gives for the autoionizing probabilities the expression

$$A^{\text{auto}}(dJ_d \rightarrow i) = 2\pi \sum_{\ell} |\langle dJ_d | V | i, \epsilon \ell \rangle|^2 , \tag{4.3}$$

if the radial functions are energy-normalized:

$$\int dr\ P_{\epsilon\ell}\ P_{\epsilon'\ell} = \delta(\epsilon - \epsilon'). \tag{4.4}$$

To perform computations we must specify a coupling scheme for the combined system of ion plus free electron. Because we will sum over the collective or intermediate quantum numbers, we are at liberty to choose the coupling scheme to simplify computations; we might use $J\ell$ coupling, and the formula

$$A^{auto}(dJ_d \to i) = 2\pi \sum_{J_i} \sum_{\ell} \sum_{K} \left| \langle dJ_d | V | iJ_i,\ \epsilon\ell\ [K] J_d \rangle \right|^2; \tag{4.5}$$

or LS coupling and the formula

$$A^{auto}(dJ_d \to i) = 2\pi \sum_{L_i} \sum_{S_i} \sum_{\ell} \sum_{L} \sum_{S} \left| \langle dJ_d | V | iL_iS_i,\ \epsilon\ell\ LSJ_d \rangle \right|^2 . \tag{4.6}$$

The preceeding formulas utilize the fact that V is diagonal in total angular momentum J. Equation (4.7) simplifies further if LS-coupling states are appropriate for d. We then obtain

the formula

$$A^{\text{auto}}(dL_dS_dJ_d \rightarrow L_iS_i) = 2\pi \sum_{\ell} |\langle dL_dS_d|V|iL_iS_i,\ \epsilon\ell\ L_dS_d\rangle|^2$$

$$= A^{\text{auto}}(dL_dS_d \rightarrow iL_iS_i). \qquad (4.7)$$

As this notation indicates, the autoionizing probability is independent of J for LS-coupling states.

Using standard angular-momentum methods (e.g., Shore and Menzel 1967), one can reduce the calculation of matrix-elements to the evaluation of 6-j symbols and radial integrals. As a simple example, consider a two-electron atom, whose doubly-excited states can be approximated by pure-configuration LS-coupling wavefunctions. The autoionizing probability is then given by the formula

$$A^{\text{auto}}(dJ_d \rightarrow i) \equiv A^{\text{auto}}(n_1\ell_1, n_2\ell_2\ LSJ_d \rightarrow n_o\ell_o)$$

$$= 2\pi \sum_{\ell'} |\langle n_1\ell_1,\ n_2\ell_2\ LSJ_d|V|n_o\ell_o,\ \epsilon\ell'\ LSJ_d\rangle|^2$$

$$= 2\pi \sum_{\ell'} \left| \sum_k \begin{Bmatrix} L & \ell_1 & \ell_2 \\ k & \ell_1 & \ell_o \end{Bmatrix} \mathcal{R}^k(\text{dir}) + (-1)^{L+S} \sum_k \begin{Bmatrix} L & \ell_1 & \ell_2 \\ k & \ell_o & \ell' \end{Bmatrix} \mathcal{R}^k(\text{ex}) \right|^2$$

$$\equiv A^{\text{auto}}(n_1\ell_1,\ n_2\ell_2\ LS \rightarrow n_o\ell_o), \qquad (4.8)$$

where $\mathcal{R}^k$ (dir) and $\mathcal{R}^k$ (ex) are expressible in terms of generalized Slater integrals R^k that involve an energy-normalized continuum orbital:

$$\mathcal{R}^k(\text{dir}) \equiv \langle \ell_1 \| \underset{\sim}{C}^{(k)} \| \ell_0 \rangle \langle \ell_2 \| \underset{\sim}{C}^{(k)} \| \ell' \rangle \; R^k(n_1\ell_1 \; n_2\ell_2 \; n_0\ell_0 \; \epsilon\ell') \tag{4.9a}$$

$$\mathcal{R}^k(\text{ex}) \equiv \langle \ell_1 \| \underset{\sim}{C}^{(k)} \| \ell' \rangle \langle \ell_2 \| \underset{\sim}{C}^{(k)} \| \ell_0 \rangle \; R^k(n_2\ell_2 \; n_1\ell_1 \; n_0\ell_0 \; \epsilon\ell') . \tag{4.9b}$$

