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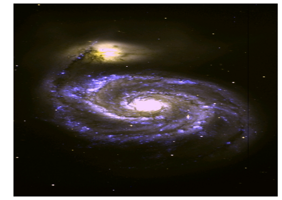

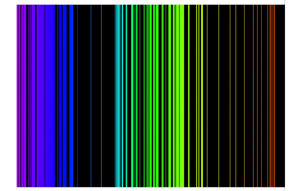

Research based online course:

"Atomic and Molecular Astrophysics and Spectroscopy with Computational workshops on R-matrix and SUPERSTRUCTURE Codes II"

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A.P.J. Abdul Kalam STEM-ER Center
(Indo-US collaboration)

- Organized under the Indo-US STEM Education and Research Center of OSU-AMU, AMU, Aligarh, India, & OSU, Columbus, USA

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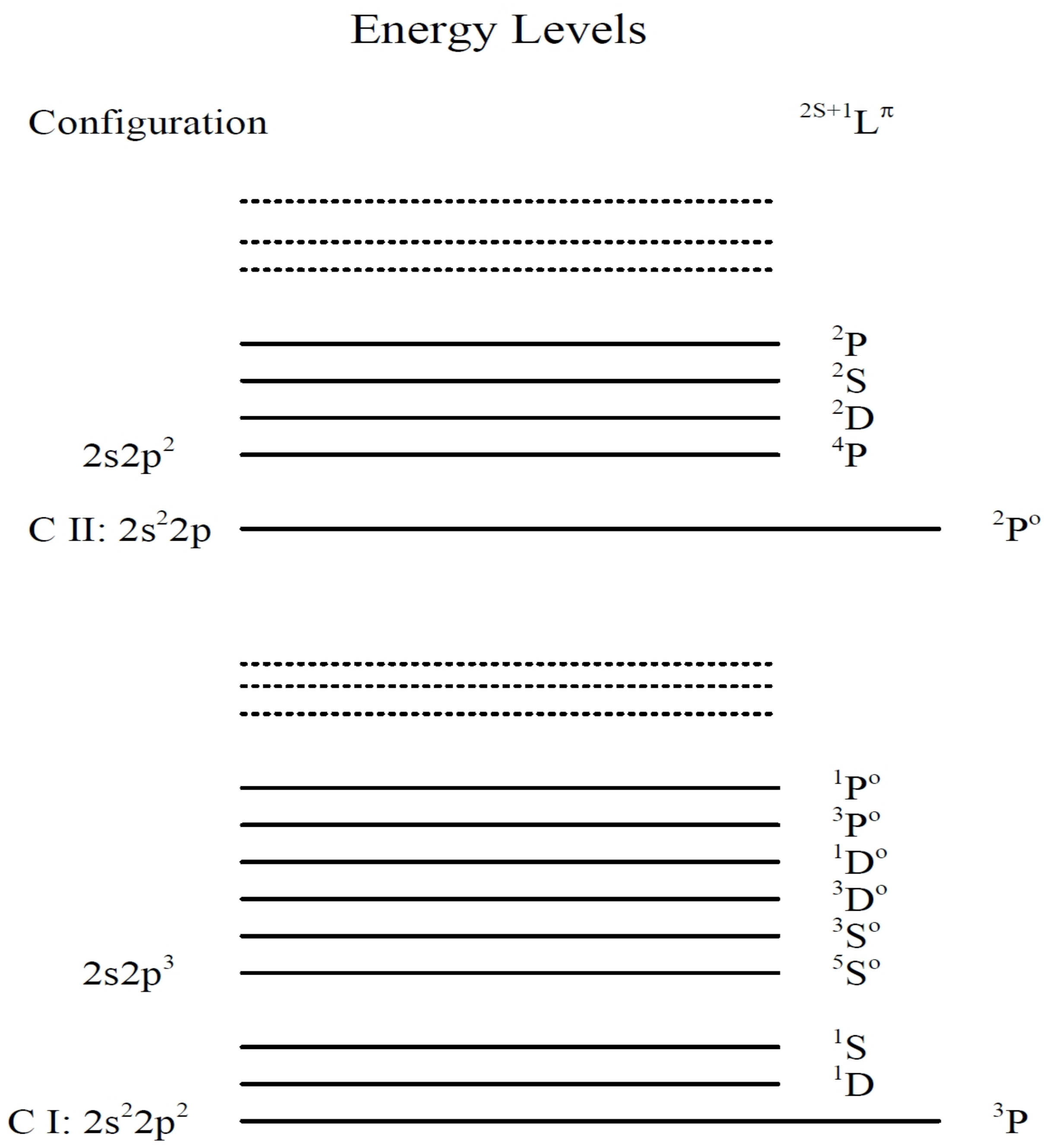
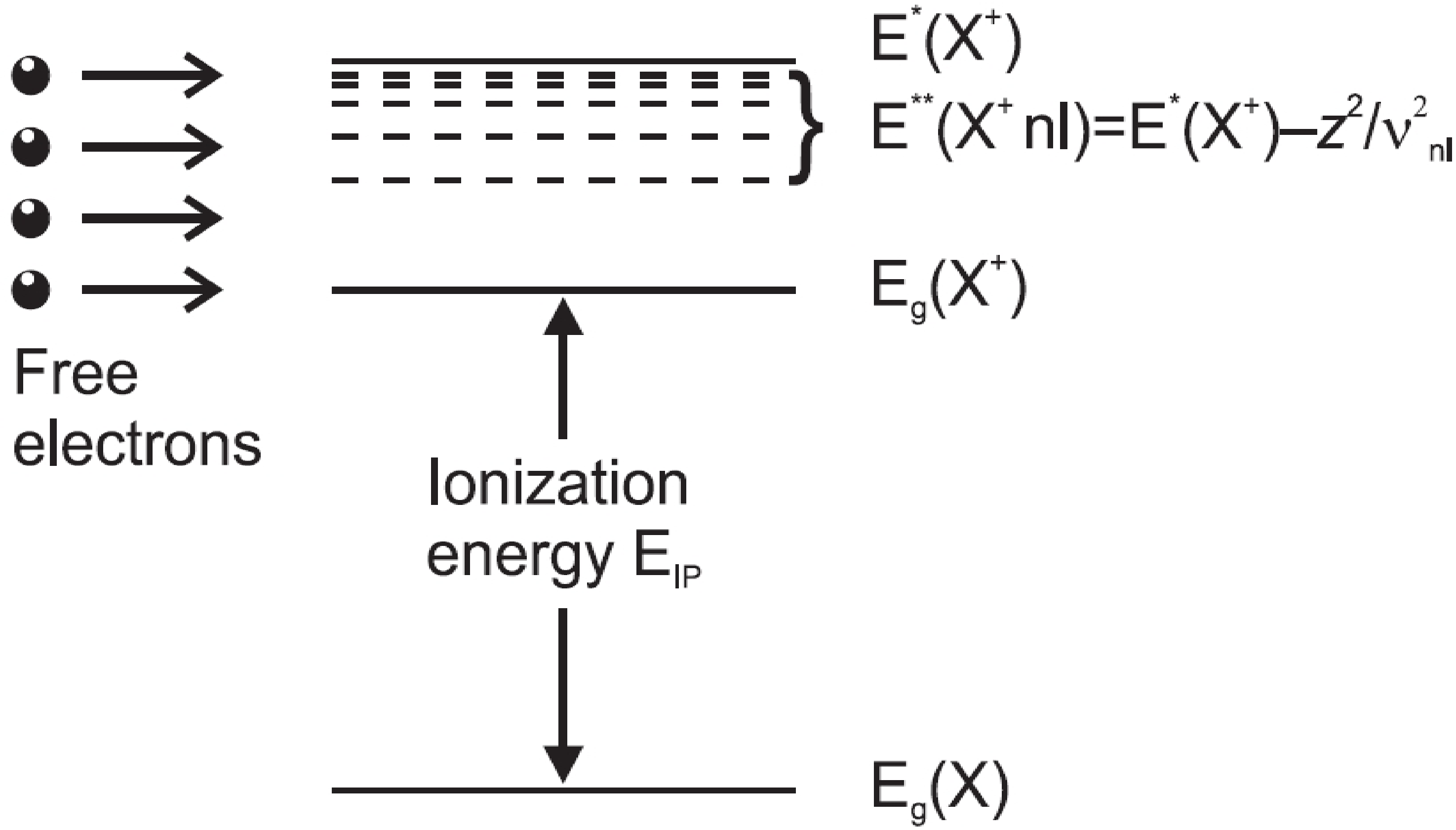
Support: OSU, OSC, OSU-AMU STEM ER Center, AMU

ATOMIC ENERGY LEVELS OF AN ATOM AND ITS ION

- Bound energy levels are negative, electron is free at zero energy. Ex: C I and C II levels



Rydberg Series of Autoionizing States: Quasi-Bound Quantum States



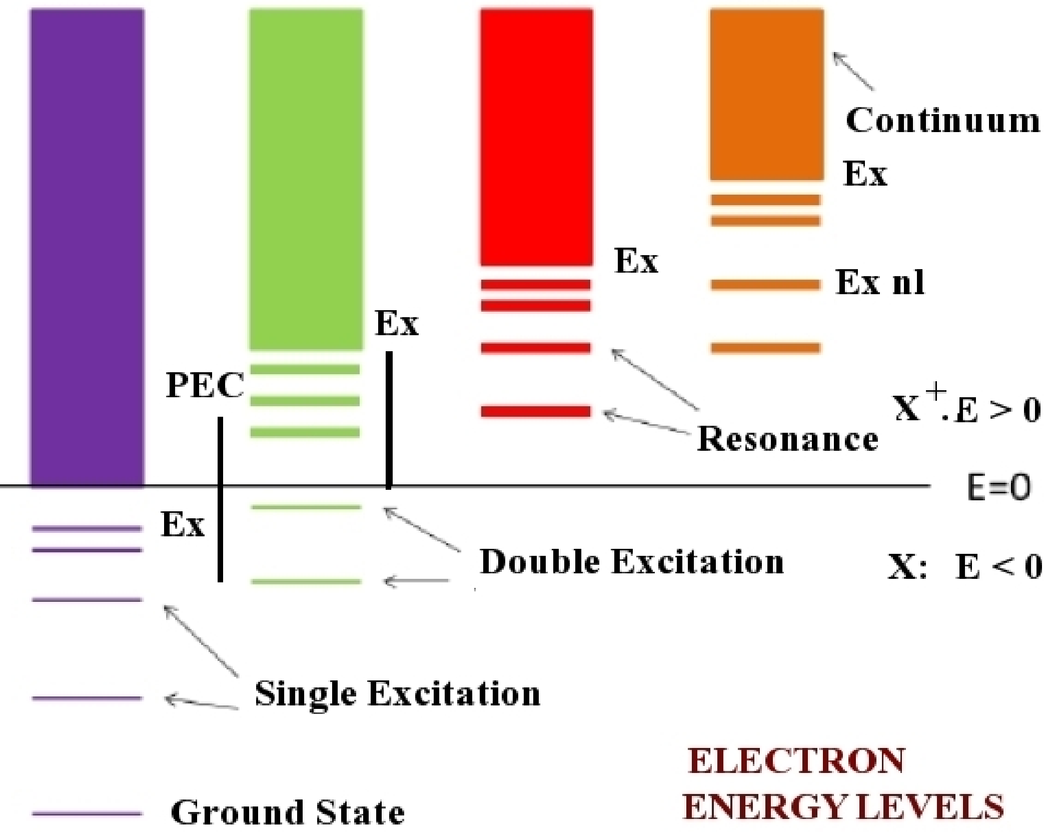
- Rydberg series of autoionizing states $(\mathbf{LS})_\mathbf{c}\nu\mathbf{l}$ lie above the ionization threshold & below an excited core state $(\mathbf{LS})_\mathbf{c}$
- Energy of the state is given by the Rydberg formula

