RADIATIVE BOUND-BOUND TRANSITIONS

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Bound-bound transition - Excitation & De-excitation:

$$X^{+Z} + h\nu \rightleftharpoons X^{+Z*}$$

- **Oscillator Strength (f), Radiative Decay Rate (A-value)**

THEORY: Breit-Pauli R-matrix Method

Quantity of Interest : S - The Line Strength

Transition Matrix elements:

$< \Psi_B||\mathbf{D}||\Psi_{B'} >$ $\rightarrow$ **Radiative Excitation and Deexcitation, D** $= \sum_i \mathbf{r}_i$ $\rightarrow$ Dipole Operator

Wave functions and energies are obtained solving, $H\Psi = E\Psi$

- **E** $< 0 \rightarrow$ **Bound (e+ion) states** Ψ_B
- **E** $\geq 0 \rightarrow$ **Continuum states** Ψ_F

Generalized line strength is defined as,

$$S = \left| \left\langle \Psi_f | \sum_{j=1}^{N+1} r_j | \Psi_i \right\rangle \right|^2 \qquad (1)$$

The oscillator strength, f_{ij}, and radiative decay rate are

$$f_{ij} = \frac{E_{ji}}{3g_i} S, \quad A_{ji}(sec^{-1}) = 0.8032 \times 10^{10} \frac{E_{ji}^3}{3g_j} S \tag{2}$$

For a multi-electron system, in nonrelativistic LS coupling:

$$\left[\sum_{i=1}^{N} \left\{ -\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N} \frac{2}{r_{ij}} \right\} \right] \Psi = E\Psi. \tag{3}$$

In close-coupling Approximation and the R-matrix method the ion is treated as a system of (N+1) electrons: a target or the ion core of N electrons with the additional interating (N+1)th electron. • Total wavefunction expansion is expressed as:

$$\Psi_E(e + ion) = A \sum_{i}^{N} \chi_i(ion)\theta_i + \sum_{j} c_j \Phi_j(e + ion)$$

$\chi_i \rightarrow$ target ion wavefunction, $\theta_i \rightarrow$ wavefunction of the interacting electron (continuum or bound) $\Phi_j \rightarrow$ correlation functions of (e+ion) • The complex resonant structures in the atomic processes are included through channel couplings.

Relativistic effects: In Breit-Pauli R-matrix (BPRM) approximation, the three one-body relativistic correction terms are added: $H^{mass} = -\frac{\alpha^2}{4} \sum_i p_i^4$, $H^{Dar} = \frac{\alpha^2}{4} \sum_i \nabla^2 \left(\frac{Z}{r_i} \right)$, $H^{so} = \frac{Ze^2\hbar^2}{2m^2c^2r^3}$**L.S**

The spin-orbit interaction H^{so} splits LS energy in to fine structure levels.
The two-body correction terms, including Breit interaction,

are:

$$H_{\rm BP} = \frac{1}{2}\sum_{i\neq j}^{N}[g_{ij}(so+so') + g_{ij}(ss') + g_{ij}(css') + g_{ij}(d) + g_{ij}(oo')]. \quad (4)$$

Substitution of $\Psi_E(e+ion)$ in $H\Psi_E = E\Psi_E$ results in a set of coupled euqations

- **Coupled equations are solved by R-matrix method**

RADIATIVE EXCITATIONS AND RADIATIVE DECAYS: f-, S, A-values for various types of transitions

Allowed electric dipole (E1) transtitions (Δ j=0,$\pm$1, parity π changes)

- **Dipole allowed (ΔL = 0, $\pm$1, $\pm$2, ΔS = 0)**
- **Intercombination (ΔL = 0, $\pm$1, $\pm$2, ΔS $\neq$ 0)**

$$A_{ji}(sec^{-1}) = 0.8032\times 10^{10}\frac{E_{ji}^3}{3g_j}S^{E1}, \qquad f_{ij} = \frac{E_{ji}}{3g_i}S^{\rm E1}(ij) \quad (5)$$

Forbidden transitions

- **Electric quadrupole (E2) transitions (Δ J = 0,$\pm$1,$\pm$2, parity does not change)**

$$A_{ji}^{E2} = 2.6733\times 10^{3}\frac{E_{ij}^5}{g_j}S^{E2}(i,j)\ {\rm s}^{-1}, \quad (6)$$

- **Magnetic dipole (M1) transitions (Δ J = 0,$\pm$1, parity does not change)**

$$A_{ji}^{M1} = 3.5644\times 10^{4}\frac{E_{ij}^3}{g_j}S^{M1}(i,j)\ {\rm s}^{-1}, \quad (7)$$

