

ELECTRON IMPACT EXCITATION OF POSITIVE IONS OF ASTROPHYSICAL INTEREST I. THEORETICAL METHOD

(Invited Paper)

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RESUMEN

Se describen los métodos teóricos desarrollados actualmente para el cálculo de las secciones eficaces de excitación de iones positivos por impacto electrónico. Se presentan resultados recientes de interés astrofísico.

ABSTRACT

The current theoretical methods developed for the calculation of electron impact excitation cross sections of positive ions are described, and illustrated with recent results of astrophysical interest.

Key words: ATOMIC PROCESSES – TRANSITION PROBABILITIES

I. INTRODUCTION

The interpretation of astronomical observations and the understanding of physical processes and conditions in stellar objects require an enormous quantity of accurate atomic data. This brings in an interesting interplay between observations and atomic physics, and in many cases it is the latter that lets the astronomer down and delays progress in such enterprises.

Emission lines, which are mainly produced by electron impact excitation of positive ions, provide useful diagnostics on the physical conditions of astronomical objects such as temperature, density and abundance of elements. Also, in the modelling of hot star atmospheres, where emission lines are present, it is necessary to consider departures from LTE, and thus take into account in detail all radiative and collisional processes that populate the levels. Consequently, a great deal of effort has been given in the past three decades to obtain accurate electron impact excitation rate coefficients of positive ions in different stages of ionization. Owing to experimental difficulties, particularly in connection with multiply-ionized species, the determination of excitation rate coefficients of astrophysical interest relies on calculation.

The original intention of this paper was to review the theoretical methods developed for the calculation of electron impact excitation rate coefficients of positive ions and to make a compilation useful to astronomers. It was soon realized, however, that this could not be done within the format of a conference talk and thus it was divided into two parts: Part I, which is hereby presented, will mainly deal with the theoretical methods, illustrated with recent results; in Part II we will review the different

computational approaches and make a compilation of rate coefficients. Part II will be submitted to the present journal for publication as a separate paper.

II. THE EXCITATION RATE COEFFICIENT

The process of excitation (or de-excitation) of an ion by electron impact is described in terms of the cross section

$$Q(i \rightarrow j) = \frac{\Omega(i,j)}{\omega_i k^2(i)} \pi a_0^2, \quad (2.1)$$

where ω_i is the statistical weight of the initial level, $k^2(i)$ is the energy of the incident electron relative to the i th level in units of Rydberg, and $\Omega(i,j)$ is a dimensionless quantity referred to as the *collision strength*. A more useful quantity, particularly in astrophysical processes, is the *rate coefficient*

$$q(i \rightarrow j; T_e) = \int_0^\infty Q(i \rightarrow j) v_i f(v_i, T_e) dv_i, \quad (2.2)$$

that is, the cross section averaged over a Maxwellian electron velocity distribution $f(v_i, T_e)$. The number of transitions per second from a level i to a level j is then given by

$$d_{ji} = N_e q(i \rightarrow j), \quad (2.3)$$

where N_e is the electron density.

For collisional de-excitation the rate coefficient in $\text{cm}^3 \text{s}^{-1}$ can be expressed by

$$q(j \rightarrow i; T_e) = \frac{8.63 \times 10^{-6} \Upsilon(j, i; T_e)}{\omega_j T_e^{1/2}} \quad (j > i) \quad (2.4)$$

where

$$\begin{aligned} \Upsilon(j, i; T_e) = & \int_0^\infty \Omega(i, j) \\ & \times \exp(-k^2(j)/\kappa T_e) d(k^2(j)/\kappa T_e) \quad (2.5) \end{aligned}$$

T_e is the electron temperature in K and κ is the Boltzmann constant. The excitation rate coefficient can be obtained from the detailed balance relation

$$\begin{aligned} q(i \rightarrow j) = & \frac{\omega_j}{\omega_i} q(j \rightarrow i) \\ & \times \exp(-(E_j - E_i)/\kappa T_e) \quad (j > i) \quad (2.6) \end{aligned}$$

Most theoretical work is concerned with the quantum mechanical calculation of the *effective collision strength* $\Upsilon(j, i; T_e)$. If the energy variation of $\Omega(j, i)$ can be neglected $\Upsilon(j, i) = \Omega(i, j)$, but for a large number of ions of astrophysical interest, particularly at low energies, the collision strength is dominated by complicated series of resonances which arise from quasi-bound states of the ion plus electron system. To be able to reproduce their effects and properties a detailed knowledge of the ionic structure and the equations that describe the collision is not only necessary, but the computations are large, modestly accurate and costly. In many cases approximate analytic approaches such as Quantum Defect Theory and semi-empirical model potential methods provide invaluable help in otherwise unaffordable calculations.

III. THE COLLISION PROCESS

In order to obtain expressions for the excitation cross section the colliding electron wave is linearly expanded in partial waves of definite angular momentum, the Schrödinger equation is solved for the ion-electron system, and from the asymptotic form of each outgoing electron wave a partial cross section can be estimated. The total cross section is obtained by adding up these partial contributions, and the convergence of the infinite partial wave expansion depends on the nature of the transition: for forbidden transitions it is relatively fast but for allowed transitions it can be very slow indeed. For electron collisions with light ions at low energies relativistic effects can be neglected and, consequently, the total spin and orbital angular momenta are sepa-

rately conserved and LS coupling can be assumed; parity is also conserved. The usual procedure then is to couple the electron and target angular momenta, and to solve the Schrödinger equation for *intermediate states* of the total system defined by the quantum numbers $SL\pi$. If cross sections between fine-structure levels are required algebraic transformations to intermediate coupling can be made, neglecting relativistic corrections in the Hamiltonian and fine-structure splittings in the target. For electron collisions with heavier ions ($Z > 20$) this approach begins to break down and relativistic effects must be somehow included.

a) Expansion of the Wave Function

If we assume that the eigenfunctions of a N-electron ion form a complete orthonormal set, the wave function for the (N + 1)-electron system can be linearly expanded in terms the ion (the target) eigenfunctions (Burke and Seaton 1971)

$$\begin{aligned} \Psi(SL\pi) = & \sum_i \mathcal{A} \chi_i(\Gamma_i S_i L_i M_{S_i} M_{L_i} | 1, 2, \dots, N) \\ & \times \theta_i(\ell_i m_{\ell_i} m_{s_i} | N + 1) \quad (3.1) \end{aligned}$$

where χ_i are the target eigenfunctions specified by the set of quantum numbers $\{\Gamma_i S_i L_i M_{S_i} M_{L_i}\}$; the expansion coefficients θ_i depend on the incident electron coordinates and take the familiar form

$$\begin{aligned} \theta_i(\ell_i m_{\ell_i} m_{s_i} | N + 1) = & \delta(m_{s_i}; \sigma_{N+1}) Y_{\ell_i m_{\ell_i}} \\ & (r_{N+1}) \frac{F_i(r_{N+1})}{r_{N+1}} \quad (3.2) \end{aligned}$$

where δ is a spin function,

$$Y_{\ell_i m_{\ell_i}}$$

is the spherical harmonic, and F_i is the electron radial function. \mathcal{A} is an antisymmetrising (Ψ must obey the exclusion principle) vector-coupling operator which gives intermediate states of the total system with quantum numbers $SL\pi$.

The electron radial functions $F_i(r)$ are obtained from the solutions of the Schrödinger equation for the total system

$$H_{N+1} \Psi = E \Psi \quad (3.3)$$

here H_{N+1} is the non-relativistic Hamiltonian and E is the total energy.

b) *Boundary Conditions and Linear Independence of the Solutions*

Since we have assumed the χ_i to be eigenfunctions of the physical system, the boundary conditions satisfied by Ψ and the number of linear independent solutions of the Schrödinger equation (3.3) are determined by the boundary conditions imposed on $F_i(r)$. Furthermore, the latter depend on the energy regime under consideration.