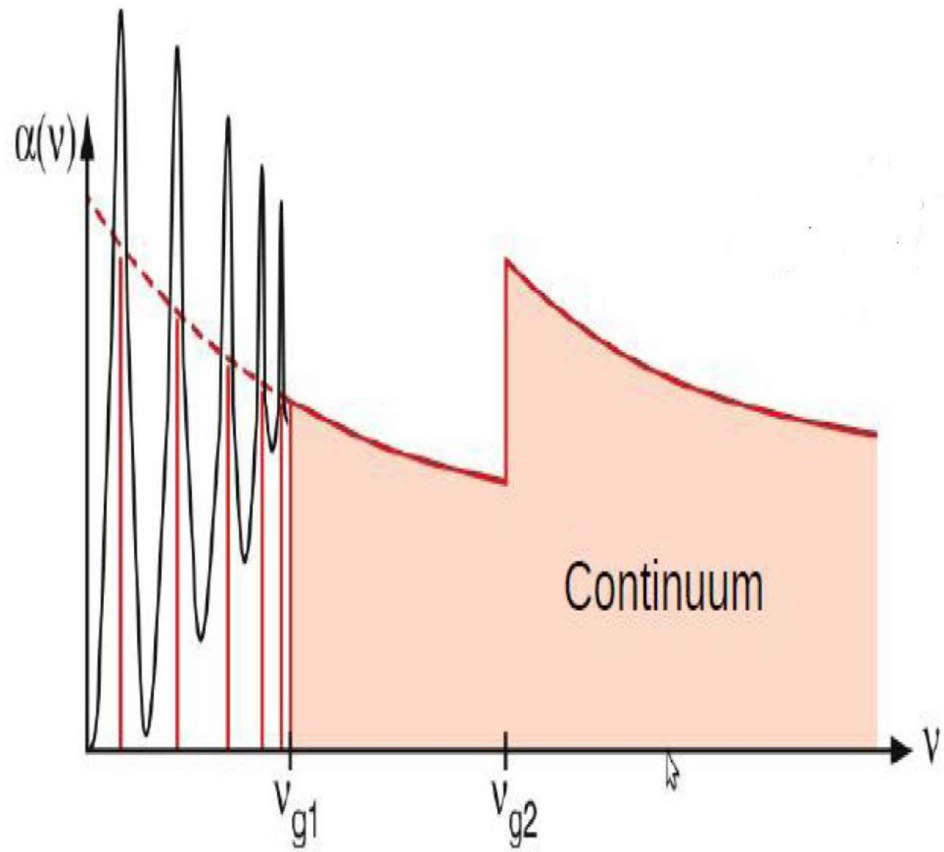
$$\mathbf{E}^{**}(\mathbf{X}^+\nu\mathbf{l}) = \mathbf{E}_{\mathbf{Res}} = \mathbf{E}_\mathbf{c} - \mathbf{z}^2/\nu^2$$

$\mathbf{E}_\mathbf{c} = \mathbf{E}^*(\mathbf{X}^+)$ = an excited threshold of the residual ion $\mathbf{X}^+$

- ν=effective quantum number, $\Delta\nu \sim 1$ for each series

Autoionizing States: RYDBERG & SEATON RESONANCES





Left: Autoionizing state: Electron at Rydberg states ($E_x nl > 0$)

$$E_x nl = E_{Res} = E^{**}(X^+ \nu l) = E_x - z^2/\nu^2$$

- PEC (Seaton) Resonance: $h\nu = Ex = Ei + Ee$
- **Right:** These introduce resonances in the continuum or smooth background of photoionization cross sections
- Details of resonances have been under investigation since the start of the Opacity Project (1987)

Close-Coupling (CC) Approximation: Produces Resonances

- CC approximation: Atomic system treated as a (N+1) electron system: - a target or an ion core of N electrons & an interating (N+1)th electron
- Total wavefunction expansion is:

$$\Psi_E(e + ion) = A \sum_i^N \chi_i(ion)\theta_i + \sum_j c_j \Phi_j(e + ion)$$

$\chi_i \rightarrow$ core wavefunction from atomic structure code
$\theta_i \rightarrow$ interacting electron wavefunction (free or bound)
$\Phi_j \rightarrow$ correlation functions of (e+ion)

- Complex resonances in the atomic processes are included via channel couplings (Not available in other approximation, e.g. DWBA)
- Substitution of $\Psi_E(e + ion)$ in

$$H\Psi_E = E\Psi_E$$

results in a set of coupled equations

- Coupled equations are solved by R-matrix method

Example: Close-Coupling Wave Function for O II

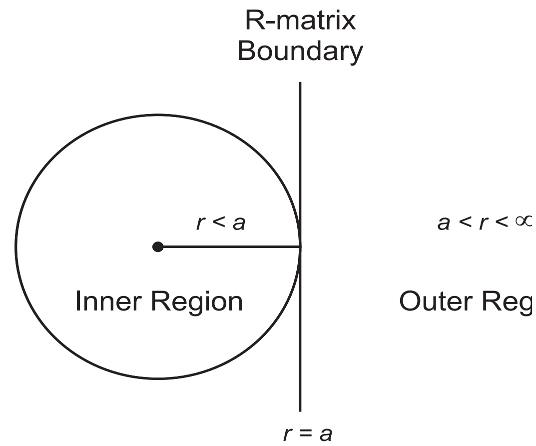
$$\Psi_E(e+\mathrm{ion}) = A\sum_{i}^{N}\chi_i(\mathrm{ion})\theta_i + \sum_{j} c_j\Phi_j(e+\mathrm{ion})$$

χ_i → **core ion wavefunction - obtained from SUPERSTRUCTuRE,**

	Level	J_t	E_t(Ry,NIST) NIST	E_t(Ry,SS) SS
1	$1s^2 2s^2 2p^2 (^3P)$	0	0.0	0.
2	$1s^2 2s^2 2p^2 (^3P)$	1	0.0010334	0.0011497
3	$1s^2 2s^2 2p^2 (^3P)$	2	0.0027958	0.003384
4	$1s^2 2s^2 2p^2 (^1D)$	2	0.18472	0.21215
5	$1s^2 2s^2 2p^2 (^1S)$	2	0.39352	0.38420
6	$1s^2 2s 2p^3 (^5S^o)$	2	0.54972	0.46200
7	$1s^2 2s 2p^3 (^3D^o)$	3	1.0938	1.12584
8	$1s^2 2s 2p^3 (^3D^o)$	2	1.0940	1.12576
9	$1s^2 2s 2p^3 (^3D^o)$	1	1.0941	1.12573
10	$1s^2 2s 2p^3 (^3P^o)$	2	1.2975	1.32510
11	$1s^2 2s 2p^3 (^3P^o)$	1	1.2975	1.32500
12	$1s^2 2s 2p^3 (^3P^o)$	0	1.2976	1.32495
13	$1s^2 2s 2p^3 (^1D^o)$	2	1.7045	1.83934
14	$1s^2 2s 2p^3 (^3S^o)$	1	1.7960	1.89708
15	$1s^2 2s 2p^3 (^1P^o)$	1	1.9178	2.02463
16	$1s^2 2s 2p 3s (^3P^o)$	0	2.4354	2.33186
17	$1s^2 2s 2p 3s (^3P^o)$	1	2.4365	2.33300
18	$1s^2 2s 2p 3s (^3P^o)$	2	2.4388	2.33186
19	$1s^2 2s 2p 3s (^1P^o)$	1	2.4885	2.40908

R-MATRIX METHOD

Substitution of CC $\Psi_E(e+ion)$ in $H\Psi_E = E\Psi_E$ introduces a set of coupled equations which are solved by the R-matrix method



• Divide the space in two regions, the inner and the outer regions, of a sphere of radius r_a
• r_a is large enough for to include electron-electron interaction potential. Wavefunction at $r > r_a$ is Coulombic due to perturbation
• In the inner region, the radial part $F_i(r)/r$ of the outer electron wave function (θ) is expanded in terms of a basis set, called the R-matrix basis,

$$F_i = \sum a_k u_k$$

which satisfies

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + V(r) + \epsilon_{lk}\right] u_{lk} + \sum_n \lambda_{nlk} P_{nl}(r) = 0.$$

& is made continuous with Coulomb functions outside r_a

RELETIVISTIC BREIT-PAULI R-MATRIX (BPRM) METHOD

- **Breit-Pauli Hamiltonian (applies for a nulti-electron system in contrast o single electron Dirac equation) is**

$$\mathbf{H}_{\mathrm{BP}} = \mathbf{H}_{\mathbf{NR}} + \mathbf{H}_{\mathrm{mass}} + \mathbf{H}_{\mathrm{Dar}} + \mathbf{H}_{\mathrm{so}} +$$

and parts of two body interaction terms.
Solve Schrodinger equation with CC expansion

$$\mathbf{H}_{\mathbf{BP}}\Psi = E\Psi$$

- **E $< 0 \rightarrow$ Bound (e+ion) states $\mathbf{\Psi_B}$**
- **E $\geq 0 \rightarrow$ Continuum states $\mathbf{\Psi_F}$**
- **Advantage of CC approximation $\rightarrow$ both +ve & -ve solutions**

The objective of the series "R-matrix calculations for opacities" is to provide high accuracy opacities obtained using the high accuracy atomic data.
• The R-matrix method is the most powerful method to obtain high accuracy parameters for the two main radiative atomic processes of photo-absorption or opacities:
i) Photo-excitation,
ii) Photo-ionization
• Relativistic Breit-Pauli R-matrix (BPRM) method implements close-coupling (CC) wavefunction expansion that generates very large number oscillator strengths for transitions and resonances in photoionization
• It can accommodate interactions of a large number of configurations that is not possible for an atomic structure calculation. This results in large Hamiltonian matrix, transition matrix elements.
• Hence, solving the Hamiltonian matrix with coupled channels becomes complex and extensive for numerical computation.
Role of R-matrix codes
• For practicability, but still producing largest sets of atomic data, R-matrix method adopts typically to compute