Here $\langle \ell \| C^{(k)} \| \ell' \rangle$ denotes the reduced matrix element of a Racah tensor. In particular, when $\ell_0 = 0$ formula (4.8) reads:

$$A^{\text{auto}}(n_1p, \; n_2\ell \; LS \rightarrow n_0s)$$

$$= \delta(L, \ell \pm 1) \; \frac{2\pi}{3} \; \frac{\text{Max}(\ell, L)}{(2L+1)} \left| R^1(n_1p \; n_2\ell \; n_0s \; \epsilon L) \right.$$

$$\left. + (-1)^S \; \frac{3}{2\ell + 1} \; R^{\ell}(n_2\ell \; n_1p \; n_0s \; \epsilon L) \right|^2 \tag{4.10}$$

where Max (ℓ, L) denotes the larger of ℓ and L. The autoionizing widths for LS-coupling states are independent of J and are

given by the formula

$$\Gamma^{\text{auto}}(\text{dLSJ}) = \Gamma^{\text{auto}}(n_1\ell_1,\ n_2\ell_2\ \text{LS})$$

$$= \sum_{n_o\ell_o} A^{\text{auto}}(n_1\ell_1,\ n_2\ell_2\ \text{LS} \rightarrow n_o\ell_o). \qquad (4.11)$$

If $\ell_o \neq 0$ the average autoionizing probability is given by the formula

$$\bar{A}^{\text{auto}}(n_1\ell_1,\ n\ell \rightarrow n_o\ell_o) \equiv \frac{\sum_{LSJ} (2J+1)\ A^{\text{auto}}(n_1\ell_1,\ n\ell\ \text{LSJ} \rightarrow n_o\ell_o)}{\sum_{LSJ} (2J+1)}$$

$$= 2\pi \sum_{\ell' SL} \frac{(2S+1)}{4} \frac{(2L+1)}{(2\ell+1)(2\ell_1+1)} \left|\langle n_1\ell_1,\ n\ell\ \text{LS}\,|V|\,n_o\ell_o,\ \epsilon\ell'\ \text{LS}\rangle\right|^2$$

$$= \frac{2\pi}{(2\ell+1)(2\ell_1+1)} \sum_{\ell} \left\{ \sum_{k} \frac{|\mathcal{R}^k(\text{dir})|^2}{2k+1} + \sum_{k} \frac{|\mathcal{R}^k(\text{ex})|^2}{2k+1} \right.$$

$$\left. - \sum_{kk'} (-1)^{k+k'} \begin{Bmatrix} \ell' & \ell_o & k \\ \ell & \ell_1 & k' \end{Bmatrix}^2 \mathcal{R}^k(\text{dir})\ \mathcal{R}^{k'}(\text{ex}) \right\}. \qquad (4.12)$$

Although LS coupling states may provide reasonable approximations for low-lying doubly excited states, they are inappropriate for the description of very highly excited

configurations $n_1 \ell_1$, $n\ell$ where n becomes very large. For example, the splitting between 2p 100ℓ and 2p 99ℓ is much smaller than the splitting between the ion levels $2p_{\frac{1}{2}}$ and $2p_{3/2}$, so one is interested in levels such as $2p_{\frac{1}{2}}$ 100ℓ and $2p_{3/2}$ 100ℓ. $J\ell$-coupling offers a better approximation for such configurations, because one is interested in a sequence of states approaching a well-defined value of J_i. The autoionizing probability in $J\ell$ coupling may be written as

$$A^{\text{auto}}(n_1 \ell_1 J_1,\ n\ell[K]J \rightarrow n_o \ell_o)$$

$$= \sum_{\ell' j_o K'} 2\pi \left| \langle n_1 \ell_1 J_1,\ n\ell[K]J | V | n_o \ell_o j_o,\ \epsilon\ell'[K']J \rangle \right|^2$$

$$= \sum_{\ell' j_o j'} 2\pi \left| \langle n_1 \ell_1 J_1,\ n\ell[K]J | V | n_o \ell_o j_o,\ \epsilon\ell' j',\ J \rangle \right|^2$$

$$= 2\pi(2K+1)(2J_1+1) \sum_{\ell' LS} (2S+1)(2L+1)$$

$$\times \left| \langle n_1 \ell_1,\ n\ell\ LS | V | n_o \ell_o,\ \epsilon\ell'\ LS \rangle \right|^2$$

$$\times \left| \sum_j (2j+1) \begin{Bmatrix} j & J_1 & J \\ K & \frac{1}{2} & \ell \end{Bmatrix} \begin{Bmatrix} \ell_1 & \ell & L \\ \frac{1}{2} & \frac{1}{2} & S \\ J_1 & j & J \end{Bmatrix} \right|^2 .$$

Although this formula shows an explicit dependence on J, K, and J_1, the average autoionizing probability is independent of J_1,

$$\bar{A}^{auto}(n_1\ell_1 J_1,\ n\ell \to n_o\ell_o) \equiv \frac{\sum_{JK}(2J+1)\, A^{auto}(n_1\ell_1 J_1,\ n\ell[K] \to n_o\ell_o)}{\sum_{JK}(2J+1)}$$

$$= 2\pi \sum_{\ell' LS} \frac{(2S+1)}{4}\,\frac{(2L+1)}{(2\ell+1)(2\ell_1+1)}$$

$$\times\ |\langle n_1\ell_1,\ n\ell\ LS|V|n_o\ell_o,\ \varepsilon\ell'\ LS\rangle|^2; \qquad (4.14)$$

in agreement with equation (4.13). The autoionizing widths exhibit the J and K dependence shown in formula (4.14):

$$\Gamma^{auto}(n_1\ell_1 J_1,\ n\ell[K]J) = \sum_{n_o\ell_o} A^{auto}(n_1\ell_1 J_1, n\ell[K]J \to n_o\ell_o). \qquad (4.15)$$