For an intermediate state $SL\pi$ every term in the expansion (3.1) gives rise to an interaction channel. If we define the channel energy in Ryd to be

$$k^2(i) = E - E_i \quad , \quad (3.4)$$

where E_i is the corresponding target energy, the channel will lead to scattering if $k^2(i) \geq 0$ and it is said to be open. Otherwise it is energetically closed ($k^2(i) < 0$). The number of linear independent solutions $\Psi_{i'}$ of (3.3) is easily shown to be equal to the number of open channels NCHOP.

As $(1/r)F_{ii'}(r)$ must be bound for all r , the behaviour at the origin is given by

$$F_{ii'}(r) \rightarrow 0 \text{ as } r \rightarrow 0 \quad (\text{all channels}) \quad . \quad (3.5)$$

where the second subscript i' denotes a specific linear independent solution.) The asymptotic behaviour of the electron functions depends on whether the channel is open or closed: for a closed channel $F_{ii'}$ has the bound-state function behaviour

$$F_{ii'}(r) \rightarrow 0 \text{ as } r \rightarrow \infty \quad (\text{closed channels}); \quad (3.6)$$

an open channel function has the asymptotic oscillatory behaviour

$$F_{ii'}(r) \sim k_i^{-1/2}$$

$$\times \{ \sin(\xi_i + \tau_i) \delta_{ii'} + \cos(\xi_i + \tau_i) R_{ii'} \} \quad , \quad (3.7)$$

alternatively,

$$F_{ii'}(r) \sim k_i^{-1/2} \{ e^{-i(\xi_i + \tau_i)} \delta_{ii'} - e^{+i(\xi_i + \tau_i)} S_{ii'} \} \quad . \quad (3.8)$$

where τ_i is the Coulomb phase

$$\xi_i = k(i)r - \frac{1}{2} \ell_i \pi + (z/k(i)) \ln(2k(i)r) + \arg \Gamma(\ell_i + 1 - iz/k(i)) \quad , \quad (3.9)$$

where $z = Z - N$ and τ_i is an arbitrary phase chosen for convenience. \mathbf{R} is referred to as the *reactance matrix* and it is real and symmetric. \mathbf{S} is the *scattering matrix* and is symmetric and unitary in order to conserve flux; it can be expressed in terms of the \mathbf{R} matrix by

$$\mathbf{S} = (1 + i\mathbf{R})(1 - i\mathbf{R})^{-1} \quad . \quad (3.10)$$

The collision strength is given by

$$\Omega(\Gamma_i S_i L_i, \Gamma_{i'} S_{i'} L_{i'}) = \frac{1}{2} \sum_{\ell} \sum_{\ell'} \sum_{SL\pi} (2S+1)(2L+1) \times |T(\Gamma_i S_i L_i \ell, \Gamma_{i'} S_{i'} L_{i'} \ell'; SL)|^2 \quad , \quad (3.11)$$

where

$$\mathbf{T} = 1 - \mathbf{S} \quad . \quad (3.12)$$

Finally, a further situation arises which is when all channels are closed. In this case all boundary conditions are rigidly specified and the problem reduces to an eigenvalue problem, that is, the conditions can only be satisfied by certain values of E which correspond to the eigenenergies of the $(N+1)$ -electron system (Eissner and Seaton 1972). This is important in the sense that the same theoretical formalism and numerical method can be used to study both the discrete spectrum and the continuum. Also, the equations to be solved have some computational advantages compared with the Hartree-Fock equations used in atomic structure calculations.

IV. COMPUTATIONAL APPROACH

a) *Truncation of the Expansion*

The summation in (3.1) is over an infinite number of bound states and includes the continuum, but in practice the expansion must be truncated. The new finite expansion

$$\Psi^{cc} = \sum_{i=1}^{NCHF} \mathcal{A}_i \chi_i \theta_i \quad (4.1)$$

is referred to as the *close-coupling expansion*. Moreover, exact solutions of the Schrödinger equation can no

longer be obtained and a new approach must be introduced, namely the *variational principle*.

It can be shown that for small variations about the exact solution

$$\delta \{(\psi_i | H-E | \psi_i') - R_{ii}'\} = (\delta \psi_i | H-E | \delta \psi_i') ; \quad (4.2)$$

or, conversely, for a trial (t) function the exact **R** matrix is given by

$$R_{ii}^{\text{exact}} = R_{ii}^t - (\psi_i | H-E | \psi_i')^t + (\delta \psi_i | H-E | \delta \psi_i'). \quad (4.3)$$

The *Kohn corrected R* matrix is defined as

$$R_{ii}^K = R_{ii}^t - (\psi_i | H-E | \psi_i')^t \quad (4.4)$$

and differs from the exact **R** matrix by a quantity of quadratic order in $\delta \psi$. If we impose on the close-coupling (CC) expansion the condition

$$(\delta \psi_i | H-E | \psi_i')^{\text{cc}} = 0 \quad (4.5)$$

for all variations $\delta \psi$, then $(\psi_i | H-E | \psi_i')^{\text{cc}} = 0$ and, hence,

$$R_{ii}^{\text{exact}} = R_{ii}^{\text{cc}} + (\delta \psi_i | H-E | \delta \psi_i') , \quad (4.6)$$

that is, the **R** matrix in the close-coupling method differs from the exact value by a quantity of second order in the order of $\delta \psi$. The equations for $F_i(r)$ are now obtained from the variational condition (4.5).

b) Bound Channels

Every term in the expansion (4.1) gives rise to a *free channel* since they contain the radial functions $F_i(r)$ which are varied freely so as to satisfy (4.5) and, as we have seen, they can be open or closed. In order to define the $F_i(r)$ uniquely (Burke and Seaton 1971) the following orthogonality conditions are imposed

$$(P_\gamma | F_i) = 0 \quad (\ell_\gamma = \ell_i), \quad (4.7)$$

where the P_γ are the target orbitals, without constraining the total wave function Ψ if a suitable linear combination of the functions Φ_j are included in the expansion. They are built up from target orbitals and take the form of bound-state functions of the $(N+1)$ -

electron system. They are referred to as the *bound channels* (Eissner and Seaton 1972).

The orthogonality conditions are incorporated in the variational formalism by the technique of Lagrange multipliers:

$$(\delta \psi_i | H-E | \psi_i') + \sum_{i\gamma} \lambda_{i\gamma} (\delta F_i | P_\gamma) = 0 , \quad (4.8)$$

and the CC expansion now takes the form

$$\Psi^{\text{cc}} = \sum_{i=1} \mathcal{A} \chi_i \theta_i + \sum_{j=1} \Phi_j c_j . \quad (4.9)$$

Furthermore, the expansion coefficients c_j are treated as variational parameters:

$$\frac{\partial}{\partial c_j} (\Psi | H-E | \Psi) = 0 . \quad (4.10)$$

c) Target Wave Functions

It should be noted that in the formulation of the variational principle exact eigenfunctions have been assumed for the target. In practice, for many-electrons, only approximate wave functions can be used introducing errors in the **R** matrix of first order in the error of the functions. Consequently, it is important to employ accurate wave functions, and for most ions it is necessary to consider electron correlation effects (*configuration interaction*), that is, the wave function for state cannot be approximated by a single configuration Γ_i , but is taken to be a linear combination of configurations of the form

$$\chi_i (\Gamma_i S_i L_i \pi_i) = \sum_m a_m \phi_m (\Gamma_m S_i L_i \pi_i) . \quad (4.11)$$

d) Approximate Solutions of the Scattering Equations

i) The close-coupling approximation.