ELECTRON-IMPACT EXCITATION (EIE)

$$e + X^{+Z} \rightarrow e' + X^{+Z*} \rightarrow e' + X^{+Z} + h\nu$$

- **Light is emitted as the excitation decays**

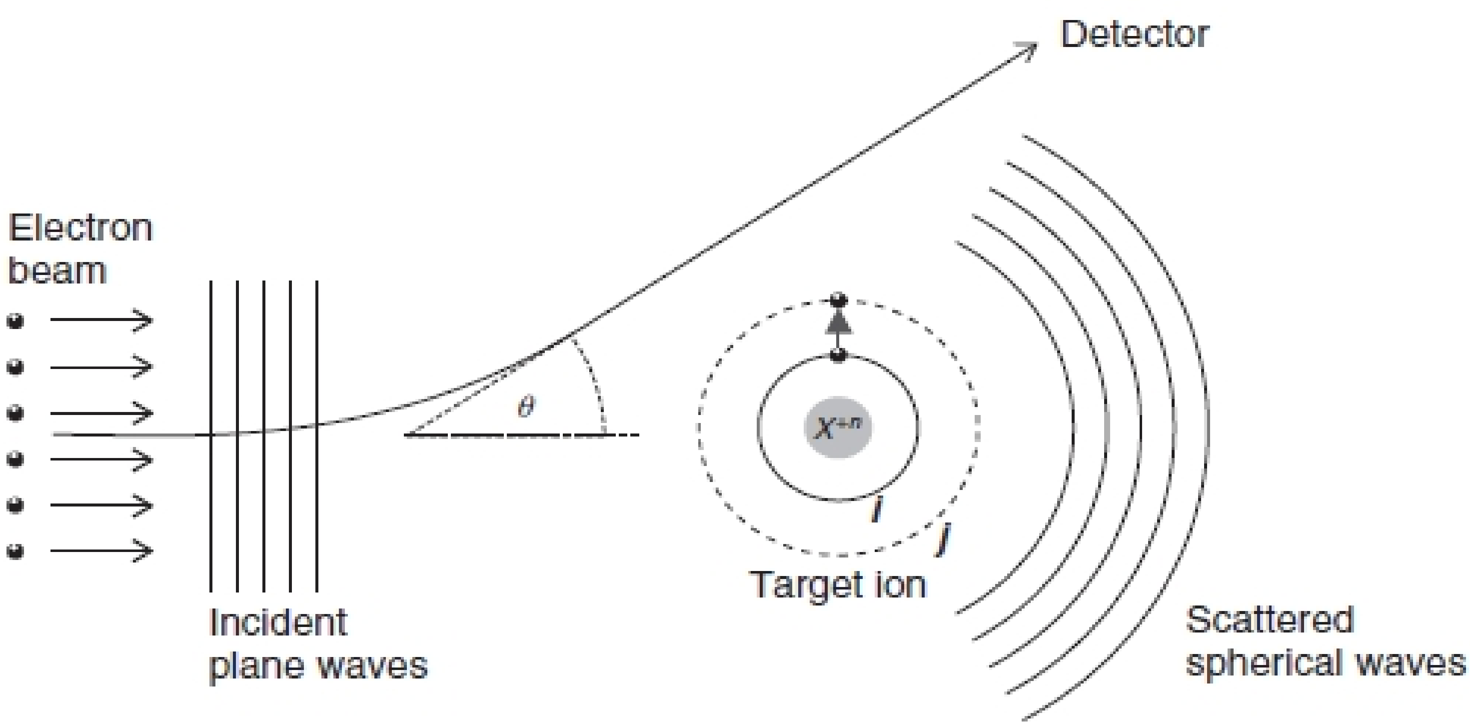
- seen as most common lines in astrophysical spectra

- mostly diagnostic forbidden lines

- **Scattered electron shows features with energy & can have autoionizing resonances**

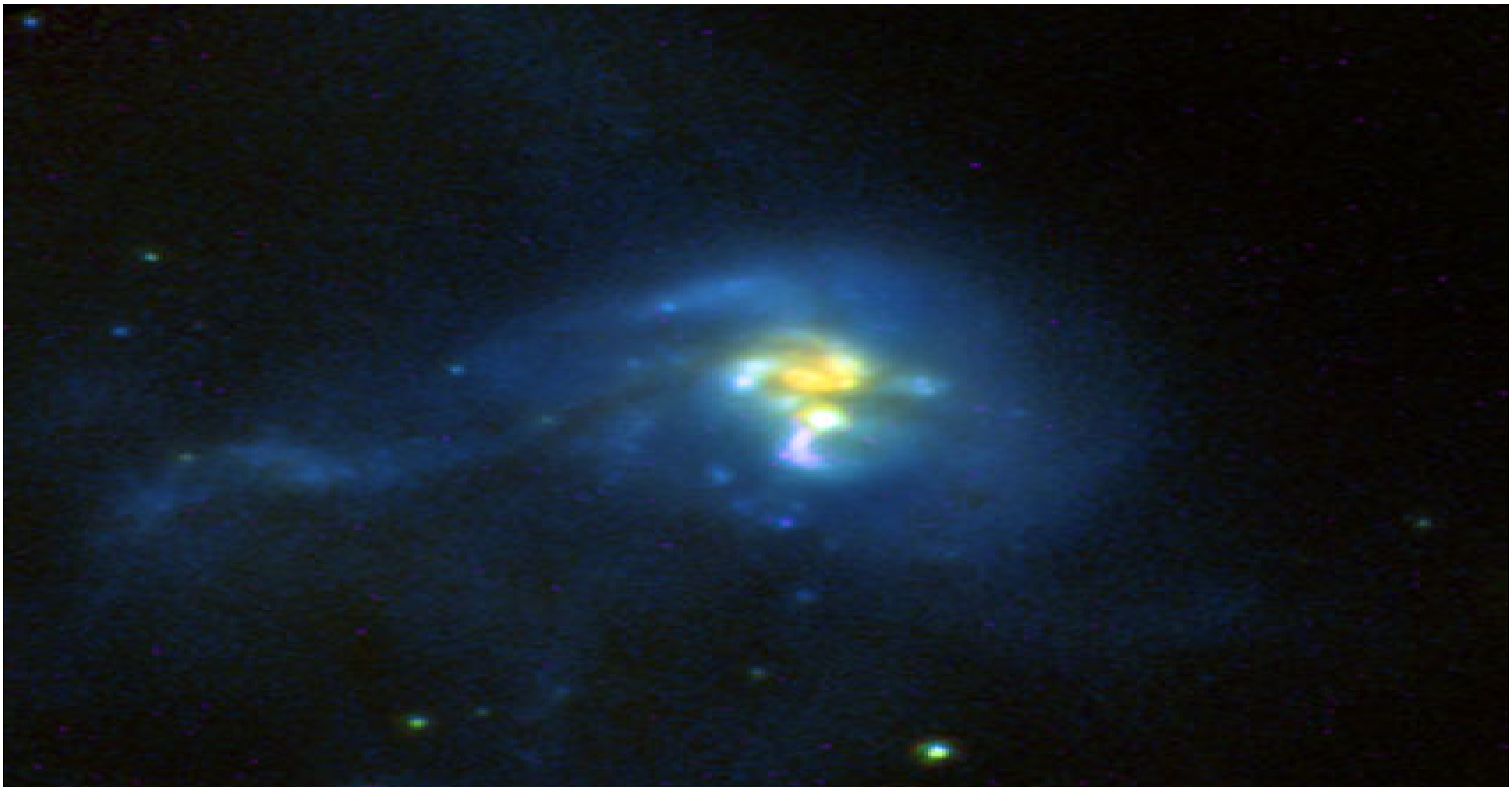
- **Atomic quantity: *Collision Strength (Ω)***

Fig. Excitation by electron impact:



ULTRA-LUMINOUS INFRA-RED GALAXY (ULIRG) IRAS-19297-0406: STUDY THROUGH FORBIDDEN LINES

- ULIRG - emits more than 10^{11} solar luminosities in IR (as stars are born), heavily dust obscured
- Only far-infrared photons (e.g. forbidden lines of Ne V) escape from absorption, observed at high redshift (by SPITZER, HERSCHEL, SOFIA) - provides information on chemical evolution of the galaxy.
- Ne V lines are observed in ULIRG



ELECTRON IMPACT EXCITATION (EIE)

• EIE Scattering matrix $\mathbf{S}_{SL\pi}(i,j)$ is obtained from the excitation transition matrix. The EIE collision strength is

$$\Omega(\mathrm{S_iL_i} - \mathrm{S_jL_j}) = \frac{1}{2}\sum_{\mathrm{SL}\pi}\sum_{\mathrm{l_il_j}}(2\mathrm{S}+1)(2\mathrm{L}+1)|\mathrm{S}_{\mathrm{SL}\pi}(\mathrm{S_iL_il_i} - \mathrm{S_jL_jl_j})|^2$$

Ω is a dimensionless quantity, introduced by Seaton. It does not diverge like the cross section, σ_{EIE} at origin,

$$\sigma_{\mathrm{EIE}} = \frac{\pi}{\mathrm{g_i k^2}}\Omega \mathrm{a_o^2},$$

• The quantity used in models is effective collision strength $\Upsilon(\mathrm{T})$, the Maxwellian averaged collision strength:

$$\Upsilon(\mathrm{T}) = \int_0^\infty \Omega_{\mathrm{ij}}(\epsilon_{\mathrm{j}})\mathrm{e}^{-\epsilon_{\mathrm{j}}/\mathrm{kT}}\mathrm{d}(\epsilon_{\mathrm{j}}/\mathrm{kT})$$