• **Electric octupole (E3) transitions (Δ J= $\pm$2, $\pm$3, parity changes)**

$$A_{ji}^{\rm E3} = 1.2050 \times 10^{-3} \frac{E_{ij}^7}{g_j} S^{\rm E3}(i,j)\ {\rm s}^{-1}, \tag{8}$$

• **Magnetic quadrupole (M2) transitions (Δ J = $\pm$2, parity changes)**

$$A_{ji}^{\rm M2} = 2.3727 \times 10^{-2} {\rm s}^{-1} \frac{E_{ij}^5}{g_j} S^{\rm M2}(i,j)\,. \tag{9}$$

The lifetime of a level,

$$\tau_k(s) = \frac{1}{\sum_i A_{ki}(s^{-1})}. \tag{10}$$

Methods:

• **Breit-Pauli R-matrix (BPRM) calculations for E1 transitions**

• **Forbidden (E2, E3, M1, M2) transitions** – SUPERSTRUCTURE

BPRM calculations:

(i) Computationally extensive due to fine structure

(ii) A major task is theoretical spectroscopy for Level identification:

$$({\bf C_t}\ {\bf S_t}\ {\bf L_t}\ {\bf J_t}\ \pi_{\bf t}{\bf n}\ell\ [{\bf K}]\ {\bf s})\quad {\bf J}\ \pi \tag{11}$$

Atomic Data: Radiative Decay Rates with Fine Structure

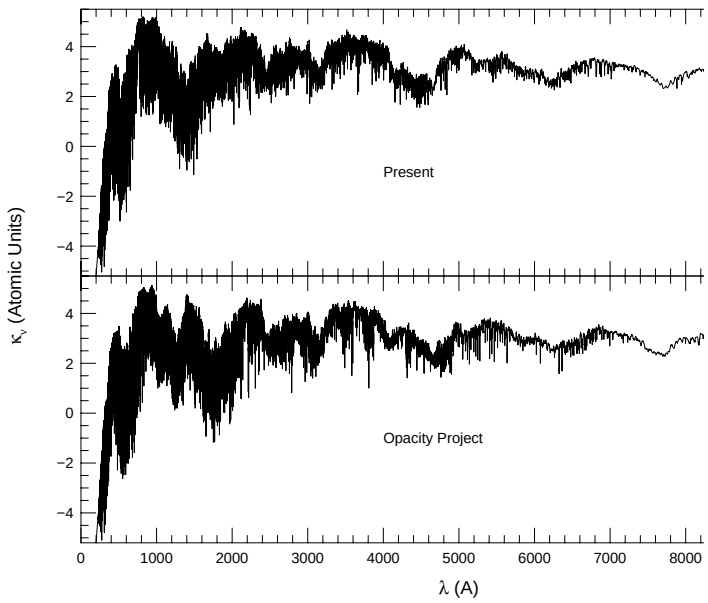
Fe ions: Fe II, Fe III, Fe IV, Fe V, Fe XIII, Fe XIV, Fe XV, Fe XVI, Fe XVII, Fe XVIII, Fe XIX, Fe XX, Fe XXI, Fe XXII, Fe XXIV, Fe XXV
Ni ions: Ni XXVI, Ni XXVII
Cr ions: Cr XXII, Cr XXIII
Ti ions: Ti XX, Ti XXI
Ca ions: Ca XV, Ca XVIII, Ca XIX
Ar ions Ar XIII, Ar XVI, Ar XVII
S ions S II, S III, S XIV
Si ions Si I, Si II, Si XII
Al ions Al XI
Mg ions Mg X
Na ions Na IX
Ne ions Ne IV, Ne VIII
F ions: F VII
O ions O II, O III, O IV, O VI
N ions: N V
C ions C II, C II, C IV

- **More extensive f-values in LS coupling for many ions**
- **Forbidden transitions for almost all iron ions**

Some example for Fe ions

Fe II (157,919 - allowed fine structure)
Fe III (124,334 - allowed fine structure, - ? E2,M1)
Fe IV (712,120 - allowed fine structure, 173,000 - E1, E2, M1)
Fe XVII (26,222 - E1; 2,312 - E2,E3,M1,M2)
Fe XVIII (141,869 - E1; 29,682 - E2,E3,M1,M2)

Monochromatic Opacities κ_ν of Fe IV at logT=4.5, $logN_e(\mathrm{cm}^{-3}) = 17.0$



- Fe IV dominates the iron opacity at this temperature and density
- κ_ν depends primarily on oscillator strengths
- Figure shows that opacity of Fe IV varies over orders of magnitute between 500 - 4000 $\AA$
- Comparison between the present and ealier atomic data indicates systematic shift in groups of OP energies