Equations (4.7), (4.8) and (4.10) lead to a set of coupled integro-differential equations for $F_i(r)$, c_j and $\lambda_{i\gamma}$ of the form

$$(h_i - k^2(i))F_i + \sum_{i'} W_{ii'} F_{i'} + \sum_{j'} U_{ij'} c_{j'} + \sum_{\gamma} \lambda_{i\gamma} P_\gamma = 0 , \quad (4.12)$$

$$\sum_{i'} (F_{i'} | U_{i'} | j) + \sum_{j'} (\mathcal{H}_{jj'} - E \delta_{jj'}) c_{j'} = 0, \quad (4.13)$$

$$(P_{\gamma} | F_i) = \delta_{\ell_{\gamma} \ell_i}, \quad (4.14)$$

where

$$h_i = \frac{d^2}{dr^2} + \frac{\ell_i(\ell_i + 1)}{r^2} - \frac{2Z}{r}, \quad (4.15)$$

and

$$\mathcal{H}_{jj'} = (\Phi_j | H | \Phi_{j'}). \quad (4.16)$$

The second term of (4.12) represents the coupling potential (direct and exchange) of the particle in all free channels i' with the target in state i . Similarly, the third term represents the interaction between the particle in all bound channels j' with the target in state i .

In the CC approximation the coupled equations are solved numerically for a small number of target terms. The number depends on the system in question and the energy regime under consideration.

ii) The Distorted Wave method.

In this approximation the inter-channel coupling is assumed to be weak which is the case for highly ionized systems ($z > 3$). It can also be used to calculate contributions from high partial waves. The electron radial functions are solutions of the equation

$$(h_i - k^2(i)) f_i^{\text{DW}} + W_{ii} f_i^{\text{DW}} = 0. \quad (4.17)$$

iii) The Coulomb-Born approximation.

The electron radial functions are taken to be solutions of the Coulomb equation

$$\left\{ \frac{d^2}{dr^2} - \frac{\ell_i(\ell_i + 1)}{r^2} + \frac{2Z}{r} + k^2(i) \right\} f_i^{\text{CB}} = 0. \quad (4.18)$$

The approximation is usually used for high partial waves in optical transitions where the convergence is slow.

V. PROBLEMS IN SCATTERING CALCULATIONS

a) Resonances

It is well known that in a variety of low energy continuum processes (e.g. photoionization, electron impact excitation, etc.) the phenomenon of resonances

takes place, that is, at some energies the scattered electron forms quasi-bound states with the target ion. This type of resonance has been observed experimentally in techniques such as UV absorption and electron spectroscopy of metallic vapours, especially the alkaline earths (Mehlman-Balloffet and Esteva 1969; Rassi *et al.* 1977). The theoretical approach to this phenomenon has received a great deal of attention (Burke 1968; Seaton 1969a).

In the calculation of excitation rate coefficients resonances must be considered as they can cause drastic changes to the cross section. In the formalism of the coupled equations resonances arise from the coupling of the open channels with closed channels and/or bound channels. If this coupling did not take place the electron would couple with the target states to give either infinite series of doubly excited bound states converging to the target terms or pure continuum states. In practice the double excitation acquires some of the character of the free state; it broadens and there is a finite probability, which depends on the coupling, for a radiationless transition into the continuum. This phenomenon is called *autoionization*.

In the calculation of the excitation cross section one must try to include the target terms which give rise to resonances in the region of interest, and this becomes more intractable as one works up the isoelectronic sequence. For instance, for transitions within the same complex ($\Delta n = 0$), the energy difference between the target terms $\Delta E_{ii}(z)$ in the sequence scales with z whereas the position of the resonances scales with z^2 and, consequently, the resonances are pulled in as z becomes larger. This effect can be appreciated in the electron impact excitation of the $2s^2 2p^2 \ ^3P - 2s^2 2p^2 \ ^1D$ forbidden transition in the carbon isoelectronic sequence (Figure 1). We consider the intermediate state $^2D^0$ which gives the largest contribution to the cross section. It can be seen that for N II the resonances converging to the excited target term $2s2p^3 \ ^3D^0$ appear fairly high and, hence, they will not contribute appreciably to the excitation rate coefficient for electron temperatures below 20000°K . On the other hand, for O III the partial cross section is dominated by the broad $2s2p^3 \ (^3D^0)3s$ resonance. For Ne V this resonance has gone below threshold, and resonances converging to higher thresholds begin to appear. Also their widths become narrower as z increases, but in no way they can be neglected in an accurate calculation.

b) Correlation Effects

One of the main problems in the close-coupling method is to be able to represent the distortion, whether long-range or short-range, of the target states by the incoming electron. These effects are unavoidable in an accurate description of the collision process, and there have been several approaches to incorporate them within the CC framework.

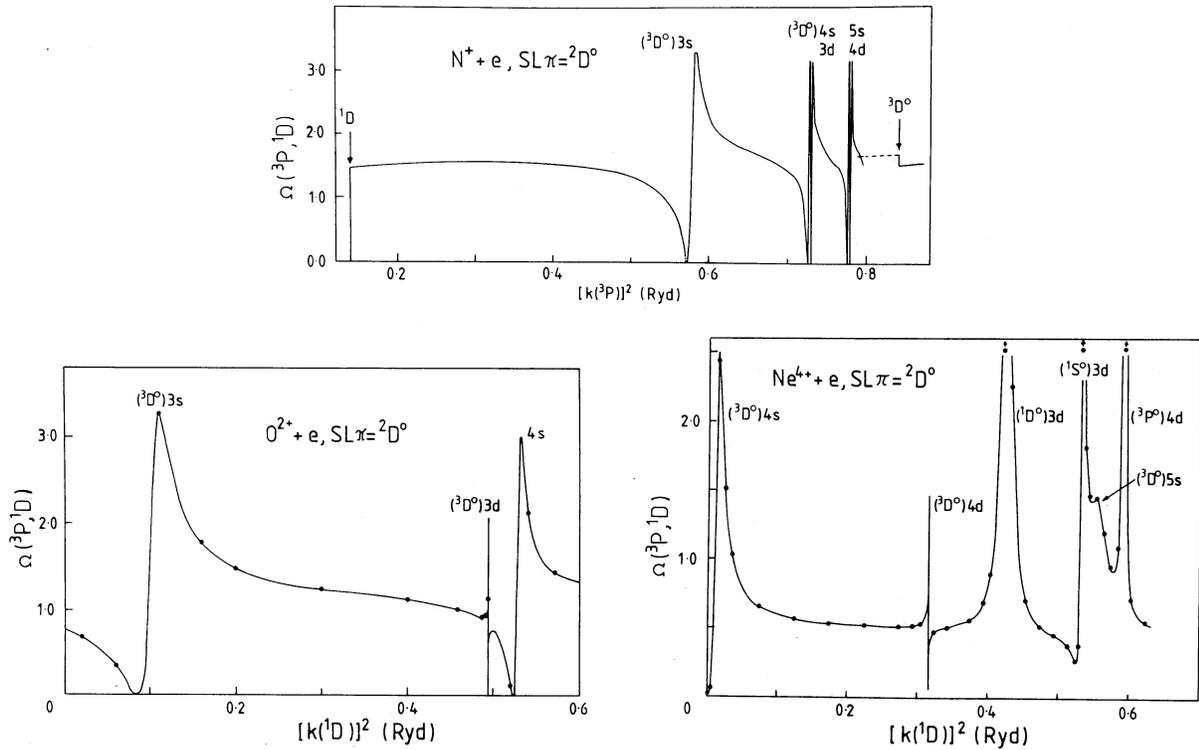


Fig. 1. Partial collision strength of the ${}^2D^0$ intermediate state for the $2s^2 2p^2 \ ^3P - \ ^1D$ transition in the carbon-like sequence showing the resonance structure. N II by Saraph and Seaton (1974); O III by Eissner and Seaton (1974); and Ne V by Giles *et al.* (1979).

One way of approximating the long-range distortion or polarization of the target states by the incident electron is by the method of *polarized pseudo-states* developed by Damburg and Karule (1967), Burke *et al.* (1969), Feautrier *et al.* (1971) and Vo Ky Lan (1971). The 2^λ -pole polarizability of an atomic state χ_0 is given in atomic units by

$$\alpha_{2\lambda} = 2 \sum_{k > 0} \frac{|\langle \chi_k | V_\lambda | \chi_0 \rangle|^2}{E_k - E_0}, \quad (5.1)$$

where

$$V_\lambda = - \sum_{i=1}^N r_i^\lambda P_\lambda(\cos \theta_i). \quad (5.2)$$

and the summation in (5.1) includes the continuum. In this method the summation in (5.1) is replaced by a single term

$$\alpha_{2\lambda} = 2 \frac{|\langle \bar{\chi}_p | V_\lambda | \chi_0 \rangle|^2}{E_p - E_0}. \quad (5.3)$$

The polarized pseudo-states $\bar{\chi}_p$ are included in the first expansion of (4.9) to account for the full 2^λ -pole polarizability of the spectroscopic target states. A problem that appears in this method, however, is that pseudo-states give rise to non-physical thresholds and pseudo-resonances, and the final cross sections must be obtained by somehow averaging over these resonances.