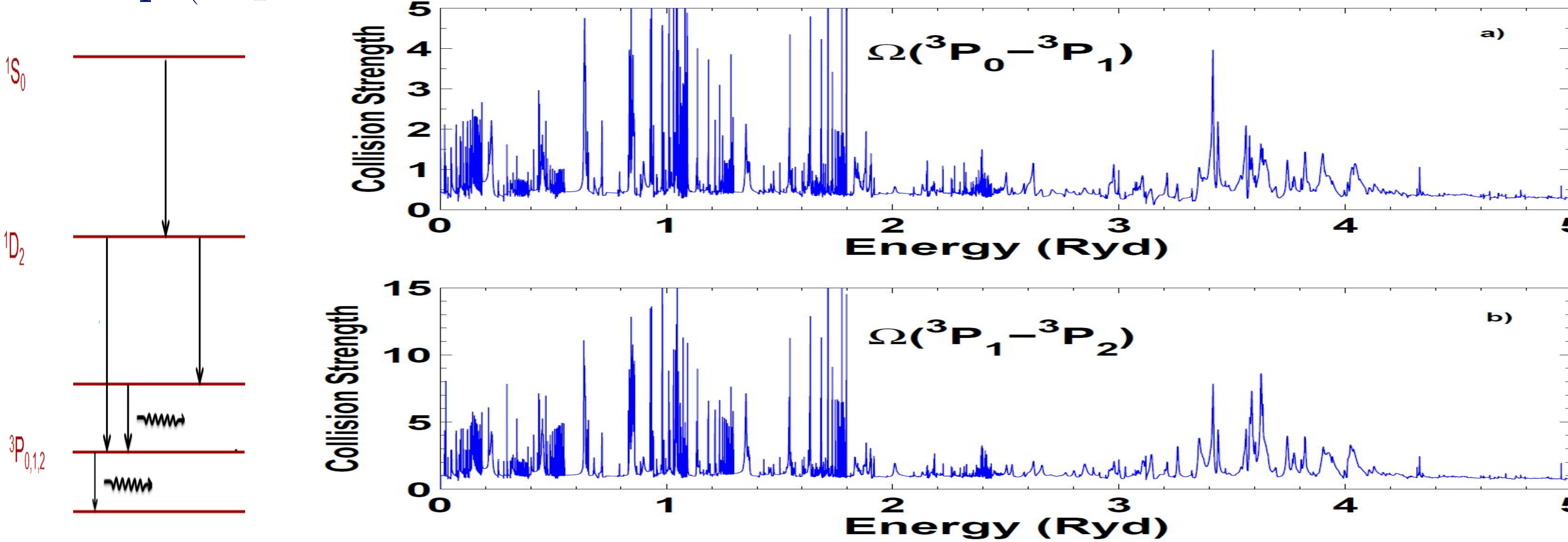
• The excitation rate coefficient $\mathrm{q_{ij}(T)}$ is given by

$$\mathrm{q_{ij}(T)} = \frac{8.63\times 10^{-6}}{\mathrm{g_i T^{1/2}}}\mathrm{e}^{-\mathrm{E_{ij}/kT}}\Upsilon(\mathrm{T})\ \mathrm{cm^3 s^{-1}}$$

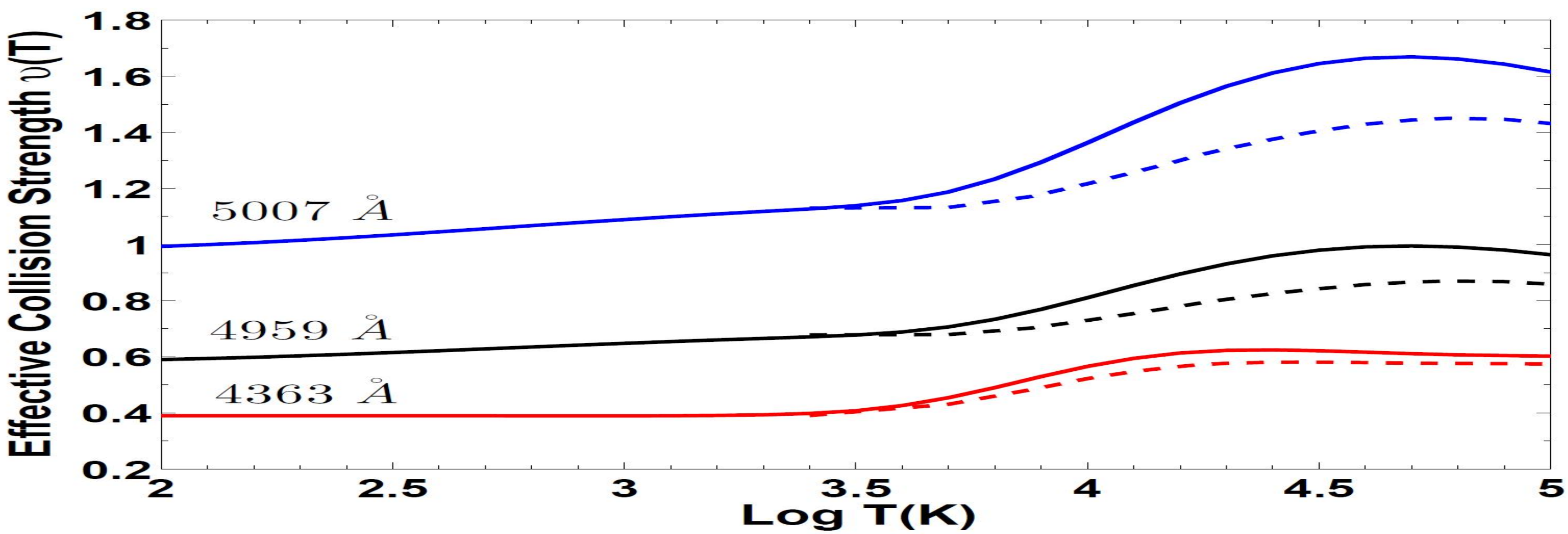
$\mathrm{E_{ij} = E_j - E_i}$ in Ry, T in K,$(1/\mathrm{kT} = 157885/\mathrm{T})$

EIE OF O III (Palay et al 2012)

- **Fig** Resonances in Ω (EIE): Top: $2p^2(^3P_0 - ^3P_1)$ $(88\mu m)$, Bottom: $2p^2(^3P_1 - ^3P_2)$ $(52\mu m)$ -IR)



- **Fig** $\Gamma(T)$ of 3 optical lines; Solid: BPRM (present), Dashed: R-matrix(LS) (Aggarwal & Keenan) Differences affect T and ρ



LINE RATIO DIAGNOSTICS

- **Collisionally Excited Lines (CEL):**

$$\mathbf{e} + \mathbf{X}^+ \rightarrow \mathbf{X}^{+*} \rightarrow \mathbf{X}^+ + \mathbf{h}\nu$$

- **The intensity of a CEL due to transition between *a* & *b***

$$\mathbf{I_{ba}}(\mathbf{X}^+, \lambda_{\mathbf{ba}}) = \frac{\mathbf{h}\nu}{4\pi}\mathbf{n_e n_{ion} q_{ba}}$$

$\mathbf{q_{ba}}$ **- EIE rate coefficient in cm^3/sec.**

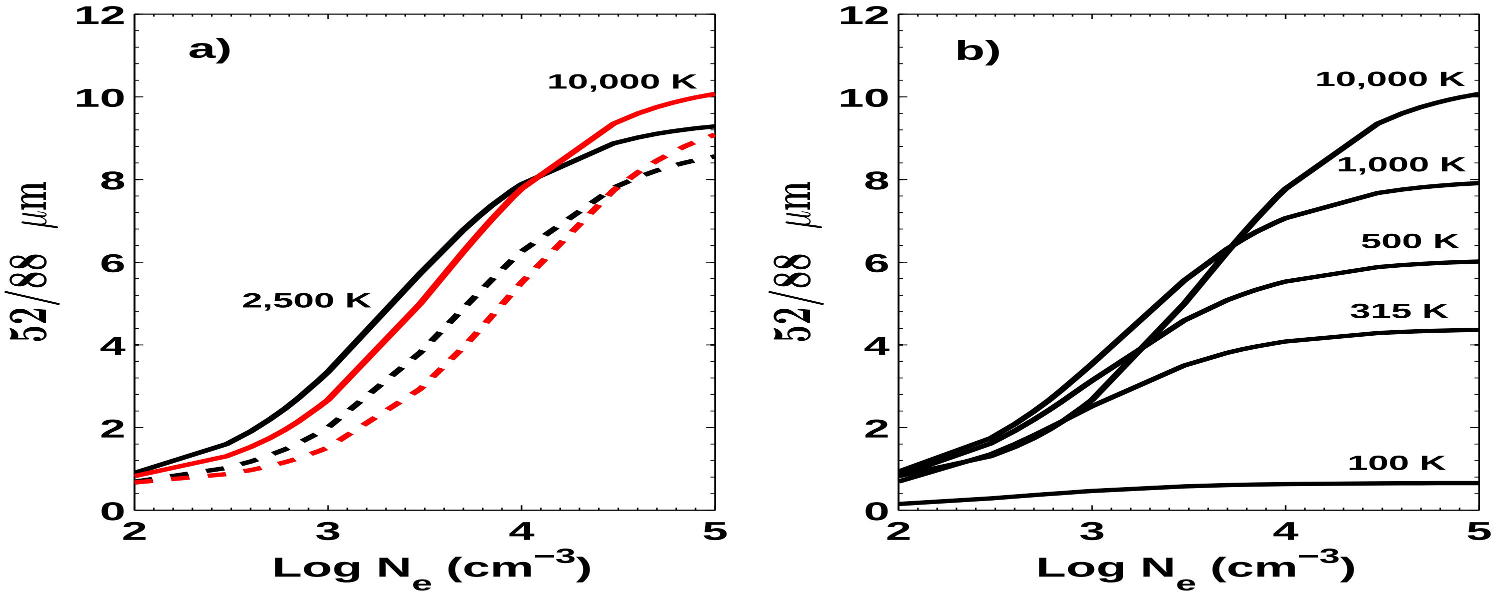
- **The ratio of intensities, mainly the emissivity ratio, of two different lines arising from the same level can be used for temperature and density diagnostics.**
- **The ratio depends on the level populations.**
- **Level populations depend on excitation rate coefficients and electron density.**

$$\frac{\mathbf{I_{ji}}(\lambda_{\mathbf{ji}})}{\mathbf{I_{lk}}(\lambda_{\mathbf{lk}})} = \frac{\nu_{\mathbf{ji}}\mathbf{n'_{ion}}}{\nu_{\mathbf{lk}}\mathbf{n''_{ion}}}\frac{\mathbf{q_{ji}}}{\mathbf{q_{lk}}}$$