The average autoionizing width is

$$\bar{\Gamma}^{auto}(S_1L_1J_1,\ n\ell) = \bar{\Gamma}^{auto}(S_1L_1,\ n\ell)$$

$$= 2\pi \sum_{S_oL_o\ell' SL} \frac{(2S+1)(2L+1)}{2(2S_1+1)(2L_1+1)(2\ell+1)}$$

$$\times\ |\langle S_1L_1,\ n\ell\ SL|V|S_oL_o,\ \varepsilon\ell'\ SL\rangle|^2, \qquad (4.16)$$

or, for a two-electron level, it is

$$\bar{\Gamma}^{auto}(n_1\ell_1,\ n\ell) = 2\pi \sum_{\ell' SL} \frac{(2S+1)(2L+1)}{4(2\ell+1)(2\ell_1+1)}$$

$$\times\ |\langle n_1\ell_1,\ n\ell\ SL|V|n_o\ell_o,\ \varepsilon\ell'\ SL\rangle|^2. \qquad (4.17)$$

V. RADIATIVE PROBABILITIES

The radiative decay rate is the Einstein spontaneous transition probability, which may be written

$$A^{rad}(d \to s) = \frac{4}{3} k^3 \frac{|\langle d \| \underset{\sim}{D} \| s \rangle|^2}{\varpi_d} = \frac{\varpi_s}{\varpi_d} A^{rad}(s \to d), \qquad (5.1)$$

$$\hbar c k \equiv |E_d - E_s|,$$

where $\langle d \| D \| s \rangle$ is the reduced matrix element of the dipole moment. If we use $J\ell$ coupling for the doubly excited state, we require the following matrix element:

$$|\langle J_1,\ n\ell[K]J \| \underset{\sim}{D} \| J_o,\ n'\ell'[K']J' \rangle|^2$$

$$= (2J+1)(2J'+1)(2K+1)(2K'+1) \begin{Bmatrix} \frac{1}{2} & K & J \\ 1 & J' & K' \end{Bmatrix}^2$$

$$\times \left[\delta(n\ell, n'\ell') \begin{Bmatrix} \ell' & J_1 & K \\ 1 & K' & J_o \end{Bmatrix}^2 |\langle J_1 \| \underset{\sim}{D} \| J_o \rangle|^2 \right.$$

$$\left. + \delta(J_1, J_1') \begin{Bmatrix} J_o & \ell & K \\ 1 & K' & \ell' \end{Bmatrix}^2 |\langle n\ell \| \underset{\sim}{D} \| n'\ell' \rangle|^2 \right]. \qquad (5.2)$$

It then follows that the radiative decay is given by the

formula

$$A^{rad}(J_1, n\ell\ [K]J \to J_o,\ n'\ell')$$

$$= \sum_{J'K'} A^{rad}(n_1\ell_1 J_1,\ n\ell\ [K]J \to n_o\ell_o J_o,\ n'\ell'\ [K']\ J')$$

$$= \begin{cases} A^{rad}(J_1 \to J_o) & \text{if } n\ell = n'\ell' \\ A^{rad}(n\ell \to n_o\ell_o) & \text{if } J_1 = J_o. \end{cases} \tag{5.3}$$

For highly excited states, transition of the inner core, $J_1 \to J_o$, is more likely than transition of the highly excited outer electron, $n\ell \to n'\ell'$, and we can write

$$A^{rad}(J_1,\ n\ell\ [K]\ J \to J_o,\ n'\ell') \cong A^{rad}(J_1 \to J_o)\,\delta(n,n')\,\delta(\ell,\ell'). \tag{5.4}$$

If the inner core is a single electron, we can write

$$A^{rad}(n,\ell_1 J_1,\ n\ell\ [K]\ J \to n_o\ell_o J_o,\ n\ell) = A^{rad}(n_1\ell_1 \to n_o\ell_o), \tag{5.5}$$

where, according to equation (5.1),

$$A^{rad}(n_1\ell_1 \rightarrow n\ell) = \frac{4}{3} k^3 \frac{|\langle n_1\ell_1 \| \underset{\sim}{D} \| n_o\ell_o \rangle|^2}{(2\ell_1+1)}$$

$$= \frac{4}{3} k^3 \frac{Max(\ell_1,\ell_o)}{(2\ell_1+1)} \left| \int_o^\infty dr\ P_{n_1\ell_1}\ P_{n_o\ell_o}\ r \right|^2 . \tag{5.6}$$

