PHOTOIONIZATION
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Photoionization & Electron-Ion Recombination:

i) Photoionization (PI) & Radiative Recombination (RR) (1-step):

$$\mathbf{X^{+Z} + h\nu \rightleftharpoons X^{+Z+1}} + \epsilon$$

ii) Autoionization (AI) & Dielectronic Recombination (DR) (2-steps):

$$\mathbf{e + X^{+Z} \rightleftharpoons (X^{+Z-1})^{**}} \rightleftharpoons \begin{cases} e + X^{+Z} & \text{AI} \\ X^{+Z-1} + h\nu & \text{DR} \end{cases}$$

The doubly excited autoionizing state [$(X^{+Z-1})^{**}$] introduces resonances

- **Radiative & Dielectronic Recombinations are inseparable in nature.**

THEORY

Close-coupling (CC) R-matrix method

Total wavefunction expansion in the CC approximation:

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

χ_i → target ion wavefunction, Φ_j → correlation functions of (e+ion)
θ_i → wavefunction of the interacting electron (continuum or bound)

- The complex resonant structures in collisional and radiative processes are included through channel couplings.

The Iron Project - The relativistic Hamiltonian in Breit-Pauli R-matrix (BPRM) approximation:

$$H_{N+1}^{\mathrm{BP}} = H_{N+1}^{NR} + H_{N+1}^{\mathrm{mass}} + H_{N+1}^{\mathrm{Dar}} + H_{N+1}^{\mathrm{so}},$$

where the non-relativisitc Hamiltonian is

$$H_{N+1}^{NR} = \sum_{i=1}^{N+1}\left\{-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N+1}\frac{2}{r_{ij}}\right\}.$$

Mass correction term → $H_{N+1}^{\mathrm{mass}} = -\frac{\alpha^2}{4}\sum_i p_i^4$, Darwin term → $H_{N+1}^{\mathrm{Dar}} = \frac{Z\alpha^2}{4}\sum_i \nabla^2(\frac{1}{r_i})$, Spin-orbit interaction term → $H_{N+1}^{\mathrm{so}} = Z\alpha^2\sum_i \frac{1}{r_i^3}\mathbf{l_i.s_i}$
Spin-orbit term splits the LS terms into fine-structure levels

Solve Schordinger equation: $H_{N+1}^{BP}\Psi = E\Psi$

The channels introduce a set of coupled equations.

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

Bound-Free Transition Matrix elements for photoionization:

$< \Psi_B||\mathbf{D}||\Psi_F >$

$\mathbf{D} \longrightarrow$ dipole operator in "length" and "velocity" forms:

$$\mathbf{D}_L = \sum_n r_n, \qquad \mathbf{D}_V = -2\sum_2 \Delta_n,$$

n = number of electrons

The photoionization cross section (σ_{PI}) is proportional to the generalized line strength (S) defined as,

$$S = | < \Psi_j||\mathbf{D}_L||\Psi_i > |^2 = \left| \left\langle \mathit{\Psi}_f | \sum_{j=1}^{N+1} r_j | \mathit{\Psi}_i \right\rangle \right|^2 ,$$

The photoionization cross section is

$$\sigma_{PI} = \frac{4\pi}{3c}\frac{1}{g_i}\omega S,$$

ω $\longrightarrow$ incident photon energy in Rydberg units

PHOTOIONIZATION CROSS SECTIONS obtained or are in progress for atoms and ions

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

- **Complete data for each ion include**

i) Total photoionization cross sections (σ_{PI}) leaving the ion in various excited core states,

ii) Level-specific photoionization cross sections (σ_{PI}(g)), leaving the ion in the core ground state.

- **Majority of the cross sections and rates are in LS coupling.**
- **However, fine structure effects are expected to be observed. Simple algebraic split of LS cross sections and rates into fine structure through statistical weight factor can be uncertain.**

- **We are carrying out calculations in relativistic BPRM approximations for ions, especially for highly charged ions.**

Photoionization Cross Sections for Fe ions

- **Extensive *narrow* resonances due to Rydberg series of autoinizing resonances.**

Resonance positions are determined from

$$(E_t - E_p) = z^2/\nu^2$$

E_t **= core threshold,** E_p **= electron energy,** ν **= effective quantum number**

- ***Wide* resonances due to photoexcitation-of-core, *PEC* resonances.**

i) Only to valence electron excited states - no PEC resonance for the ground state and equivalent electron states.

ii) Resonances occur at core threshold energies where these thresholds are allowed for dipole allowed transition to the core ground state.