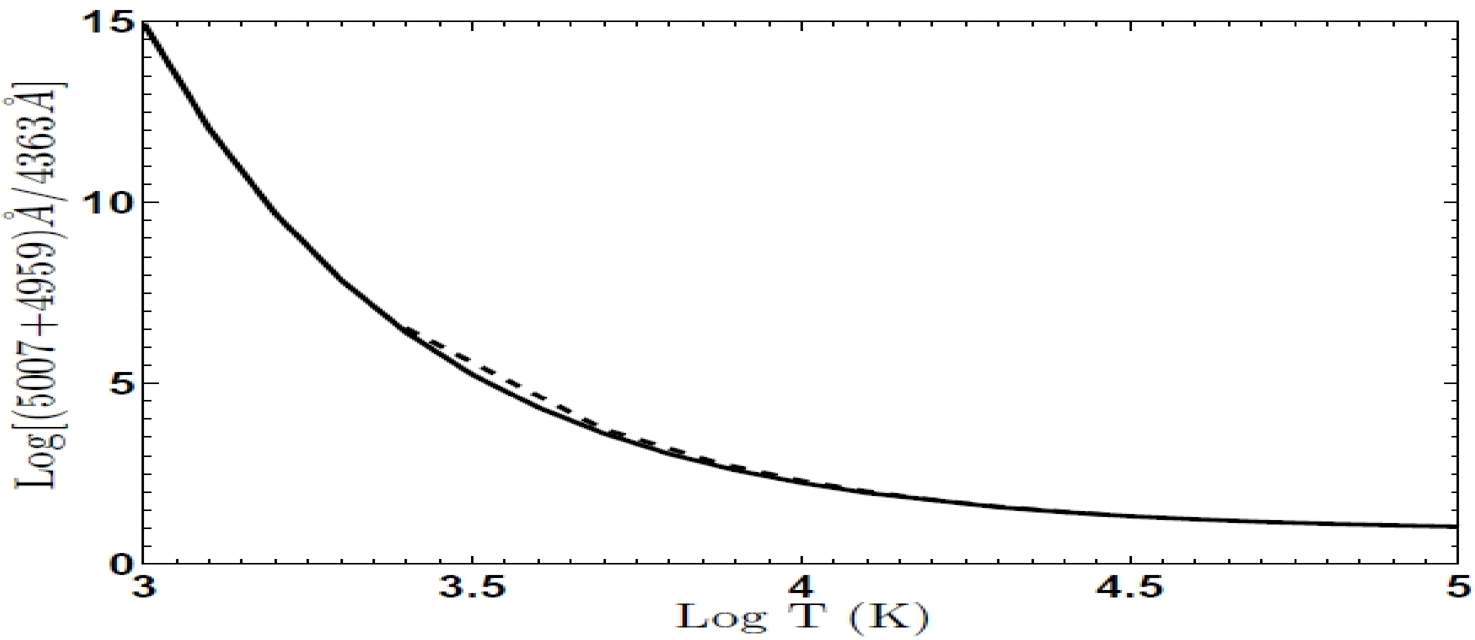
The density or T are varied for the line ratios to carry out the diagnostics of plasmas.

LINE RATIO: DENSITY ρ & T DIAGNOSTICS (Palay et al 2012)

- Intensity ratio of two observed lines can be compared to the calculated curves for density (ρ) & T diagnostics. Significant FS effect on ρ diagnostics, 100 - 10,000 K

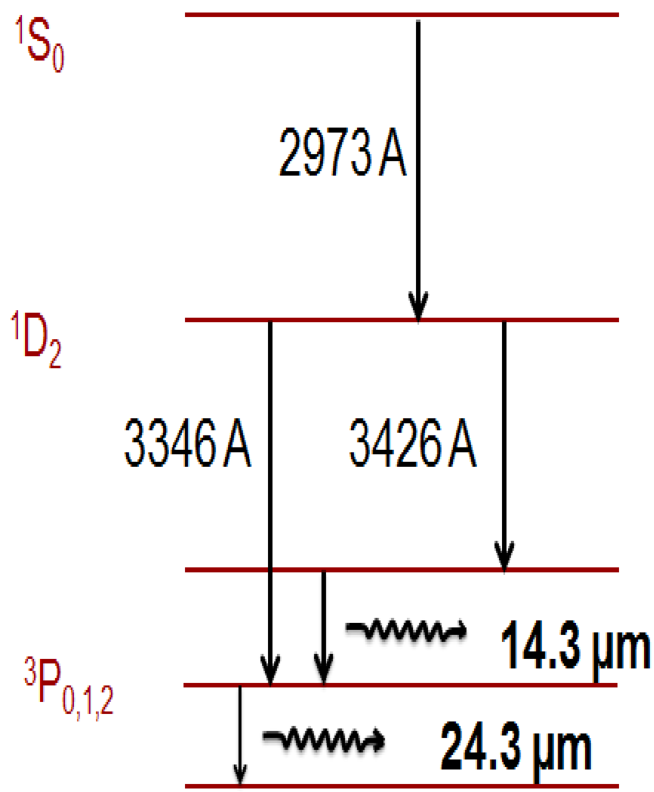


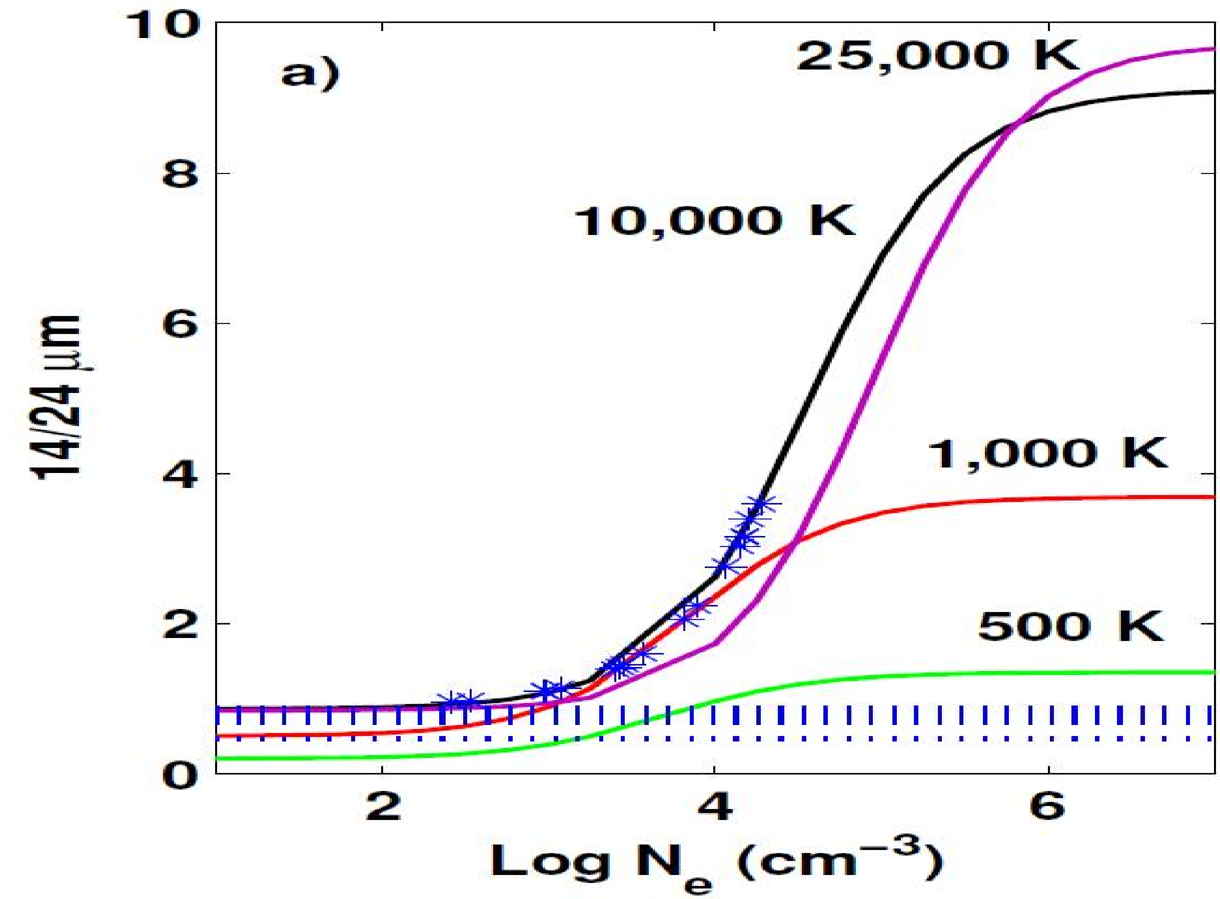
Blended line ratio with T at $N_e = 10^3 cm^{-3}$ indicates considerable rise in low T region



EIE: LINE RATIOS OF Ne V (Dance et al 2010)

• The intensity of a CEL of ion X_i: $\mathbf{I_{ba}(X_i, \lambda_{ba}) = \left[\frac{h\nu}{4\pi} n_e n_{ion}\right] q_{ba}}$





• **Comparison:** IR 14/24 μm line emissivity ratios: a) Present curves (solid) at different T, Asterisks (observed from PNe at T = 10,000 K with assigned densities, Rubin 2004), Dotted curves (observed line ratios, outside typical nebular T-ρ range except at low T, Rubin 2004),

• Better agreement at T = 10,000 (10 PNe) and 500 K (anomalously low, 11 PNe)

DETERMINATION OF ELEMENTAL ABUNDANCES

From the intensity of a line

$$\mathbf{I_{ba}(X^+, \lambda_{ba}) = \frac{h\nu}{4\pi} n_e n_{ion} q_{ba}}$$

population of a level b can be written as

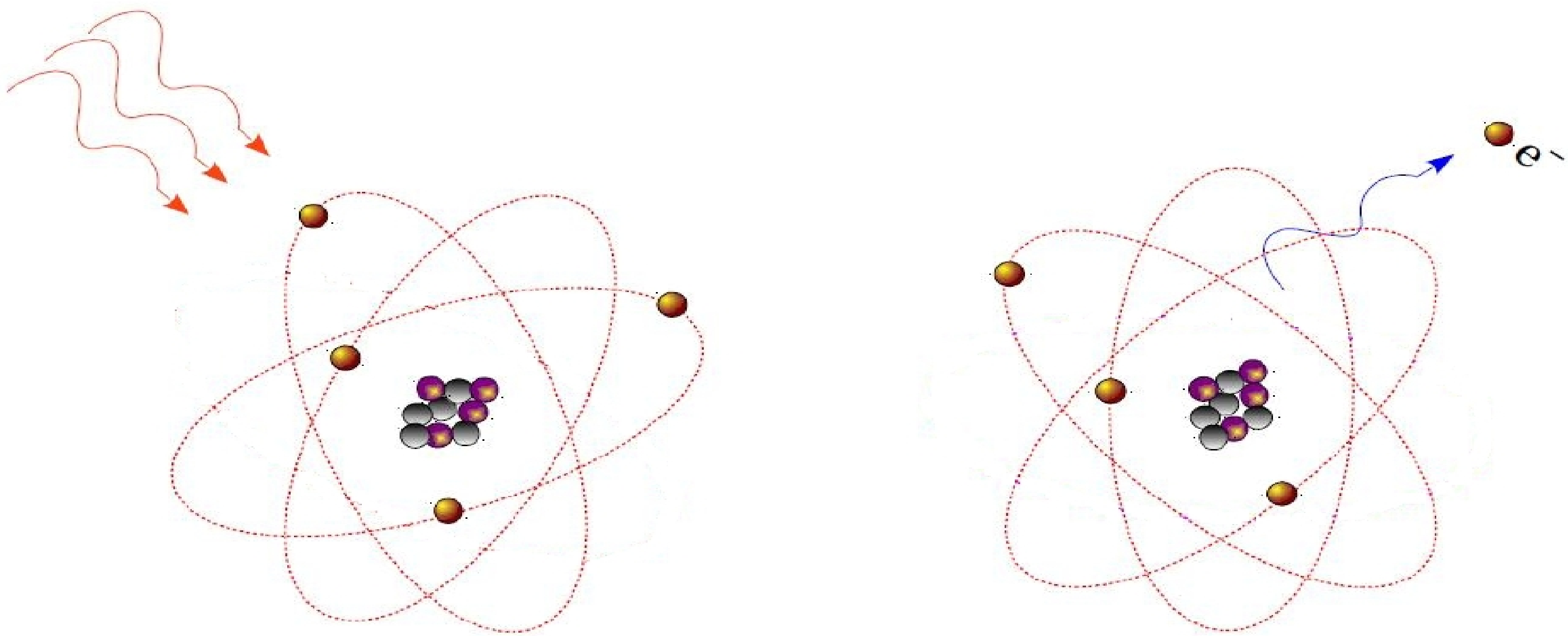
$$\mathbf{N(b) = n_{ion} q_{ba} = \frac{1}{n_e} \frac{4\pi}{h\nu} I_{ba}}$$