In a similar manner additional bound channels or *correlation functions* can be included in (4.9) to account for short-range correlation effects (Burke and Taylor 1966). These functions usually contain pseudo-orbitals generated by optimizing target energy separations.

An alternative approach is to approximate the target distortion by *analytic model potentials*. For instance, Seaton and Steenman-Clark (1977) showed that the dipole distortion of the 1s state of hydrogen can be represented by a model potential with asymptotic form

$$V \sim - \frac{\alpha}{r^4} + \frac{(6\beta + 24\gamma k^2 (1s))}{r^6}, \quad (5.4)$$

where α is the dipole polarizability of the 1s state, and the parameters β and γ can be obtained from f-value estimates. Model potentials usually contain empirical parameters which are adjusted to reproduce experimental data and have been widely used in atomic calcula-

ons of simple systems (Laughlin and Victor 1973; orcross and Seaton 1976; Mendoza 1981a).

At intermediate energies, that is at energies several mes the threshold value, the problem becomes more complicated: there are too many channels to include in the CC expansion and the inter-channel coupling is still strong and cannot be neglected. There have been several attempts to account for neglected open channels based on the pseudo-states method (Burke and Mitchell 1973), but again the presence of pseudo-resonances brings in difficulties. Recently, some progress has been made at intermediate energies using a new method based on a L^2 discretization of the continuum (Reinhardt 1979) from which scattering information can be extracted (Berrington *et al.* 1981).

c) Relativistic Effects

Relativistic effects in electron-ion collisions have been discussed by Walker (1974) and Jones (1975). The way in which they have been included in computational work can be summarized as follows:

i) When the relativistic effects are small and the fine-structure energy splittings in the target can be neglected, it is possible to obtain expressions for the excitation cross section between fine-structure levels using algebraic transformations, from LS coupling to intermediate coupling, for the R matrix (Saraph 1972). They are of the form

$$\begin{aligned} R^{J\pi}(\Gamma_1 S_1 L_1 J_1 \ell K, \Gamma_1' S_1' L_1' J_1' \ell' K') \\ = \sum_{LS} C(SLJ; S_1 L_1 J_1; \ell K) \\ {}^{SL\pi}(\Gamma_1 S_1 L_1 \ell s, \Gamma_1' S_1' L_1' \ell' s') C(SLJ; S_1' L_1' J_1'; \ell' K'), \end{aligned} \quad (5.5)$$

where C are algebraic recoupling coefficients and

$$J_1 + L_1 = J, \quad J_1' + \ell = K, \quad \text{and} \quad K + s = J; \quad (5.6)$$

is the total angular momentum of the new intermediate state $J\pi$.

If relativistic effects cannot be neglected in the target they can still be treated as perturbations, the target Hamiltonian re-diagonalized in intermediate coupling to obtain *term coupling coefficients*, and the expressions for $R^{J\pi}$ are now obtained in terms of $R^{SL\pi}$ and these coefficients.

ii) For intermediate weight ions ($Z > 20$) relativistic effects in the target and in the collision process begin to show up in such a manner that they cannot be neglected. They can be treated by a perturbative Breit-Pauli method (Jones 1975) which has been recently incorporated in the close-coupling formalism by Scott and Burke (1981).

iii) For very heavy ions the only satisfactory approach is based on solutions of the Dirac equation (Walker 1974).

VI. QUANTUM DEFECT THEORY

The complexity and cost of formal atomic calculations, and the frequent unavailability of large enough computers have encouraged the development of alternative analytic methods to approximate some of the problems for which there has been urgent need. Quantum Defect Theory (QDT), developed by Seaton and collaborators (Seaton 1970), is one of such methods and is at present widely used in the analysis of the data obtained from close-coupling computations.

The mathematical formalism of QDT is based on the analytic properties of the solutions of the Coulomb equation. The coupled equations of the scattering problem take the general form in matrix notation

$$\left\{ \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2z}{r} + \epsilon \right\} \mathbf{F} + \mathbf{W} \mathbf{F} = 0 \quad (6.1)$$

For a positive ion the asymptotic potential is dominated by the Coulomb term and no essential error arises by assuming that

$$W_{ii'}(r) = 0 \quad \text{for } r > r_0, \quad (6.2)$$

where r_0 is finite. Consequently, for $r > r_0$, \mathbf{F} can be expanded in terms of the analytic solutions of the Coulomb equation $f(\epsilon|r)$ and $g(\epsilon|r)$

$$\mathbf{F}(\epsilon|r) = f(\epsilon|r) \mathbf{I}(\epsilon) + g(\epsilon|r) \mathbf{J}(\epsilon) \quad (6.3)$$

Furthermore, it has been shown (Ham 1955) that, assuming certain continuity conditions near the origin, $\mathbf{F}(\epsilon|r)$ is an entire analytic function of ϵ for all finite values of r and, hence \mathbf{I} and \mathbf{J} , which contain the expansion coefficients, will also be analytic functions of ϵ and can be represented by convergent expansions.

If we consider a region with all channels open we can define a matrix \mathcal{R} such that

$$\mathbf{F} \sim k^{-1/2} \{ (\sin \zeta) + (\cos \zeta) \mathcal{R} \}, \quad r > r_0 \quad (6.4)$$

and a matrix $\mathcal{X} = (1 + i\mathcal{R})(1 - i\mathcal{R})^{-1}$. \mathcal{R} and \mathcal{X} are slowly varying functions of energy and, with the above approximation, we can define the analytic continuations of \mathcal{R} and \mathcal{X} for all finite values of the energy, and develop extrapolation and interpolation expressions for

scattering parameters in terms of these analytic continuations. For instance, in the region of some channels closed \mathcal{R} can be partitioned according to the scheme

$$\mathcal{R} = \begin{pmatrix} \mathcal{R}_{oo} & \mathcal{R}_{oc} \\ \mathcal{R}_{co} & \mathcal{R}_{cc} \end{pmatrix} \quad \begin{array}{l} o = \text{open} \\ c = \text{closed} \end{array} \quad (6.5)$$

and the reactance matrix \mathcal{R} can be expressed in this region by (Seaton 1969b)

$$\mathcal{R} = \mathcal{R}_{oo} - \mathcal{R}_{oc} \{ \mathcal{R}_{cc} + \tan \pi \nu_c \}^{-1} \mathcal{R}_{co}, \quad (6.6)$$

where

$$k^2(c) = -z^2/\nu_c^2 \quad (6.7)$$

Similarly, the S matrix is given by

$$\mathcal{S} = \mathcal{X}_{oo} - \mathcal{X}_{oc} \{ \mathcal{X}_{cc} - \exp(-2\pi i \nu_c) \}^{-1} \mathcal{X}_{co} \quad (6.8)$$

The resonance structure which characterises this region is contained in the second term of (6.6) or (6.8).

Another useful quantity is the collision strength averaged over resonances in the region just below threshold, referred to as the *Gailitis average*. It has been shown by Seaton (1969b) that for one closed channel c

$$\langle |S_{ii'}|^2 \rangle = |X_{ii'}|^2 + \frac{|X_{ic}|^2 |X_{ci'}|^2}{\sum_i |X_{ci'}|^2}, \quad (6.9)$$

and that it is discontinuous across the threshold for new transitions (*Gailitis jump*).