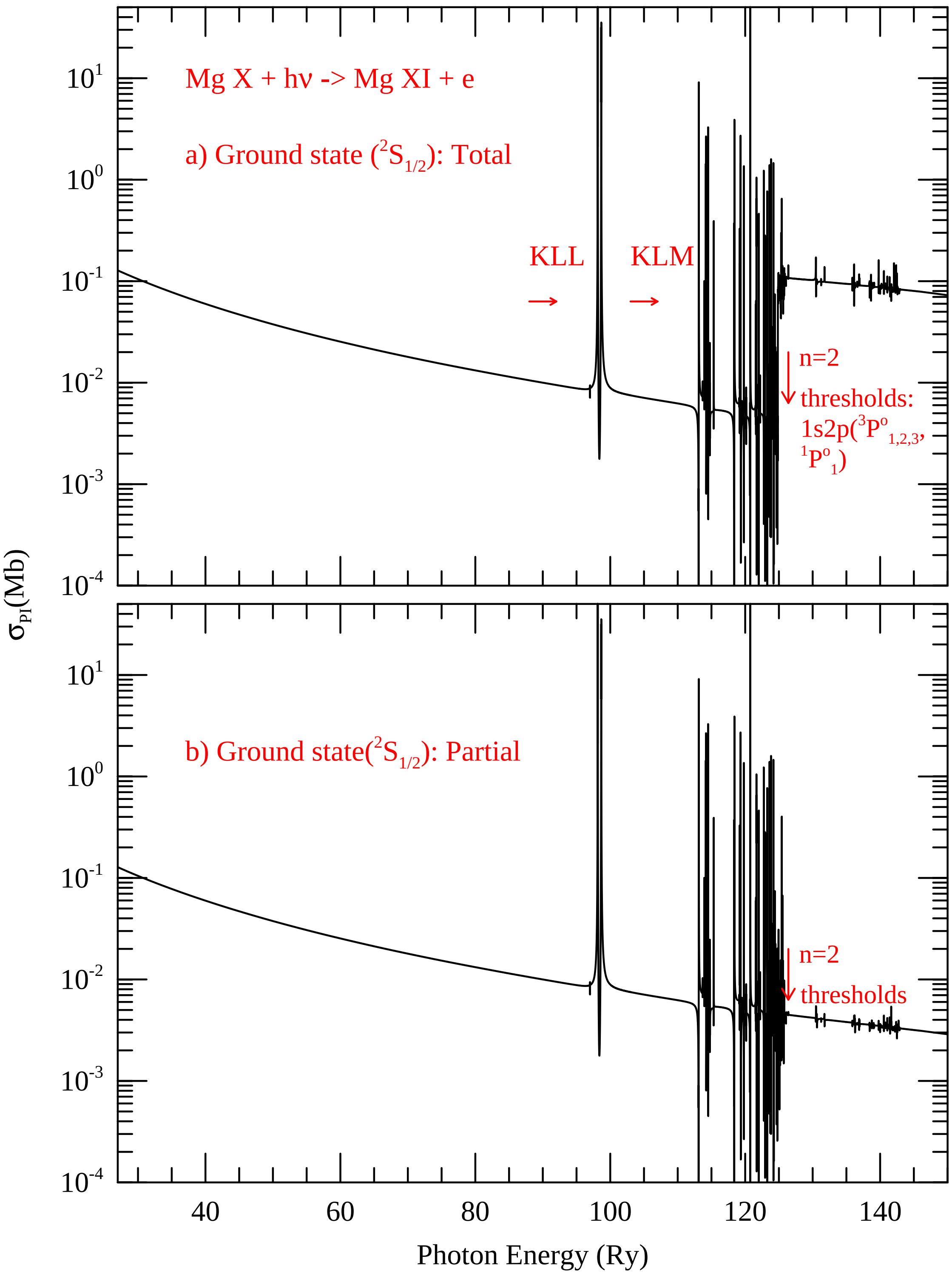
- **Closely spaced core levels cause overlapping of various Rydberg series of resonances**
- **Most of the calculations are in LS coupling. However, fine structure effects are expected to be observed. This means that there can be additional narrow resonances allowed in fine structure, but not allowed in LS coupling.**