Abundance of element X w.r.t. H, $\mathbf{n(X)/n(H)}$, can be obtained from the intensity I of a collisional exited line of wavelength λ_{ba} from its ionization state X_i using several quantities. as

$$\mathbf{I(X^+, \lambda_{ba}) = \frac{h\nu}{4\pi} A_{ba} \frac{N(b)}{\sum_j N_j(X^+)} \frac{n(X^+)}{n(X)} \left[\frac{n(X)}{n(H)}\right] n(H)}$$

$\mathbf{A_{ba}}$ = radiative decay rate, $\mathbf{\sum_j N_j}$ = total populations of all excited levels, $\mathbf{N(b)/\sum_j N_j(X^+)}$ = population fraction, $\mathbf{\frac{n(X^+)}{n(X)}}$ - ionization fraction (from photoionization model)

PHOTOIONIZATION (PI):



i) Direct Photoionization (background):

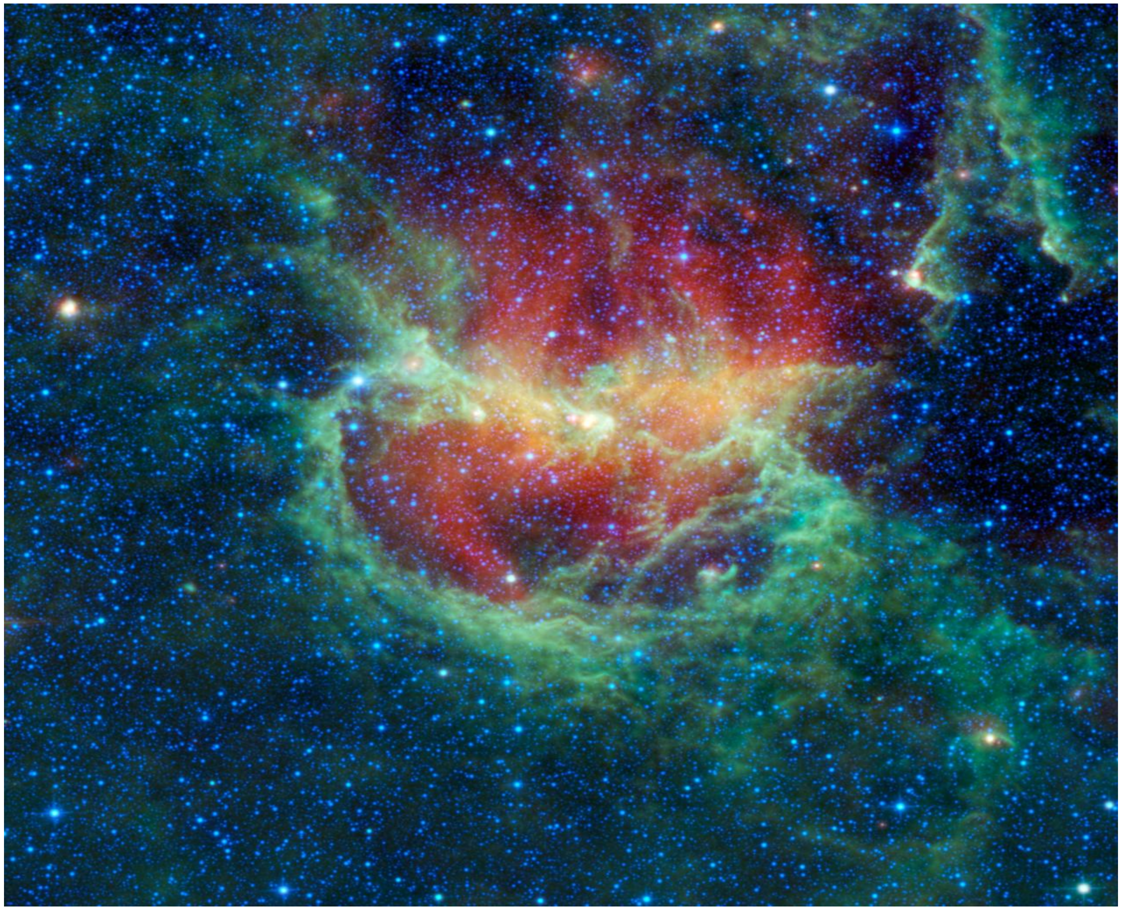
$$\mathbf{X^{+Z}} + \mathbf{h}\nu \rightleftharpoons \mathbf{X^{+Z+1}} + \epsilon$$

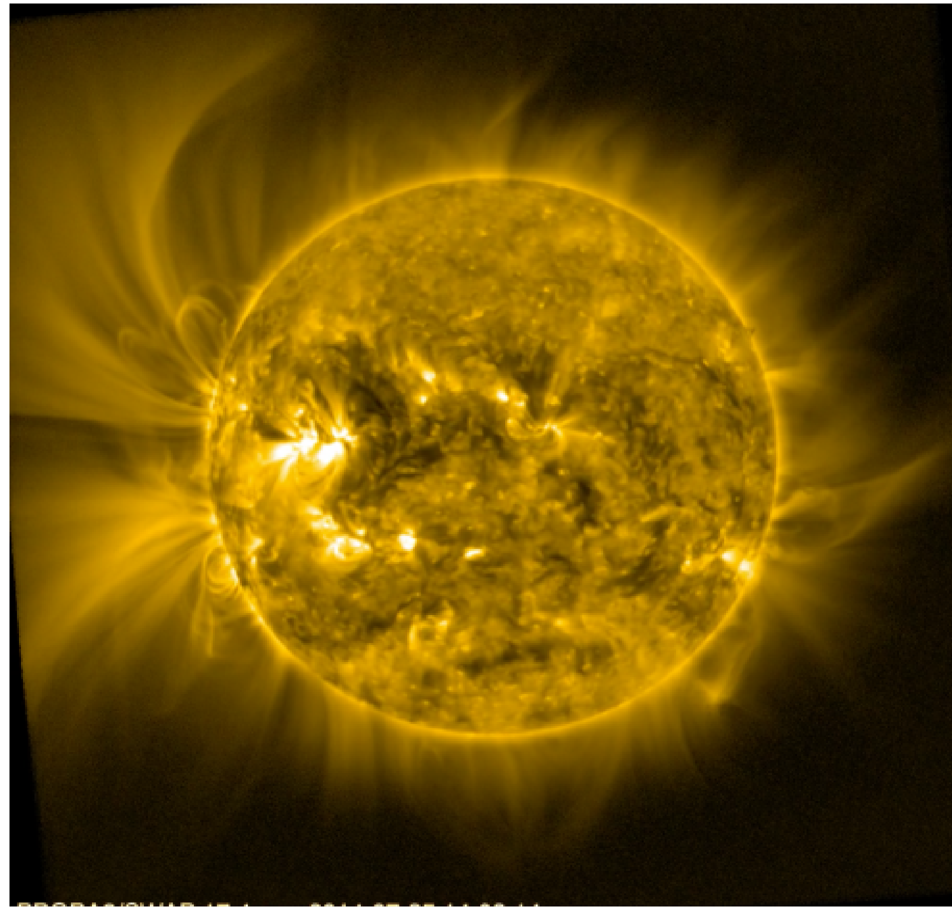
ii) Resonant Photoionization: an intermediate state before ionization → "Autoionizing state" → RESONANCE

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

- **Autoionizing states form in nature all the time and hence require to be treated in the calculations.**

PHOTOIONIZED PLASMAS





- Photoionization occurs with any light source
- L: Lambda Centauri nebula with radiation sources of stars, R: Solar corona
- Ionization fractions in plasmas at photoionization equilibrium is obtained from equation of balance:

$$\mathbf{N}(\mathbf{z})\int_{\nu_0}^{\infty}\frac{4\pi \mathbf{J}_\nu}{\mathbf{h}\nu}\sigma_{\mathbf{PI}}(\mathbf{z},\nu)\mathbf{d}\nu = \mathbf{N_e}\mathbf{N}(\mathbf{z}+\mathbf{1})\alpha_{\mathbf{RC}}(\mathbf{T_e})$$

where $\sigma_{\mathbf{PI}}(\mathbf{z},\nu)$ is photoionization cross sections

PHOTOIONIZATION (PI) CROSS SECTIONS

Radiative Transition Matrix:

Transition Matrix elements with a Photon

$< \Psi_B||D||\Psi_F >$ **Dipole operator:** $\mathbf{D} = \sum_i \mathbf{r}_i$

- Selection rules (E1-dipole) for photoionization,

$$\begin{aligned} \Delta l &= l_j - l_i = \pm 1, \Delta L = L_j - L_i = 0, \pm 1, \\ \Delta M &= M_{L_j} - M_{L_i} = 0, \pm 1 \\ \Delta J &= J_j - J_i = 0, \pm 1; \text{ Parity changes} \end{aligned} \quad (1)$$

- Ex: $\mathbf{np} \to \epsilon\mathbf{s}, \epsilon\mathbf{d}, \ ^3\mathbf{P} \to ^3\mathbf{S^o}, ^3\mathbf{P^o}, ^3\mathbf{D^o}$