In Figure 2 we illustrate some of these features in connection again with the $2s^2 2p^2 \ ^3P - 2s^2 2p^2 \ ^1D$ transition in the carbon-like sequence for the 2P intermediate state of the total system. In contrast with the $^2D^0$ intermediate state (Figure 1), the 1S threshold now gives rise to a free channel which below threshold produces resonances of the type $2s^2 2p^2 \ (^1S)np$ and above threshold leads to the new transitive $2s^2 2p^2 \ ^3P - 2s^2 2p^2 \ ^1S$. The high $(^1S)np$ resonances are obtained by extrapolation from above threshold using QDT expressions, and it is seen that the agreement with the close-coupling values is very good. Also, the Gailitis average is shown to be discontinuous across the 1S and $^3D^0$ thresholds and this is a direct consequence of conservation of flux. Even in the case of Ne V, where there is a resonance sitting at threshold, it is still possible to implement this approach. Above the 1S threshold the QDT formulae are used to interpolate the CC values and thus obtain a complete description of the cross section in the region of interest.

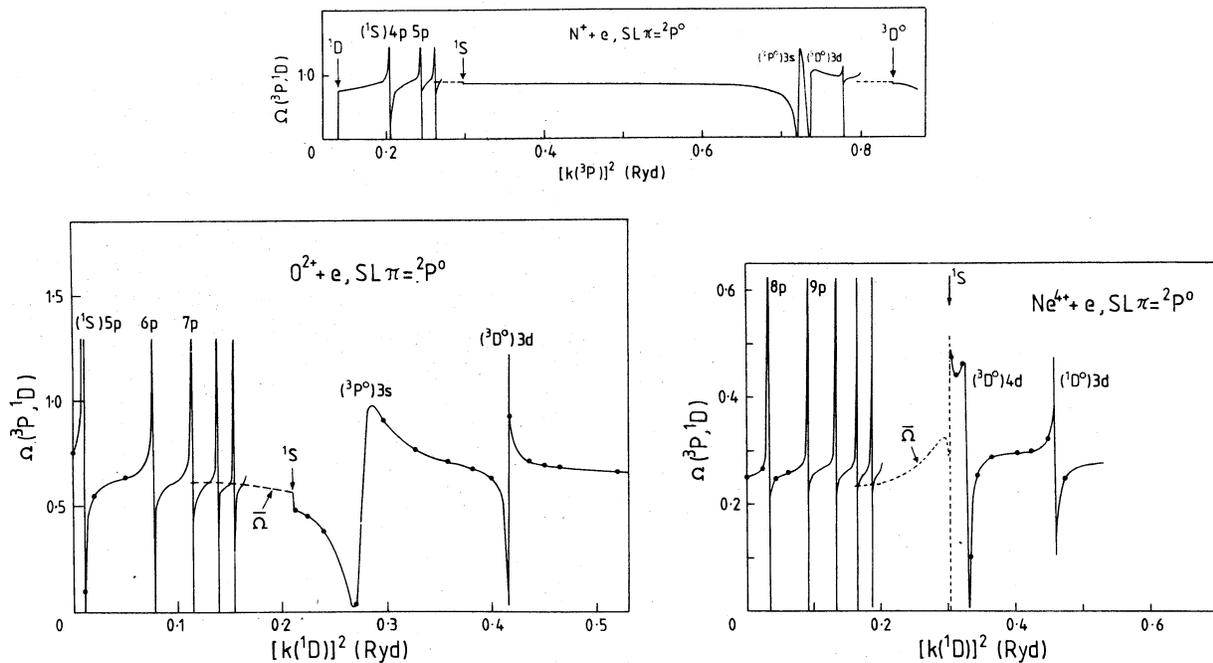


Fig. 2. Partial collision strength of the $^2P^0$ intermediate state for the $2s^2 2p^2 \ ^3P - ^1D$ transition in the carbon-like sequence showing some of the QDT features. N II by Saraph and Seaton (1974), O III by Eissner and Seaton (1974) and Ne V by Giles *et al.* (1979); filled circles, CC approximation; solid lines QDT fit; broken line *Gailitis average*.

VII. SELECTED RESULTS

a) *The Lithium Isoelectronic Sequence*

It is convenient to start the discussion of results with the lithium-like sequence as there are extensive calculations in different approximations and accurate experimental measurements which bring out the main features encountered in scattering problems.

Transitions in the lithium isoelectronic sequence are used in temperature diagnostics in the solar corona (Heroux 1964). The level spacings in the $1s^2 2s - 1s^2 2p$ and $1s^2 2s - 1s^2 3p$ transitions make the ratio $R = q(2s - 2p)/q(2s - 3p)$ temperature dependent. Moreover, at low densities (Saraph and Seaton 1970)

$$R \cong I(2s-2p)/I(2s-3p), \quad (7.1)$$

where $I(2s - np)$ is the line intensity of radiation. Thus from a knowledge of the line-intensity ratio and R the plasma temperature can be estimated.

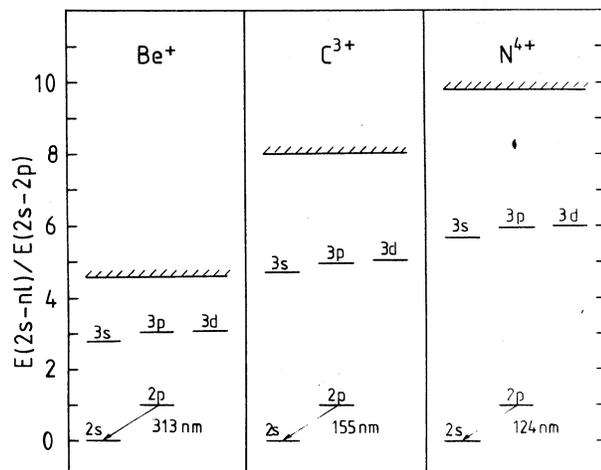


Fig. 3. Energy level structure of Be II, C IV and N V in units of the $2s - 2p$ excitation energy.

In Figure 3 we show the energy level structure of Be II, C IV and N V. The relative spacing between the $n=2$ and $n=3$ levels increases along the sequence and, consequently, the effect of the coupling with higher thresholds on the cross section of the $2s - 2p$ transition is expected to decrease with z . On the other hand, for the $2s - 3p$ transition this coupling will always be important.

In Figure 4 we show the calculated and experimental cross sections for the $2s - 2p$ transition for these ions. The main features can be summarized as follows:

i) The excitation cross section for $\text{Be}^+ + e^-$; has

been calculated in a variety of approximations. It can be seen that the Coulomb-Born approximation grossly overestimates the cross section near threshold but converges to the experimental limit at high energies. Unitarization of the S matrix and exchange are also important, and they are found to lower the cross section in the low energy region. Also, as the contribution to the cross section for intermediate states with $L \leq 3$ is relatively small for this transition the unitarized Coulomb-Born approximation with exchange gives reasonable results. The close-coupling method gives fairly good results at low energies, but even a 5-state (5CC) approximation gives results which are 20% above experiment suggesting slow convergence of the CC expansion.

ii) The agreement with experiment for the higher members of the sequence is much better: for C IV a 5CC approximation and for N V a 2CC are sufficient to give satisfactory agreement with experiment. In fact, for the latter case, the distorted wave, Coulomb-Born and CC results are in 10% agreement (results not shown).

iii) A usual feature found in experimental measurements is that the threshold for a transition is not sharp due to the energy distribution of the electron beam. If theoretical values are averaged over the electron beam energy distribution, and in the case of NV it has a FWHM of $\sim 3\text{eV}$, the agreement with the experimental trend is greatly improved.

b) *The Beryllium Isoelectronic Sequence*

Transitions in the $n=2$ complex of ions in the Be-like sequence are observed in a variety of astronomical objects. However, astrophysical interpretations from these transitions (e.g. in the upper atmosphere of the sun) are sensitive to small errors (25%) in the atomic data, and a great deal of effort has been given to obtain rate coefficients for these transitions to an accuracy better than 10%.