In turn, the radiative width of the doubly excited level is

$$\Gamma^{rad}(J_1,\ n\ell\ [K]\ J) = \sum_{J_o} A^{rad}(J_1 \rightarrow J_o) + \sum_{n_o\ell_o} A^{rad}(n\ell \rightarrow n_o\ell_o)$$

$$= \Gamma^{rad}(J_1) + \Gamma^{rad}(n\ell), \tag{5.7}$$

or, approximately,

$$\Gamma^{rad}(J_1,\ n\ell\ [K]\ J) \cong \Gamma^{rad}(J_1). \tag{5.8}$$

The radiative width is independent of the coupling scheme and of quantum numbers K and J.

VI. RATE COEFFICIENTS

The preceding sections give, for dielectronic recombination through $J\ell$-coupling resonances,

$$J_i\ \varepsilon\ell' \rightarrow J_1\ n\ell\ [K]\ J_d \rightarrow J_o\ n\ell,$$

the rate coefficient

$$\alpha^{di}(J_i \rightarrow J_o,\ n\ell) = \frac{(2J_o+1)}{(2J_i+1)} \left(\frac{2\pi}{kT}\right)^{3/2} \sum_{J_1} \exp(-\varepsilon/kT) \times A^{rad}(J_o \rightarrow J_1)(2\ell+1)b(J_1,n\ell) \qquad (6.1)$$

where

$$(2\ell+1)b(J_1,n\ell) = \sum_{\ell' K J_d} \frac{(2J_d+1)}{2(2J_1+1)} \frac{A^{auto}(J_1,n\ell\ [K]\ J_d \rightarrow J_i,\varepsilon\ell')}{\Gamma^{rad}(J_1) + \Gamma^{auto}(J_1,n\ell\ [K]\ J_o)}. \qquad (6.2)$$

For recombination onto a one-electron atom, through LS-coupling resonances,

$$n_i\ell_i,\ \varepsilon\ell' \rightarrow n_1\ell_1,\ n\ell\ LS \rightarrow n_o\ell_o,\ n\ell,$$

the rate coefficient is

$$\alpha^{di}(n_i \ell_i \rightarrow n_o \ell_o,\ n\ell) = \frac{(2\ell_o+1)}{(2\ell_i+1)} \left(\frac{2\pi}{kT}\right)^{3/2} \sum_{n_1 \ell_1} \exp(-\epsilon/kT) \times A^{rad}(n_o \ell_o \rightarrow n_1 \ell_1)(2\ell+1) b(n_1 \ell_1, n\ell) \tag{6.3}$$

where

$$(2\ell+1) b(n_1 \ell_1, n\ell) = \sum_{\ell' LS} \frac{(2S+1)(2L+1)}{4(2\ell_1+1)} \times \frac{A^{auto}(n_1 \ell_1, n\ell\ LS \rightarrow n_i \ell_i,\ \epsilon\ell')}{\Gamma^{rad}(n_1 \ell_1) + \Gamma^{auto}(n_1 \ell_1, n\ell\ LS)} . \tag{6.4}$$

The coefficients for recombination onto the ground level or ground configuration are

$$\alpha^{di}(J_o \rightarrow J_o, n\ell) = \left(\frac{2\pi}{kT}\right)^{3/2} \sum_{J_1} \exp(-\epsilon/kT)\ A^{rad}(J_o \rightarrow J_1)(2\ell+1) b(J_1, n\ell) \tag{6.5}$$

$$(2\ell+1) b(J_1, n\ell) = \sum_{KJ} \frac{(2J+1)}{2(2J_1+1)} \frac{\Gamma^{auto}(J_1,\ n\ell\ [K]\ J_o)}{\Gamma^{rad}(J_1) + \Gamma^{auto}(J_1, n\ell\ [K]\ J_o)}, \tag{6.6}$$

and

$$\alpha^{di}(n_o\ell_o \rightarrow n_o\ell_o, n\ell) = \left(\frac{2\pi}{kT}\right)^{3/2} \sum_{n_1\ell_1} \exp(-\epsilon/kT) \times A^{rad}(n_o\ell_o \rightarrow n_1\ell_1)(2\ell+1)b(n_1\ell_1, n\ell) \tag{6.7}$$

$$(2\ell+1)b(n_1\ell_1, n\ell) = \sum_{LS} \frac{(2S+1)}{4} \frac{(2L+1)}{(2\ell_1+1)} \frac{\Gamma^{auto}(n_1\ell_1,\ n\ell\ LS)}{\Gamma^{rad}(n_1\ell_1)+\Gamma^{auto}(n_1\ell_1, n\ell\ LS)}. \tag{6.8}$$