Matrix element is reduced to generalized line strength

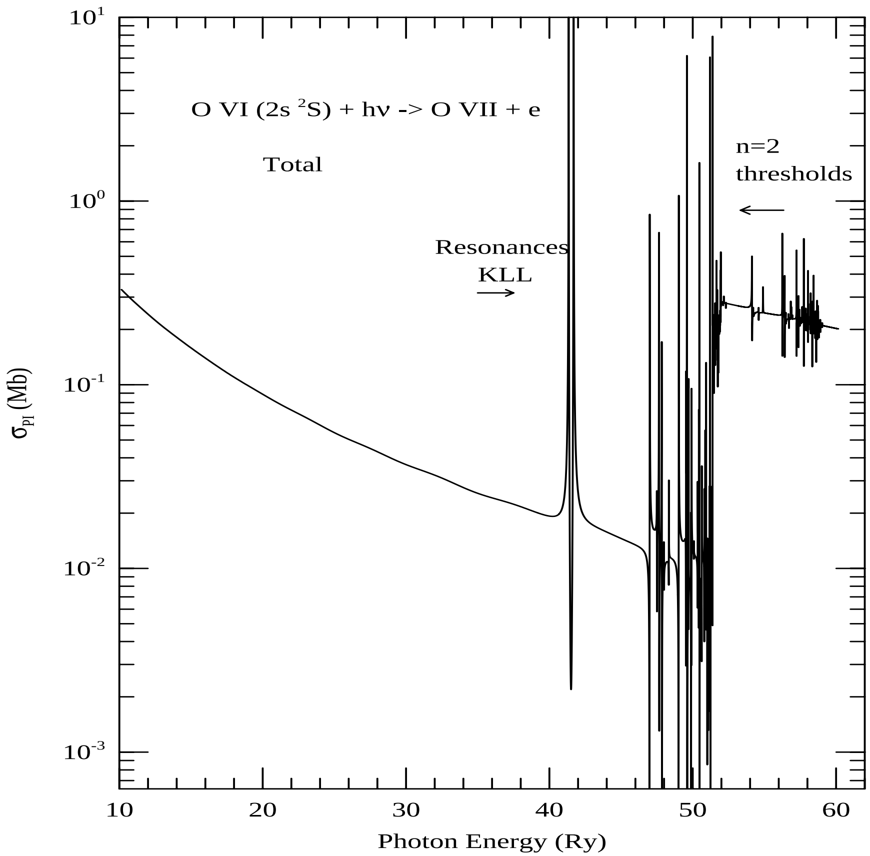
$$\mathbf{S} = | < \Psi_j||\mathbf{D}||\Psi_i > |^2 = \left| \left\langle \Psi_f | \sum_{j=1}^{N+1} \mathbf{r}_j | \Psi_i \right\rangle \right|^2$$

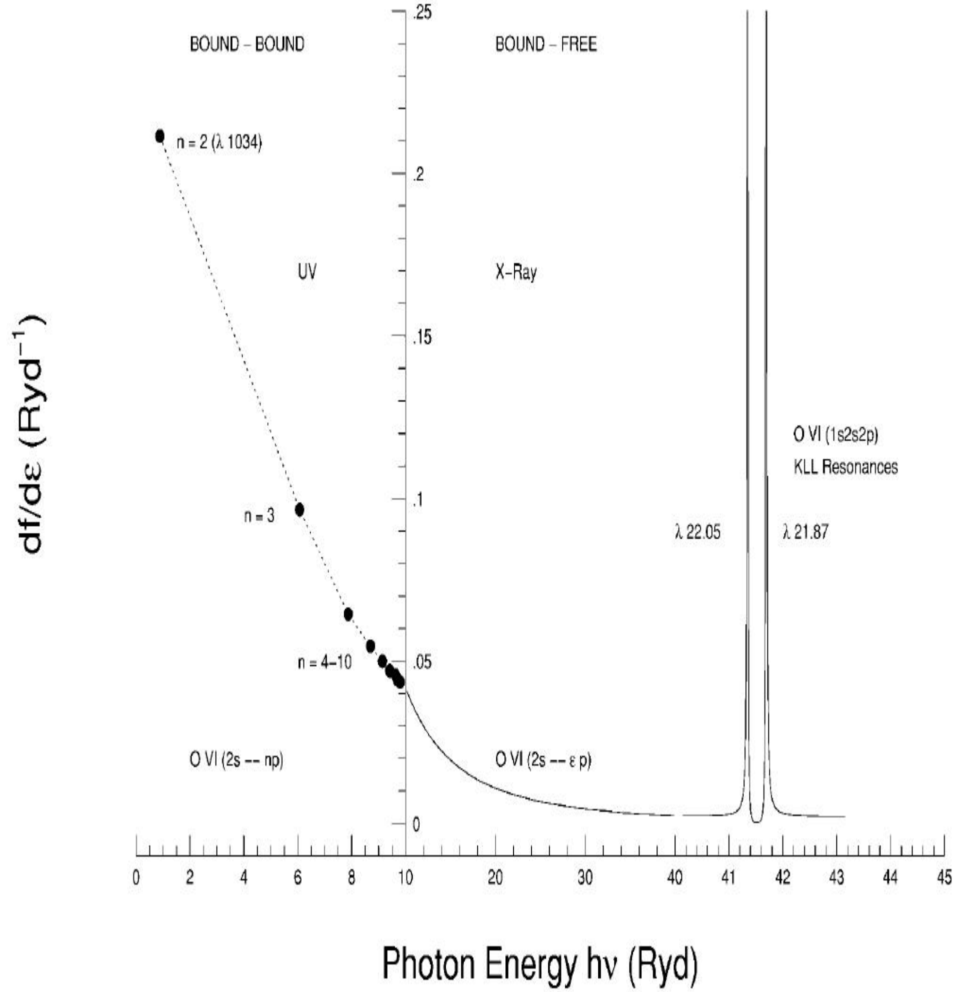
Photoionization: The cross section is

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

$\omega \to$ **incident photon energy in Rydberg unit**

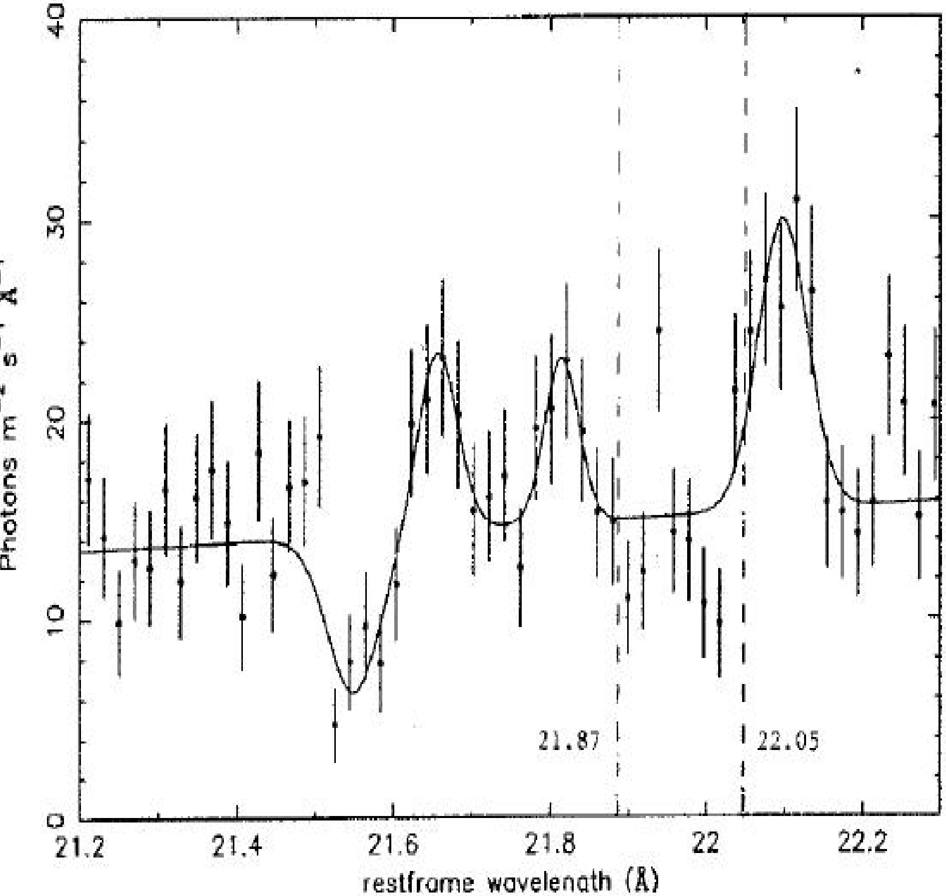
PHOTOIONIZATION RESONANCE CAN BE SEEN IN ABSORPTION SPECTRUM

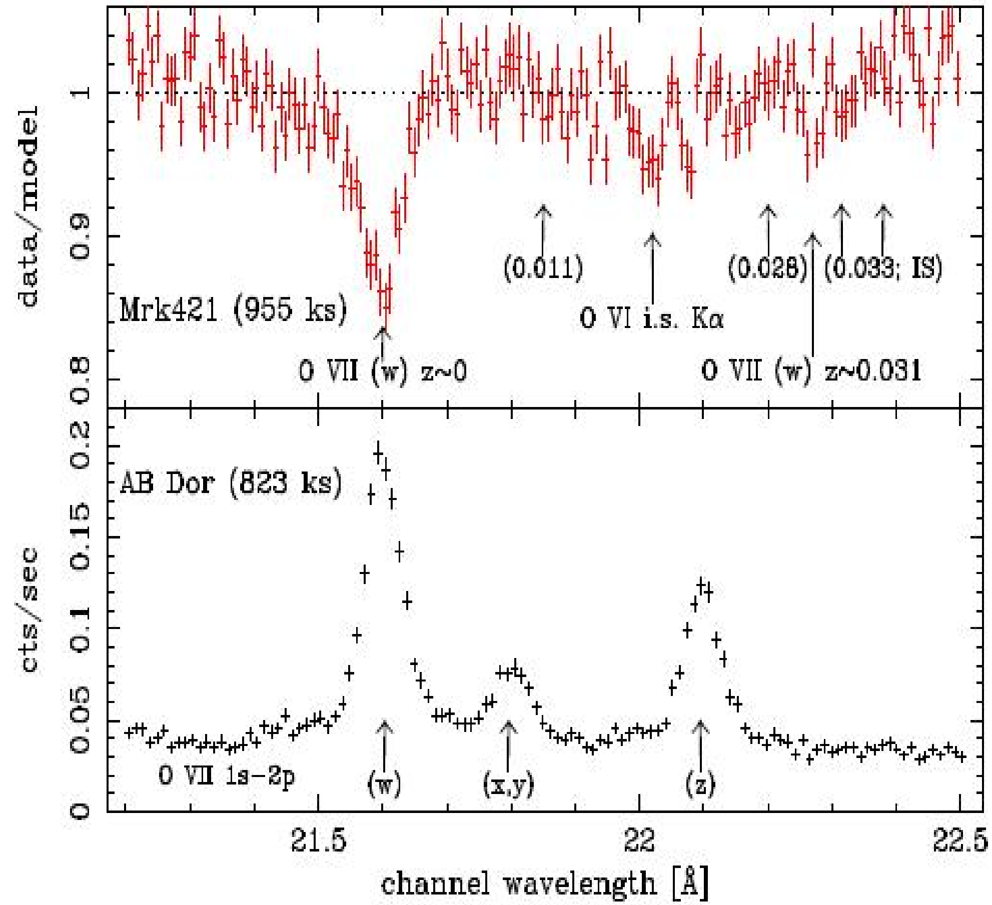




L) KLL ($1s^22s - 1s2s2p$) or Kα resonances in photoionization of Li-like O VI (Nahar 1998).
R) Pradhan (2000) calculated the resonant oscillator strength and predicted the presence of the absorption KLL lines at 22.05 and 21.87 $\AA$ between the two emission lines i and f of He-like O VII at 21.80 and 22.01 $\AA$