Firstly, it is found that the target wave functions are sensitive to configuration interaction, and correlation configurations containing $3l$ and $4l$ pseudo-orbitals must be included to reproduce the experimental term energy separations and f -values to $\sim 2\%$. Secondly, the cross section at low energies is dominated by resonances converging to the $2l$ thresholds, and at higher temperatures ($> 10000^\circ\text{K}$) the rate coefficients are also sensitive to resonances converging to the $2s3l$ thresholds. Calculations have been carried out by Berrington *et al.* (1977, 1979) for C III in a 6CC approximation, for O V in 6CC and 12CC, and by Dufton *et al.* (1979) for Ne VII in a 6CC approximation. These calculations also include correlation functions for the $(N+1)$ -electron system which make some allowance for neglected thresholds.

In Figure 5 we show the results for the $1s^2 2s^2 \ ^1S - 1s^2 2s 2p \ ^3P^0$ and $1s^2 2s^2 \ ^1S - 1s^2 2s 2p \ ^1P^0$ transitions in O V in 6CC and 12CC approximations. Below the resonances converging to the $n=3$ thresholds

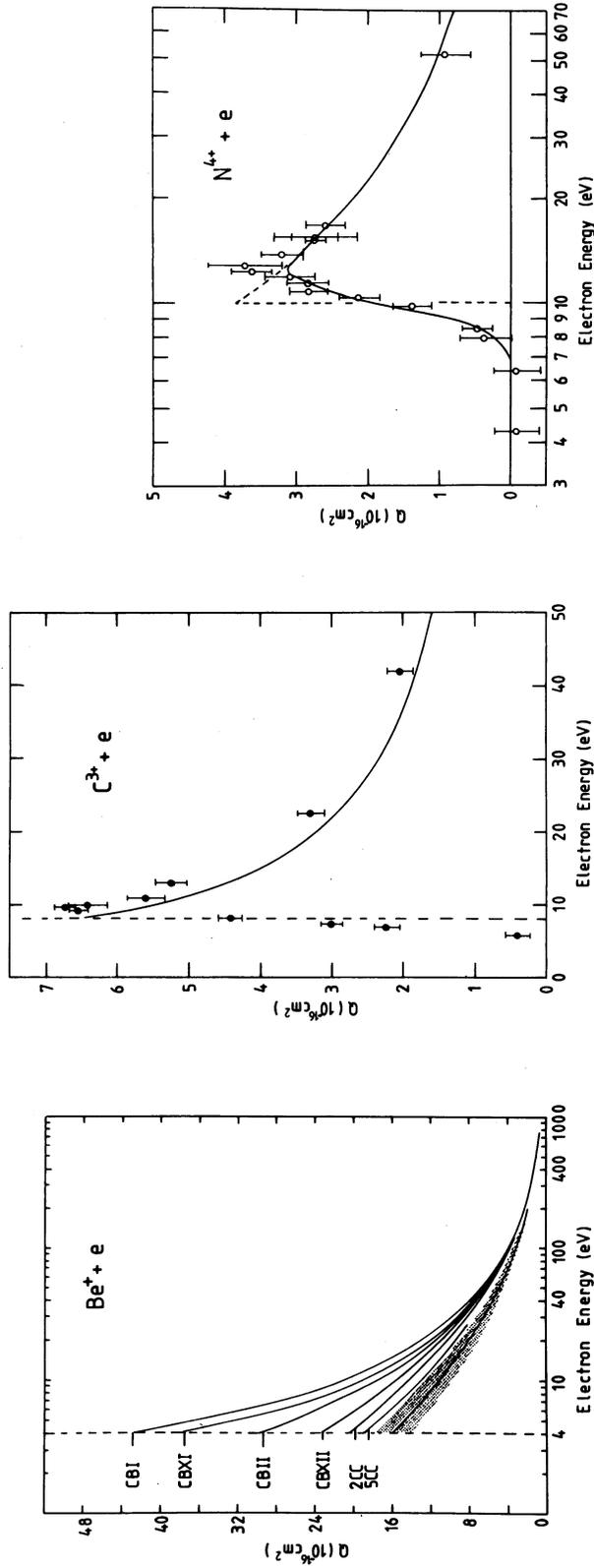


Fig. 4. Electron impact excitation cross section for the $2s - 2p$ transition in the lithium-like sequence. Be II by Hayes *et al.* (1977); CBI, Coulomb-Born; CBXI, Coulomb-Born with exchange; CBII, unitarized Coulomb-Born with exchange; 2CC, 2-state close-coupling; 5CC, 5-state close-coupling; hatched curve, experiment by Taylor *et al.* (in press). C IV: Solid curve, 5CC by Gau and Henry (1977); experiment by Taylor *et al.* (1977). N V: dashed curve, 2CC by van Wyngaarden and Henry (1976); solid curve, 2CC values averaged over the electron beam energy profile; experiment by Gregory *et al.* (1979).

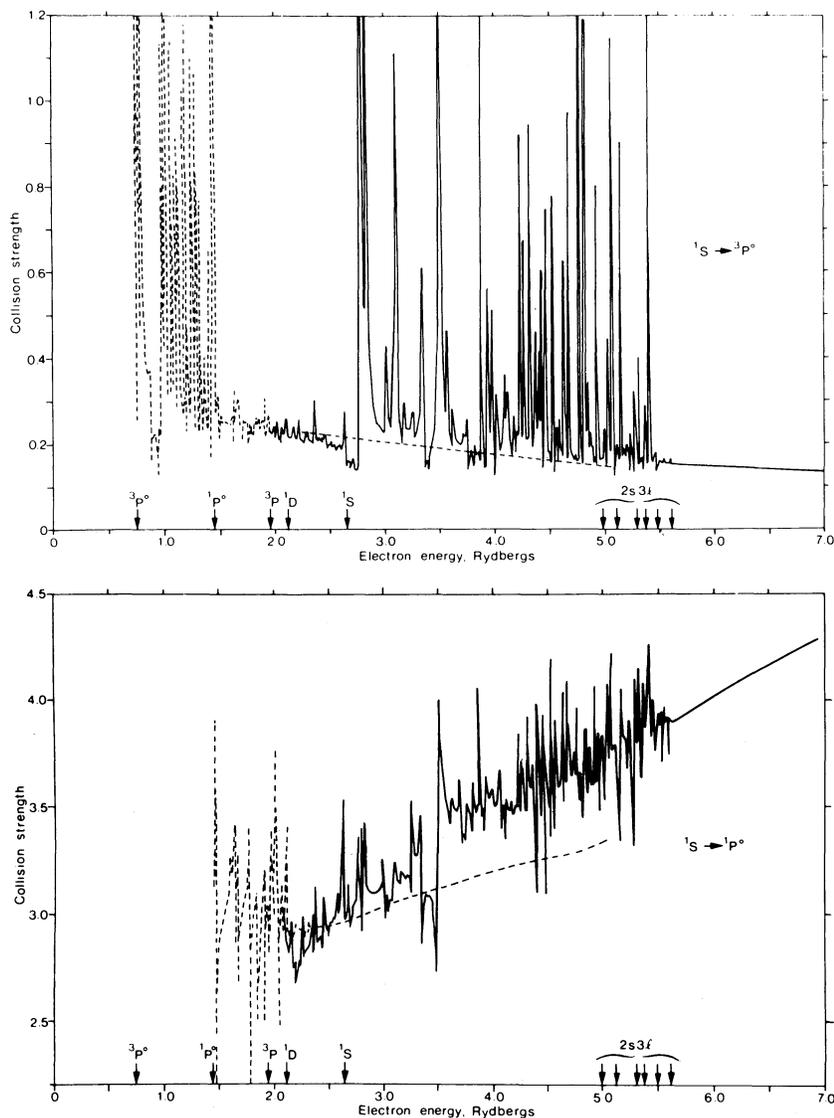


Fig. 5. Total collision strength for the $1S - 3P^0$ and $1S - 1P^0$ transitions in O V by Berrington *et al.* (1977, 1979). Solid curve, 12CC; dashed curve, 6CC.