If $\ell_o = 0$, the latter formula becomes

$$\alpha^{di}(n_o s \rightarrow n_o s,\ n\ell) = \left(\frac{2\pi}{kT}\right)^{3/2} \sum_{n_1} \exp(-\epsilon/kT) \times A^{rad}(n_o s \rightarrow n_1 p)\ (2\ell+1)\ b\ (n_1 p, n\ell) \tag{6.9}$$

$$(2\ell+1)\ b\ (n_1 p, n\ell) = \sum_{LS} \frac{(2S+1)}{4} \frac{(2L+1)}{3} \delta(L, \ell\pm1) \times \frac{\Gamma^{auto}(n_1 p, n\ell\ LS)}{\Gamma^{rad}(n_1 p) + \Gamma^{auto}(n_1 p, n\ell\ LS)}. \tag{6.10}$$

The total rate coefficient for recombination onto the ground configuration may be written

$$\alpha^{di}(n_o\ell_o;tot) = 4.141 \times 10^{-16} \sum_{n_1\ell_1} \frac{\exp(-1.44\tilde{\nu}/T)}{T^{3/2}} \times A^{rad}(n_o\ell_o \rightarrow n_1\ell_1) \times \sum_{n\ell} (2\ell+1)b(n_1\ell_1,n\ell)$$

$$= 2.7622 \times 10^{-9} \sum_{n_1\ell_1} \frac{\exp(-1.44\tilde{\nu}/T)}{T^{3/2}} \times f(n_o\ell_o \rightarrow n_1\ell_1) \times (10^{-4}\tilde{\nu})^2 \sum_{n\ell} (2\ell+1)b(n_1\ell_1,n\ell), \qquad (6.11)$$

where T is expressed in degrees Kelvin, $\tilde{\nu}$ is the wavenumber (in cm^{-1}) of the $n_o\ell_o \rightarrow n_1\ell_1$ transition, and

$$(2\ell+1)b(n_1\ell_1,n\ell) = \sum_{LS} \frac{(2S+1)}{4} \frac{(2L+1)}{(2\ell_1+1)} \frac{\Gamma^{auto}(n_1\ell_1,n\ell\ LS)}{\Gamma^{rad}(n_1\ell_1)+\Gamma^{auto}(n_1\ell_1,n\ell\ LS)}$$

$$= \sum_{j_1KJ} \frac{(2J+1)}{4(2\ell_1+1)} \frac{\Gamma^{auto}(n_1\ell_1j_1,n\ell\ [K]\ J)}{\Gamma^{rad}(n_1\ell_1)+\Gamma^{auto}(n_1\ell_1j_1,n\ell[K]J)} . \qquad (6.12)$$

These formulas also apply to more complex atoms, with the replacement

$$n_1\ell_1 \rightarrow S_1L_1 \quad \text{and} \quad 4(2\ell_1+1) \rightarrow 2(2S_1+1)(2L_1+1).$$

When recombination occurs onto an s level, formula (6.12) must be replaced by

$$(2\ell+1)b(n_1 p,\ n\ell) = \sum_{LS} \frac{(2S+1)}{4}\,\frac{(2L+1)}{3}\,\delta(L,\ell\pm1) \times \frac{\Gamma^{auto}(n_1 p, n\ell\ LS)}{\Gamma^{rad}(n_1 p) + \Gamma^{auto}(n_1 p, n\ell\ LS)} \quad . \tag{6.13}$$

Formula (6.11) is similar to the general formula given by Burgess, which may be written approximately as

$$\alpha^{di}(n_o\ell_o;tot) \cong 3.0 \times 10^{-3} \sum_{n_1\ell_1} \frac{\exp(-1.44\tilde{\nu}/T)}{T^{3/2}} \times f(n_o\ell_o \rightarrow n_1\ell_1) \times \left(10^{-4}\tilde{\nu}\right)^{\frac{1}{2}} \times \left[\frac{Z(Z+1)^4}{Z^2 + 13.4}\right]^{\frac{1}{2}} . \tag{6.14a}$$

The Burgess Formula requires

$$\sum_{n\ell} (2\ell+1)b(n_1\ell_1, n\ell) = \frac{1.09 \times 10^5}{(10^{-4}\ \tilde{\nu})^{3/2}} \left[\frac{Z^2 + 13.4}{Z(Z+1)^4}\right]^{\frac{1}{2}} . \tag{6.14b}$$

Future computational studies of $b(n_1\ell_1, n\ell)$ will establish the range of validity for this equality; several obvious inconsistencies (concerning recombination onto $\ell_o = 0$ and onto excited states) are noted below.