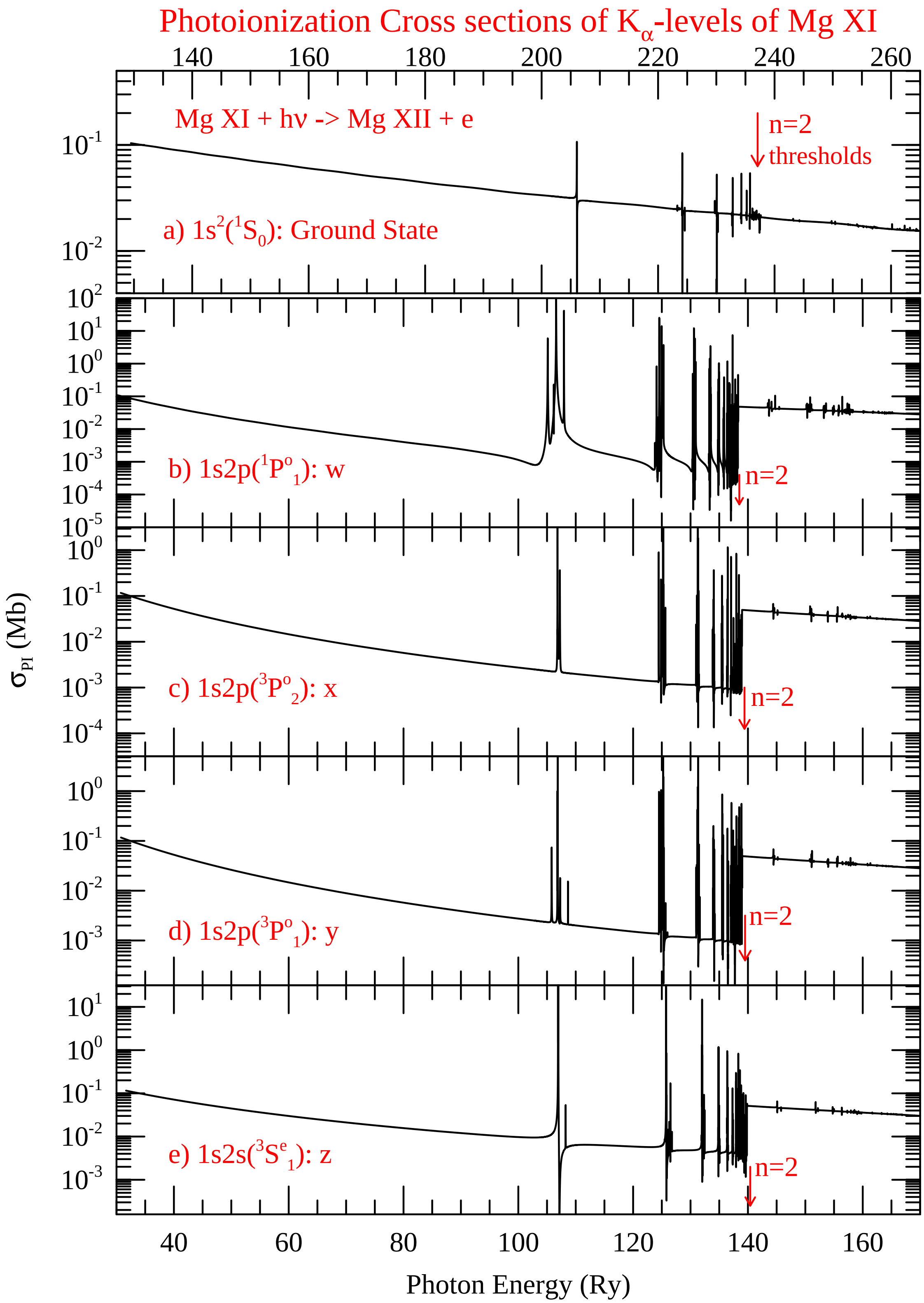
Data Accessibility - Ohio State University:

1. **Anonymous ftp: ftp.astronomy.ohio-state.edu**
2. **Email: nahar@astronomy.ohio-state.edu**

Examples of photoionization cross sections - next few pages

Photoionization Cross sections of ground state of Mg X




Photoionization Cross sections of K_α-levels of Mg XI
140
160
180
200
220
240
260
Mg XI + hν -> Mg XII + e
n=2
thresholds
10^{-1}
10^{-2}
a) $1s^2(^1S_0)$: Ground State
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
b) $1s2p(^1P^o_1)$: w
n=2
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
c) $1s2p(^3P^o_2)$: x
n=2
10^{0}
10^{-1}
10^{-2}
10^{-3}
d) $1s2p(^3P^o_1)$: y
n=2
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
e) $1s2s(^3S^e_1)$: z
n=2
σ_{PI} (Mb)
40
60
80
100
120
140
160
Photon Energy (Ry)

Photoionization Cross Sections of Fe XXI