The 6CC and 12CC results are in good agreement, but in the resonance region the collision strength for the $1S - 3P^0$ is increased on average by a factor of 2 and for the $1S - 1P^0$ by $\sim 10\%$. This difference in contributions is due to the fact that for the $1S - 3P^0$ transition, being spin-forbidden, the convergence of the CC expansion is quite fast and the main contributions come from the lower partial waves where resonances dominate. On the other hand, the $1S - 1P^0$ is an allowed transition and the convergence is much slower and contributions to the cross section come from higher partial waves where resonances are less important. These new results have been used to resolve outstanding discrepancies in the interpretation of observations in the upper solar atmosphere (Dufton *et al.* 1978, 1979).

c) $2p^q$ Isoelectronic Sequences

Transitions in ions with ground configuration $2p^q$ ($q = 1, 2, 3, 4, 5$) play an important role in a wide range of astrophysical problems. For example, the analysis of the forbidden transitions within the ground configuration of such ions ($q = 2, 3, 4, 5$) provides reliable estimates of the electron temperature and density and abundances in gaseous nebulae. Also, the semi-forbidden and allowed transitions between levels in the $n = 2$ and $n = 3$ complexes are used in the interpretation of observations from quasars, the solar corona and hot stars. In many cases the electron impact excitation rate coefficients for the lower members of the sequences are dominated by resonances, and detailed close-coupling

calculations have been carried out attaining accuracies of 10% – 20%. For the higher members the Distorted Wave method has been widely used, and results are quoted to be accurate to better than 50%.

Here we will only discuss an interesting technique developed by Pradhan (1976) to calculate the cross section for the $2s^2 2p^3 \ ^2D_{3/2}^0 - 2s^2 2p^3 \ ^2D_{3/2}^0$ fine-structure transition in O II. Fine-structure transitions within the np^3 ground configuration are used in electron density estimates in nebulae. He uses a 5CC approximation and the algebraic method by Saraph (1972) (section 5.3) to obtain cross sections for these transitions neglecting relativistic effects and fine-structure energy splitting in the target. However, the cross section for the above transition is populated by resonances converging to the $2s^2 2p^3 \ ^2P^0$ threshold which in intermediate coupling mix strongly to give a complicated pattern. He makes use of an extrapolation method based on QDT which gives impressive results (Figure 6).

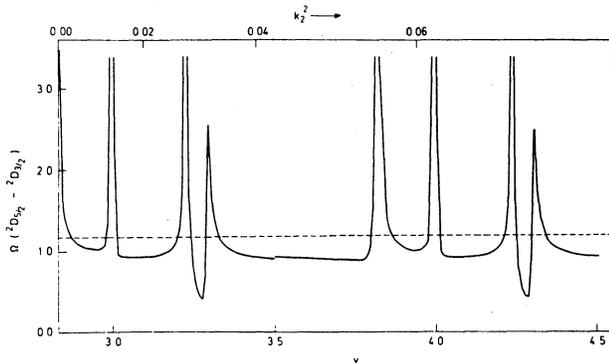


Fig. 6 Total collision strength by Pradhan (1976) for the $^2D_{3/2}^0 - ^2D_{3/2}^0$ transition in O II as a function of the effective quantum number at energies just above the $^2D^0$ threshold. Dashed curve, Gailitis average.

$R^{SL\pi}$ in LS coupling are calculated at a few points above the $^2P^0$ threshold, where they are slowly varying with energy, and they are fitted to low order polynomials. They are then extrapolated below threshold with the QDT formula (6.6) to two points corresponding to $\nu = 3.0$ and $\nu = 4.0$, where $k^2(^2P^0) = -1/\nu^2$ (Figure 6). The extrapolated $R^{SL\pi}$ at these two points are now transformed to intermediate coupling ($R^{J\pi}$) using the relation (5.5), and the slowly varying $\chi^{J\pi}$ matrices are calculated with

$$\chi^{J\pi} = (1 + iR^{J\pi})(1 - iR^{J\pi})^{-1} \quad (7.1)$$

The $\chi^{J\pi}$ matrices calculated at $\nu = 3.0$ are used to obtain collision strengths with the QDT formula (6.8) between $\nu = \nu_t$ and $\nu = 3.5$, and those calculated at $\nu = 4.0$ are used to obtain collision strengths in the range

$\nu = 3.5$ and $\nu = 4.5$. For $\nu > 4.5$ the resonances are closely spaced and the Gailitis average may be implemented. Thus he is able to obtain a complete description of the cross section in this difficult region and calculate the effective collision strength $\Upsilon(3/2, 5/2; T_e)$ for this transition.

d) The Sodium Isoelectronic Sequence

As an example of calculations done for ions in this sequence we will mention the results by Mendoza (1981b) on the electron impact excitation of the $3s - 3p$ transition of Mg II (Figure 7).

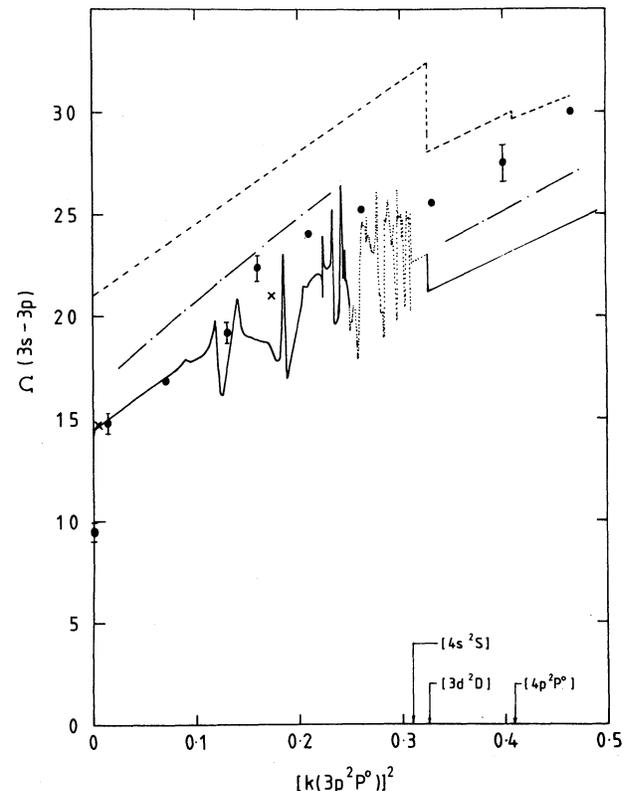


Fig. 7. Total collision strength for the $3s - 3p$ transition in Mg II. Solid line, 4CC by Mendoza (1981b); dot-dashed line, 3CC by Burke and Moores (1968); dashed line; CB by Blaha (1972); crosses DW by Kennedy *et al.* (1978); filled circles, experiment by Zapesochnyi *et al.* (1975).

A 4CC ($3s, 3p, 3d, 4s$) approximation is used, and the distortion of the $2p^6$ core by the two outer electrons is approximated by semi-empirical model polarization potentials which include a term to account for the valence-valence interaction by the polarized core (dielectronic polarization, Norcross and Seaton 1976). The special feature of his method is that the $n\ell$ wave functions of Mg^+ are calculated by considering the

$Mg^{++} + e^{-}$ system in a single closed channel representation (i.e. an eigenvalue problem), and adjusting the empirical parameters of the polarization potential to fit the spectral series of Mg^{+} . Thus these orbitals are expected to be more accurate than those obtained by the usual atomic structure methods. Results are compared with experiment and other theoretical results in Figure 7. Again, as the $3s - 3p$ is an allowed transition and the convergence of the partial wave expansion is low, the agreement with simpler approximations, e.g. the Distorted Wave and unitarized Coulomb-Born with exchange, is fairly good.

e) The Second Row Sequences

Recently there have been some attempts to extend the close-coupling approach used with considerable success for first-row ions to the larger ions of the second row of the periodic table. The target term structures show many similarities, but the open $n = 3$ shell and the increased atomic radius make the problem much more difficult.