For the lowest-lying doubly-excited levels, autoionization is far more probable than competing modes of radiative decay; the resonance state d, once formed, promptly yields a free electron and an ion. Thus the autoionizing levels which one recognizes in optical spectra have widths that greatly exceed their radiative widths. (It is this property that makes the broad autoionizing lines so conspicuous.) This balance of probabilities reverses for very highly excited states; state d then decays with greatest likelihood through

photon emission, usually resulting in a stabilized state s. If the autoionizing width greatly exceeds the radiative width, formula (6.12) becomes

$$\sum_{n\ell}(2\ell+1)b(n_1\ell_1,n\ell) \cong \sum_{n\ell jKJ}\frac{(2J+1)}{4(2\ell_1+1)} = \sum_{n\ell LS}\frac{(2S+1)(2L+1)}{4(2\ell_1+1)}$$

$$= \sum_{n\ell}(2\ell+1) = \sum_{n} n^2 . \qquad (6.15)$$

Note, however, that formula (6.13) gives

$$\sum_{n\ell}(2\ell+1)b(n_1p,n\ell) \cong \sum_{n\ell LS}\frac{(2S+1)}{4}\,\frac{(2L+1)}{3}\,\delta(L,\ell\pm1)$$

$$= \frac{2}{3}\sum_{n\ell}(2\ell+1)\left[1+\tfrac{1}{2}\delta\ell_o\right] = \frac{2}{3}\sum_{n}(n^2+\tfrac{1}{2}) . \qquad (6.16)$$

Thus the recombination rate onto an s electron is roughly $\frac{2}{3}$ the recombination rate onto an $\ell_o \neq 0$ electron, because the parity selection rule permits autoionization only in accordance with the rule

$$n_1p,\ n\ell\ LS \rightarrow n_os,\ \varepsilon L\ LS \quad \text{if } L = \ell+1 \text{ or } L = \ell-1.$$

Approximations (6.15) and (6.16) hold only if

$$\Gamma^{auto}(n_1 \ell_1, n\ell) >> \Gamma^{rad}(n_1 \ell_1). \tag{6.17}$$

This condition fails when ℓ grows sufficiently large (typically $\ell > 7$). As n grows large, the autoionizing width diminishes as $(n^*)^{-3}$, where n^* is the effective quantum number corresponding to n. Thus for sufficiently large n or ℓ, we obtain

$$\Gamma^{auto}(n_1 \ell_1, n\ell) << \Gamma^{rad}(n_1 \ell_1). \tag{6.18}$$

For large values of n, only a few values of ℓ need be considered, and we find

$$\sum_{\ell} (2\ell+1) b(n_1 \ell_1, n\ell) \rightarrow \frac{\text{constant}}{(n^*)^3} . \tag{6.19}$$

Because of the strong dependence of $A^{auto}(J_1, n\ell \rightarrow J_i, \epsilon\ell')$ on ℓ, we can obtain a good approximation to the rate coefficient by using average autoionization rates and widths. We thereby obtain the formulas

$$(2\ell+1) b(J_1, n\ell) = (2\ell+1) \frac{\bar{\Gamma}^{auto}(J_1, n\ell)}{\Gamma^{rad}(J_1) + \bar{\Gamma}^{auto}(J_1, n\ell)} \tag{6.20}$$

$$(2\ell+1) b(n_1 \ell_1, n\ell) = (2\ell+1) \frac{\bar{\Gamma}^{auto}(n_1 \ell_1, n\ell)}{\Gamma^{rad}(n_1 \ell_1) + \bar{\Gamma}^{auto}(n_1 \ell_1, n\ell)} . \tag{6.21}$$

For recombination to a one-electron ion, the use of average widths eliminates any reference to the coupling scheme. Formula (6.21) is basically the formula used by Burgess (1964, 1965, 1966). Formula (6.21) does not apply when $\ell_o = 0$; that case requires the substitution

$$(2\ell+1) \rightarrow (2\ell+1)\left[\tfrac{2}{3} + \tfrac{1}{3}\,\delta(\ell,0)\right].$$

To obtain the rate coefficient $\alpha^{di}(n_i\ell_i \rightarrow n_o\ell_o,n)$ for recombination onto an excited ion configuration, we multiply formula (6.11) by the fraction of autoionization that proceeds into the $n_i\ell_i$ continuum:

$$\frac{\overline{A}^{auto}(n_1\ell_1,\ n\ell \rightarrow n_i\ell_i)}{\sum_i \overline{A}^{auto}(n_1\ell_1, n\ell \rightarrow n_i\ell_i)}\ .$$

The formula is

$$\alpha^{di}(n_i\ell_i \rightarrow n_o\ell_o,n) = \frac{(2\ell_o+1)}{(2\ell_i+1)}\left(\frac{2\pi}{kT}\right)^{3/2} \sum_{n_1\ell_1} \exp(-\epsilon/kT)$$

$$\times\ A^{rad}(n_o\ell_o \rightarrow n_i\ell_i)\ x \sum_{\ell} (2\ell+1)\ \frac{\overline{A}^{auto}(n_1\ell_1,n\ell \rightarrow n_i\ell_i)}{\overline{\Gamma}^{rad}(n_1\ell_1)+\overline{\Gamma}^{auto}(n_1\ell_1,n\ell)}\ . \qquad (6.22)$$

The preceeding remarks suggest that a formula such as

$$\alpha^{di}(n_o \rightarrow n_o,n) = \left(\frac{2\pi}{kT}\right)^{3/2} \sum_{n_1} \exp(-\epsilon/kT) \quad A^{rad}(n_o \rightarrow n_1)$$

$$x\ n^2\ \frac{\bar{\Gamma}^{auto}(n_1,n)}{\Gamma^{rad}(n_1)+\bar{\Gamma}^{auto}(n_1,n)} \qquad (6.23)$$

used in a previous paper (Tucker and Gould 1966), must be applied with caution.