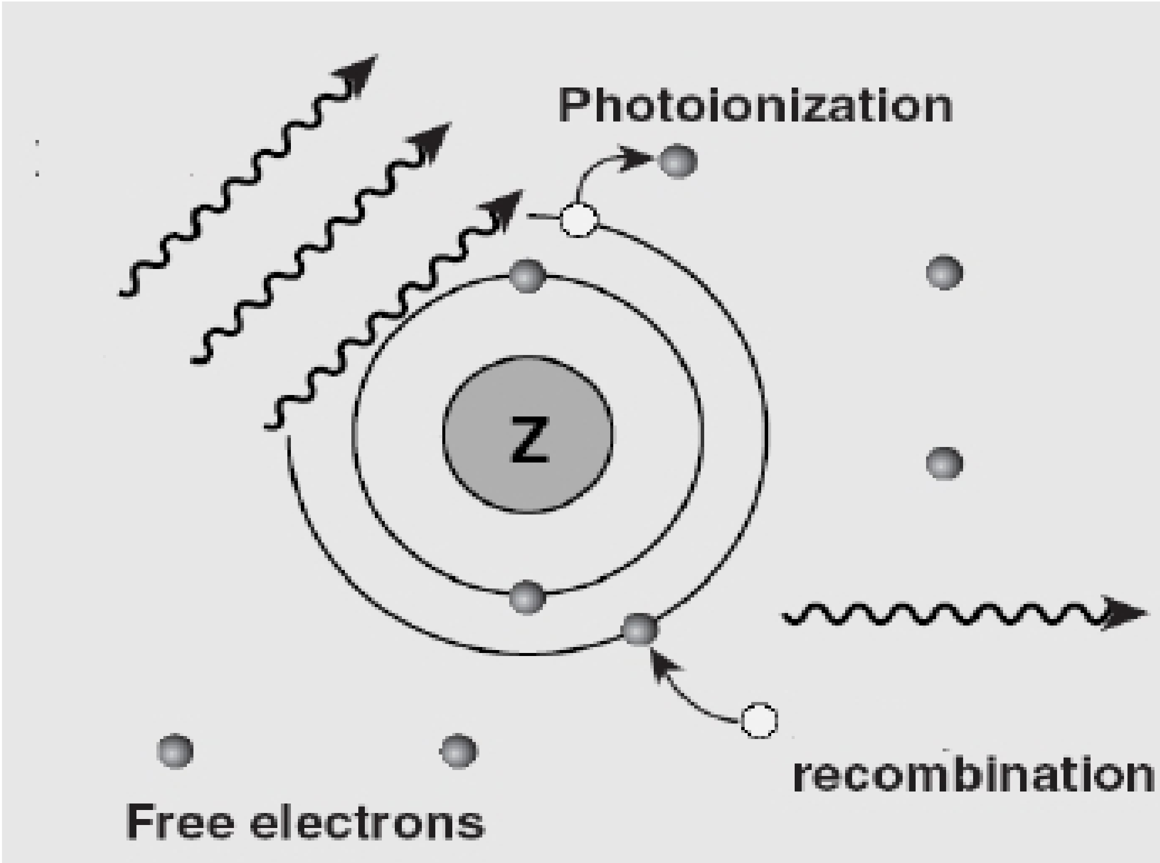
PHOTOIONIZATION RESONANCE SEEN IN ABSORPTION SPECTRUM (Seen for the first time under the OP)





L) Pradhan (APJL 2000) identified the O VI absorption lines in between the two x-ray emission lines of O VII in the spectra of Seyfert galaxy NGC5548 (Kastra et al 2000).
R) These lines were later detected in the X-ray spectra of Mrk 421 observed by XMM-Newton (Rasmussen et al 2007) and led to estimation of oxygen abundance

PHOTOIONIZATION (PI) & ELECTRON-ION RECOMBINATION



i) Photoionization (PI) & Radiative Recombination (RR):

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

ii) Indirect PI & Dielectronic Recombination (DR) with intermediate autoionizing state → RESONANCE:

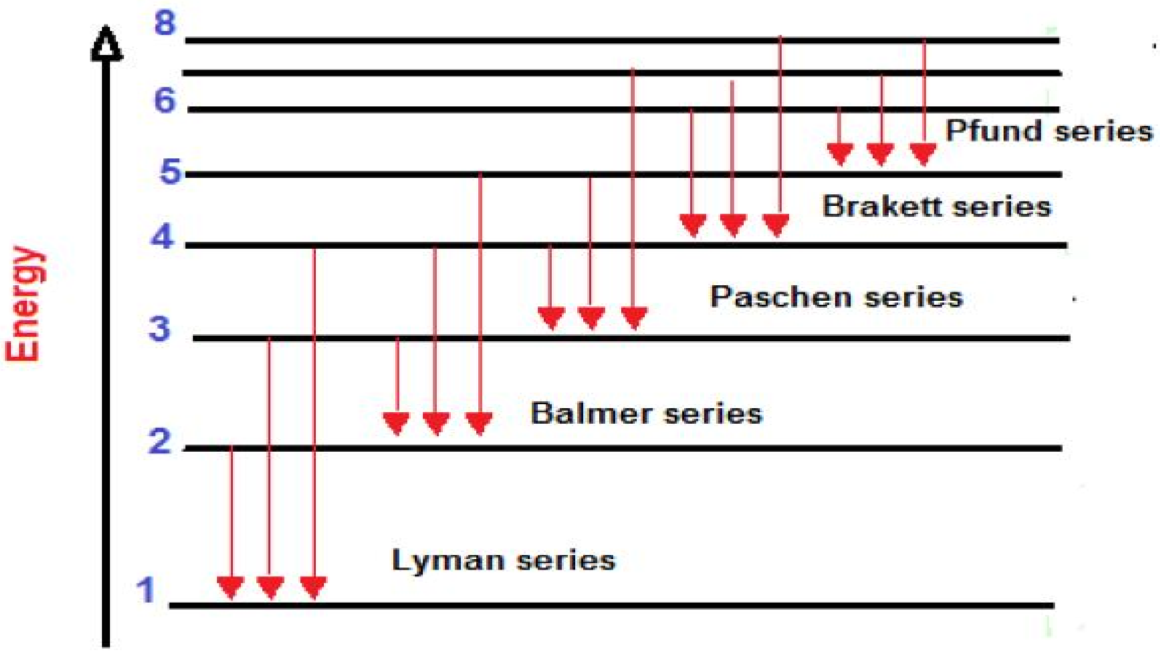
$$\mathbf{X^{+Z} + h\nu \rightleftharpoons (X^{+Z})^{**} \rightleftharpoons X^{+Z+1} + \epsilon}$$

- **Unified method (Nahar and Pradhan 1992, 1994) combines the two processes for the total recombination**

ELECTRON-RECOMBINATION IS COMMON IN ALL ASTRONOMICAL OBJECTS

- Crab nebula with stars radiating the plasma - photoionization and electron ion recombination are the dominating atomic processes
- Intergalactic region with no light source - recombination occurs. - Even in dark, cold space there are electrons and ions which go through recombination process
- Recombination - in emission spectra, Photoionization - absorption spectra
- Recombination determines the ionization fractions in astrophysical plasma

ELECTRON-ION RECOMBINATION LINES (REL):



• In thin and cooler nebular plasmas, electrons are not excited - the observed high lying emission lines form from recombination. • The intensity of lines depend on level population where recombination can contribute directly or by cascading

• Elemental Abundances ($N(X^+)$) is related to emissivity intensity of a REL & the effective recombination rate coefficient: ($\alpha_{\rm eff}$)

$$\epsilon(\lambda_{\bf pj}) = \left[\mathbf{N_e N(X^+) h\nu_{pj}}\right] \alpha_{\rm eff}(\lambda_{\bf pj})[\text{arg cm}^{-1}\text{s}^{-1}]$$

• Ionization fractions in plasmas at coronal equilibrium:

$$\mathbf{N(z-1)S_{EII}(z-1) = N(z)\alpha_{RC}(z)}$$

ELECTRON-ION RECOMBINATION: UNIFIED METHOD
(NAHAR & PRADHAN 1992, 1994)

$$\mathbf{X^{z} + h\nu \rightleftharpoons X^{z+} +}\ \ \epsilon \begin{cases} \rightarrow \text{Photoionization} \\ \leftarrow \text{(e,Ion) Recombination} \end{cases}$$

<u>**TRANSITION MATRIX:**</u> **Photoionization & Recombination:**

$$\mathbf{T_{BF} = <\Psi_B||D||\Psi_F>, \quad D_L = \sum_n r_n}$$

D $\rightarrow$ **dipole operator in "length" form,** n **= number of electrons he generalized line strength (S) is defined as,**

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

Photoionization: **The cross section is**

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

ω $\rightarrow$ **incident photon energy in Rydberg unit**

Recombination: **Cross section,** σ_{RC} **is related to** σ_{PI}**:**

$$\sigma_{\mathbf{RC}} = \sigma_{\mathbf{PI}}\frac{\mathbf{g_i}}{\mathbf{g_j}}\frac{\mathbf{h^2}\omega^\mathbf{2}}{\mathbf{4}\pi^\mathbf{2}\mathbf{m^2c^2v^2}}.$$

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ELECTRON-ION RECOMBINATION: UNIFIED METHOD (NAHAR & PRADHAN 1992, 1994)

Typical Approximation

- **Separate calculations of Radiative Recombination (RR) rate & Dielectronic recombination (DR) rate**

$$\alpha_{\mathbf{RC}} = \alpha_{\mathbf{RR}} + \alpha_{\mathbf{DR}}$$

- **Unified Method → total recombination**

$$\alpha_{\mathbf{RC}} = \mathbf{Unified}[\alpha_{\mathbf{RR}} + \alpha_{\mathbf{DR}}]\ \&\ \mathbf{Interference!of\ RR + SR}$$

- **Recombination cross section, σ_{RC}, from principle of detailed balance (Milne Relation):**

$$\sigma_{\mathbf{RC}} = \sigma_{\mathbf{PI}} \frac{\mathbf{g_i}}{\mathbf{g_j}} \frac{\mathbf{h^2\omega^2}}{\mathbf{4\pi^2 m^2 c^2 v^2}}.$$

The recombination rate coefficient:

$$\alpha_{\mathbf{RC}}(\mathbf{T}) = \int_0^\infty \mathbf{v f(v) \sigma_{RC} dv},$$

$\mathbf{f(v,T)} = \frac{4}{\sqrt{\pi}}(\frac{\mathbf{m}}{\mathbf{2kT}})^{3/2}\mathbf{v^2 e^{-\frac{mv^2}{2kT}}}$ = **Maxwellian distribution function**

Total α_{RC}: Contributions from infinite number of recombined states