Following Layzer (1959) all configurations in the same complex must be included in the description of the target wave functions and this implies that a large number of configurations must be taken into account. Even so, the term energy separations and f-values are

generally poor and correlation configurations containing $4l$ and sometimes $5l$ pseudo-orbitals must be considered. For forbidden and semi-forbidden transitions in the first-row ions the contributions to the cross section from channels containing f and g waves are small and can be calculated with the Distorted Wave or Coulomb-Born approximations, and in some cases neglected. This is not the situation for the larger ions where it is usually necessary to include these channels explicitly in the CC expansion.

There are two recent detailed CC calculations by Baluja *et al.* (1980) on the $3s^2\ ^1S - 3s3p\ ^3P^0$ transition in Si III and by Dufton and Kingston (1980) on the $3s^23p\ ^2P^0 - 3s3p^2\ ^4P$ transition in S IV. In both of these cases accurate target functions and the resonance contribution to the cross section play a dominant role. In the former calculation it is found that the effective collision strength at $5000^{\circ}K$ is larger by a factor of six compared with earlier DW results; even at high temperatures ($25 \times 10^4\ ^{\circ}K$) it is larger by a factor of 2. A similar situation is found in the S IV calculation.

The author is at the moment involved in an extensive study of the forbidden transitions for ions in the silicon and phosphorus isoelectronic sequences. In Figure 8 we illustrate a problem encountered in the calculation of the cross section for the transition $3s^23p^2\ ^3P - 3s^23p^2\ ^1D$ of S III. There are large shifts in

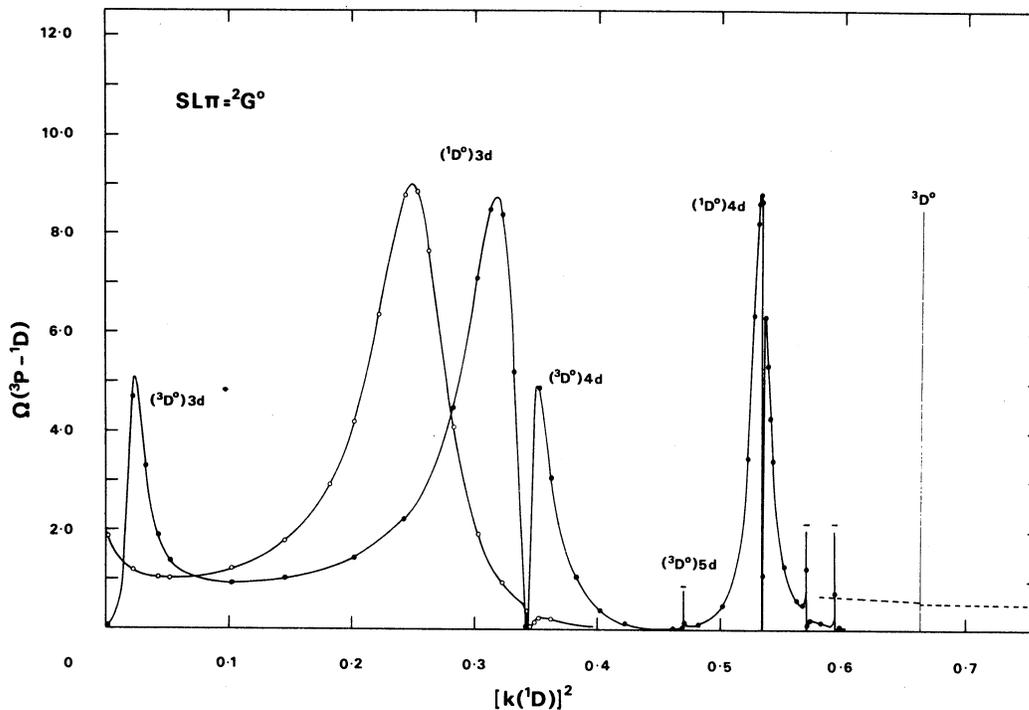


Fig. 8. Partial collision strength of the $^3G^0$ intermediate state for the $3s^23p^2\ ^3P - ^1D$ transition in S III showing the shift in the position of the 3d resonances caused by including correlation for the excited configurations. Dots, without correlation; open circles, with correlation.

the position of the 3d resonances when configurations in the $n = 3$ complex which correlate with the excited odd configurations are included. There are also shifts when channels containing g waves are neglected. The other resonances are only slightly affected.

f) Heavier Ions

The problems encountered in the calculation of excitation cross sections for heavy ions are innumerable, some of them intractable with present computational methods and facilities: open shells, large number of close-lying levels leading to strong correlation effects in the target and in the close-coupling expansion for the $(N + 1)$ -electron system, relativistic effects in the target and in the collision process, complicated resonance structure and poor experimental measurements. We illustrate the way in which these problems have been tackled with a recent calculation by Nussbaumer and Storey (1980) on atomic data for the astrophysically important Fe II. There is hardly any astronomical object which does not show lines of Fe II in its spectrum and the atomic data are very poor indeed.

Fe II has 25 electrons, 7 of which are in open shells. The lowest 4 configurations $3d^6 4s$, $3d^7$, $3d^5 4s^2$ and

$3d^6 4p$ give rise to 116 terms and 299 fine-structure levels. They calculate energy levels and transition probabilities for allowed and forbidden transitions with the atomic structure program SUPERSTRUCTURE Eisner *et al.* 1974). They restrict the configuration basis and consequently, some of the term energies are very poor (Table 1), in particular the $3d^7 \ ^4F$. This term is greatly improved if the $3d^6 4d$ configuration is included. Experimental f-values for allowed transitions show large discrepancies (\sim factor of 2) among themselves to provide a guide to the accuracy of their calculated values. However, their calculated transition probabilities for the forbidden transitions are in reasonable agreement with the semi-empirical results by Garstang (1962): for transitions within the ground term it is better than 10%; for the strong transitions to higher levels it is in general better than 20%, but there are large discrepancies for the feeble ones.

They also calculate collision strengths for all the fine-structure transitions of the lowest four terms. The close-coupling expansion is generated in the two-configuration basis $3d^6 4s$, $3d^7$ and limited to the 4 terms 6D , 4F , 4D and 4P , and electron partial waves with $\ell < 3$. Collision strengths are calculated in LS coupling at three energies thus neglecting resonances, and the fine-structure cross sections are obtained by the algebraic method of Saraph (1972) neglecting relativistic effects and fine-structure in the target which for Fe II is not really valid. They find that the contribution to the cross section from partial waves with $\ell > 3$ is small and can be ignored, and the largest errors arise from neglecting resonances and from using poor target wave functions, an uncertainty of 50% is quoted. A more ambitious calculation, based on the Breit-Pauli treatment, is at the moment being prepared by the group at the Queen's University of Belfast.

I would like to thank Professor M.J. Seaton for encouraging me to give this talk. A research grant from the Science Research Council of Great Britain is acknowledged.

TABLE 1

OBSERVED AND CALCULATED TERM ENERGIES OF Fe II (cm^{-1})^a

State	Observ.	Calc.
$3d^6 4s \ ^6D$	0	0
$3d^7 \ ^4F$	2003	34879
$3d^6 4s \ ^4D$	7904	9521
$3d^7 \ ^4P$	13196	52248
$3d^6 4p \ ^6D^0$	38294	35091
$\ ^6F^0$	41754	38690
$\ ^6p^0$	42649	40689
fine-structure:		
$3d^6 4s \ ^6D_{9/2}$	0	0
$\ ^6D_{7/2}$	385	391
$\ ^6D_{5/2}$	668	684
$\ ^6D_{3/2}$	863	888
$\ ^6D_{1/2}$	977	1009
$3d^7 \ ^4F_{9/2}$	0	0
$\ ^4F_{7/2}$	567	662
$\ ^4F_{5/2}$	965	1152
$\ ^4F_{3/2}$	1245	1490
$3d^6 4p \ ^6D^0_{9/2}$	0	0
$\ ^6D^0_{7/2}$	201	257
$\ ^6D^0_{5/2}$	400	479
$\ ^6D^0_{3/2}$	554	647
$\ ^6D^0_{1/2}$	650	750

a. Results by Nussbaumer and Storey (1980).

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