VII. CONFIGURATION MIXING

Pure-configuration wavefunctions, though adequate for some purposes, often give a poor description of actual wavefunctions, and one must then introduce appropriate mixing of configurations. As an example, $^1P_1^\circ$ autoionizing series in helium are attributable, in a first approximation (Fano and Cooper 1965), to the resonance states

$$\Psi(2n\pm\ ^1P_1) = \frac{1}{\sqrt{2}}\left[\psi(2s,np\ ^1P_1) \pm \psi(2p,ns\ ^1P_1)\right]. \qquad (7.1)$$

Such mixing of configurations with the same sets of principal quantum numbers is a natural consequence of the Z^{-1} expansion approach to nonrelativistic atomic structure (Layzer 1959). However, if n is sufficiently large, the configuration mixing caused by the Coulomb interaction is less significant than the spin-orbit interaction of the unexcited electron. In the above example, when the configuration splitting is appreciably less than the level splitting $2p_{\frac{1}{2}} - 2p_{3/2}$,

$$\frac{\hbar c R_\infty}{2n^3} \ll E(2p_{3/2}) - E(2p_{\frac{1}{2}}), \qquad (7.2)$$

the resonance states can be expected to tend toward $J\ell$ coupling states, $\psi(2p_j, n\ell\ [K]\ J)$:

$$\psi(2p_{\frac{1}{2}}, ns\ [\tfrac{1}{2}]\ 1),\ \psi(2p_{3/2}, ns\ [\tfrac{3}{2}]\ 1).$$

For singly ionized beryllium, this occurs for $n \geq 30$. For the sodium sequence, $\psi(3p_j, n\ell\ [K]\ J)$, $J\ell$ coupling should occur for $n \geq 15$. Because the bulk of dielectronic recombination occurs for $10 \leq n \leq 200$, the neglect of configuration mixing with the use of $J\ell$ coupling may not introduce serious errors, even for helium and the light elements.

VIII. OVERLAPPING RESONANCES

The derivation of equations (2.15) and (2.16) from equation (2.12) assumes that overlapping resonances do not interfere. To see why this is so, consider the expression

$$\Upsilon(i\epsilon \to s) \equiv \sum_{(is)} \left| \sum_{d} \frac{\langle s|D|d\rangle \langle d|V|i\epsilon\rangle}{\epsilon+E_i-E_d+i\frac{1}{2}\Gamma(d)} \right|^2 . \tag{8.1}$$

Let us introduce $J\ell$ coupling states, so that formula (8.1) reads

$$\Upsilon(J_i\epsilon \to J_o,n\ell) = \tag{8.2}$$

$$\sum_{\ell''K''} \sum_{KJ_sM_s\mu} \left| \sum_{J_1n'\ell'K_dJ_dM_d} \langle J_o,n\ell\ [K]\ J_sM_s|D_\mu|J_1,n'\ell'\ [K_d]\ J_dM_d\rangle \right.$$
$$\left. \times \frac{\langle J_1',n'\ell'\ [K_d]\ J_dM_d|V|J_i,\epsilon\ell''\ [K'']\ J_dM_d\rangle}{\epsilon+E(J_i)-E(J_1,n'\ell'\ [K']\ J_dM_d)+\frac{1}{2}i\Gamma(J_1,n'\ell'\ [K']\ J_dM_d)} \right|^2 .$$

We then use the result

$$\sum_{KJ_sM_s\mu} \langle J_o,n\ell\ [K]\ J_sM_s|D_\mu|J_1,n'\ell'\ [K_d]\ J_dM_d\rangle$$
$$\times \langle J_o,n\ell\ [K]\ J_sM_s|D_\mu|J_1',n''\ell''\ [K_d']\ J_d'M_d'\rangle^*$$
$$= \delta(M_d,M_d')\ \delta(J_d,J_d')\ \delta(K_d,K_d')\ \delta(\ell,\ell'')\ \delta(n',n'')$$
$$\times \langle J_o \| D \| J_1\rangle \langle J_o \| D \| J_1'\rangle^*/(2J_o+1) \tag{8.3}$$

to write

(8.4)

