**RADIATIVE BOUND-BOUND TRANSITIONS**

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Bound-bound transition - Excitation & De-excitation:

\[ X^+Z + h\nu \iff X^+Z^* \]

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

**THEORY:** Breit-Pauli R-matrix Method

Quantity of Interest : \(S\) - The Line Strength

Transition Matrix elements:

\[ <\Psi_B||D||\Psi_{B'}> \rightarrow \text{Radiative Excitation and Deexcitation}, \quad D = \sum_i r_i \rightarrow \text{Dipole Operator} \]

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

- \(E < 0 \rightarrow \text{Bound (e+ion) states } \Psi_B\)
- \(E \geq 0 \rightarrow \text{Continuum states } \Psi_F\)

Generalized line strength is defined as,

\[
S = \left| \left< \Psi_f \left| \sum_{j=1}^{N+1} r_j |\Psi_i \right> \right> \right|^2
\]  

(1)
The oscillator strength, $f_{ij}$, and radiative decay rate are

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

(2)

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

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

(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: $H^{mass} = -\frac{\alpha^2}{4} \sum_i p_i^4$, $H^{Dar} = \frac{\alpha^2}{4} \sum_i \nabla_i^2 \left( \frac{Z}{r_i} \right)$, $H^{so} = \frac{Ze^2\hbar^2}{2m^2c^2r^3} \text{L.S}$

The spin-orbit interaction $H^{so}$ splits LS energy in to fine structure levels.

The two-body correction terms, including Breit interaction,
are:

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

(4)

Substitution of \( \Psi_E(e + \text{ion}) \) 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) transitions (\( \Delta j=0,\pm1, \) parity \( \pi \) changes)

- Dipole allowed (\( \Delta L = 0, \pm1, \pm2, \Delta S = 0 \))
- Intercombination (\( \Delta L = 0, \pm1, \pm2, \Delta S \neq 0 \))

\[ A_{ji}(sec^{-1}) = 0.8032 \times 10^{10} \frac{E_{\text{ji}}^3}{3g_j} S^{E1}_i, \quad f_{ij} = \frac{E_{ji}^3}{3g_i} S^{E1}(ij) \]  

(5)

Forbidden transitions

- Electric quadrupole (E2) transitions (\( \Delta J = 0,\pm1,\pm2, \) parity does not change)

\[ A^{E2}_{ji} = 2.6733 \times 10^{3} \frac{E_{ij}^5}{g_j} S^{E2}(i, j) \text{ s}^{-1}, \]  

(6)

- Magnetic dipole (M1) transitions (\( \Delta J = 0,\pm1, \) parity does not change)

\[ A^{M1}_{ji} = 3.5644 \times 10^{4} \frac{E_{ij}^3}{g_j} S^{M1}(i, j) \text{ s}^{-1}, \]  

(7)
• **Electric octupole (E3) transitions** ($\Delta J = \pm 2, \pm 3$, parity changes)

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

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

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

The lifetime of a level,

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

**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:

$$(C_t \ S_t \ L_t \ J_t \ \pi_t n\ell \ [K] \ s) \ J \ \pi \quad (11)$$
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 $\kappa_\nu$ of Fe IV at $
abla \log T=4.5$, $\log N_e (\text{cm}^{-3}) = 17.0$

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