$$\Upsilon(J_i \epsilon \rightarrow J_o, n\ell) = \sum_{\ell'' K''} \sum_{J_1 J_1'} \frac{\langle J_o \| \underset{\sim}{D} \| J_1 \rangle \langle J_o \| \underset{\sim}{D} \| J_1' \rangle^*}{(2J_o+1)}$$

$$\times \sum_{K_d J_d M_d} \frac{\langle J_1, n\ell\ [K_d]\ J_d M_d | V | J_i, \epsilon\ell''\ [K'']\ J_d M_d \rangle}{\epsilon + E(J_i) - E(J_1, n'\ell'\ [K']\ J_d) + i\frac{1}{2}\Gamma(J_1, n'\ell'\ [K']\ J_d)}$$

$$\times \frac{\langle J_1', n\ell\ [K_d]\ J_d M_d | V | J_i, \epsilon\ell''\ [K'']\ J_d M_d \rangle^*}{\epsilon + E(J_i) - E(J_1', n'\ell'\ [K']\ J_d) + i\frac{1}{2}\Gamma(J_1', n'\ell'\ [K']\ J_d)} .$$

Integration over energy then gives

$$\int d\epsilon\ \Upsilon(J_i\ \epsilon \rightarrow J_o, n\ell) = \sum_{J_1 J_1'} \frac{\langle J_o \| \underset{\sim}{D} \| J_1 \rangle \langle J_o \| \underset{\sim}{D} \| J_1' \rangle^*}{(2J_o+1)}$$

$$\times 2\pi \sum_{\ell'' K''} \sum_{K_d J_d} \langle J_1,\ \alpha \| V \| J_i, \epsilon\ell''\ [K'']\ J_d \rangle$$

$$\times \langle J_1', \alpha \| V \| J_i, \epsilon\ell''\ [K'']\ J_d \rangle^*$$

$$\times \frac{[\Gamma(J_1', \alpha) + \Gamma(J_1, \alpha)]}{[E(J_1, \alpha) - E(J_1', \alpha)]^2 + \frac{1}{4}[\Gamma(J_1', \alpha) + \Gamma(J_1, \alpha)]^2} ,$$

(8.5)

where, for typographical convenience, α denotes $n\ell\ [K_d]\ J_d$. We see here that the only significant contribution comes from the cases where the splitting $E(J_1) - E(J_1')$ of the ion

levels is much less than the widths: the overlapping doubly excited states contribute independently to the recombination coefficient. Similarly, if $E(J_1)$ and $E(J_1')$ lie close together, our interest centers on recombination onto a term, L, S: summation over J_1 and J_1' then again eliminates interference. As a result of these selection rules, we can write

$$\int d\epsilon \;\; \Upsilon(J_i \epsilon \rightarrow J_o, n\ell) = \sum_{J_1} \frac{|\langle J_o \| D \| J_1 \rangle|^2}{(2J_o+1)}$$

$$\times \sum_{\ell'' K''} \sum_{K_d J_d} \frac{2\pi |\langle J_1, n\ell \;\; [K_d]\; J_d \| \underset{\sim}{V} \| J_i, \epsilon \ell'' \;\; [K'']\; J_d \rangle|^2}{\Gamma(J_1, n\ell \;\; [K_d]\; J_d)} \; . \tag{8.6}$$

This is the result used in writing equations (2.15) and (2.16). [Note that $|\langle J \| \underset{\sim}{V} \| J \rangle|^2 = (2J+1) \; |\langle J | V | J \rangle|^2$].

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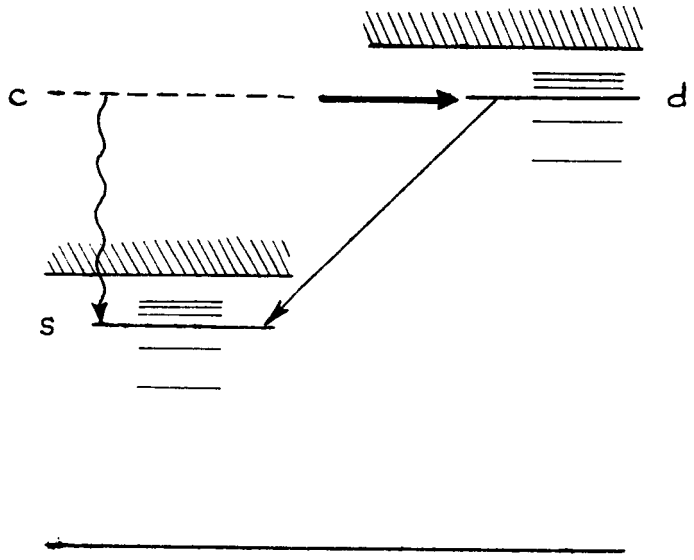

Figure 1. Schematic illustration of electron capture from continuum c to doubly excited state d (bold arrow), followed by stabilizing radiative transition to singly excited state s (thin arrow). Wavy line shows direct capture.

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