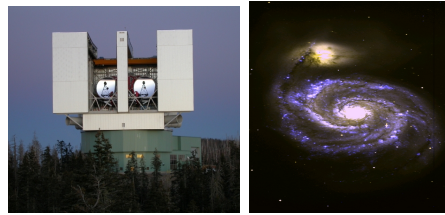




THE OHIO STATE UNIVERSITY



Lectures and Workshop on:

**”ATOMIC STRUCTURE AND TRANSITIONS:
THEORY AND USE OF SUPERSTRUCTURE PRO-
GRAM”**

PROF. SULTANA N. NAHAR

Astronomy, Ohio State U, Columbus, Ohio, USA

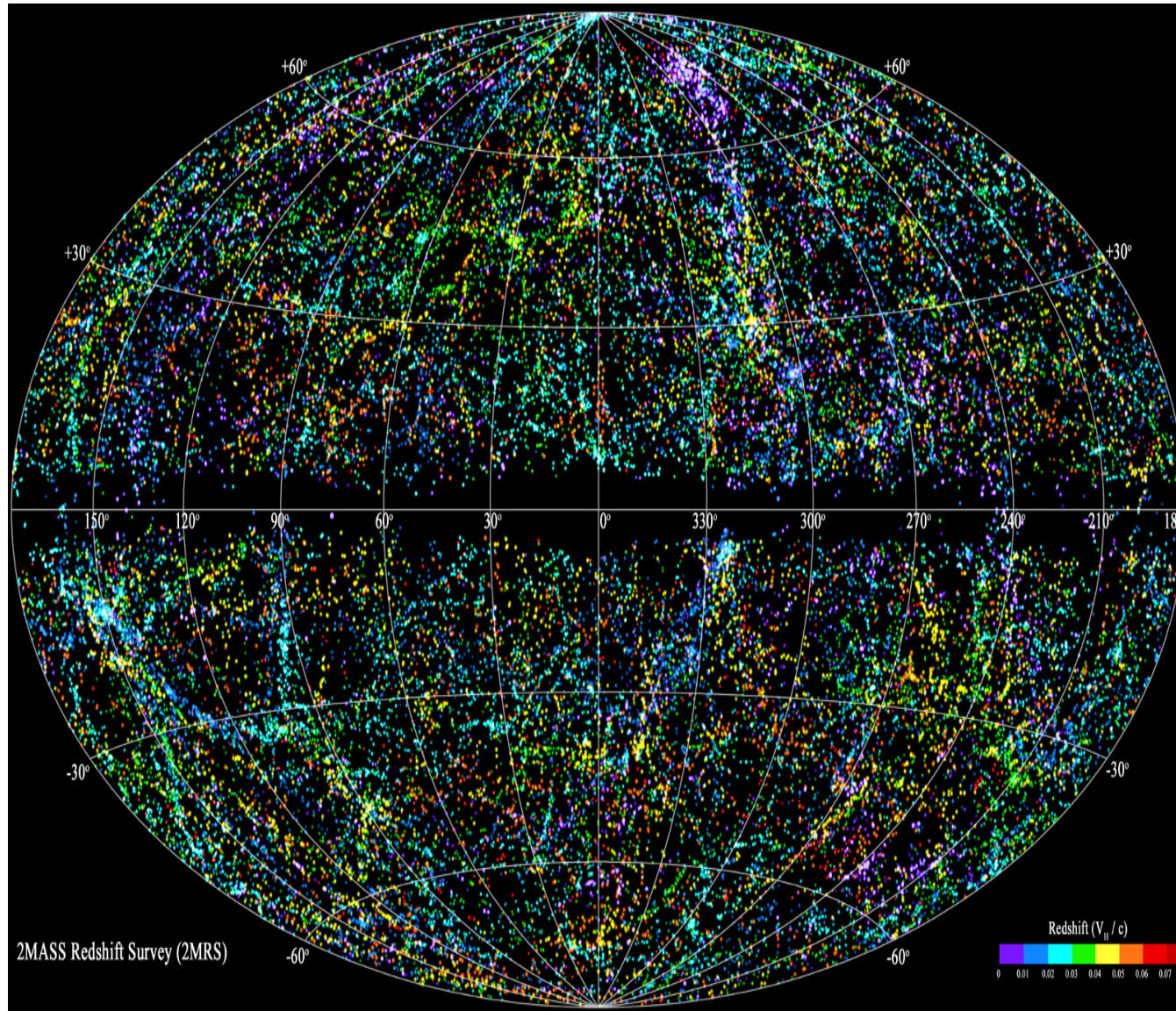
Email: nahar.1@osu.edu

<http://www.astronomy.ohio-state.edu/~nahar>

- **Textbook: ”Atomic Astrophysics and Spectroscopy”
A.K. Pradhan & S.N. Nahar (Cambridge U Press, 2011)**
- **Computation: Ohio Supercomputer Center (OSC) ‘**
 - **OSU, June - July, 2020**

Study the UNIVERSE through RADIATION:

Most Complete 3D Map of the universe (Created: By 2MASS - 2-Micron All Sky Survey over 3 decades)

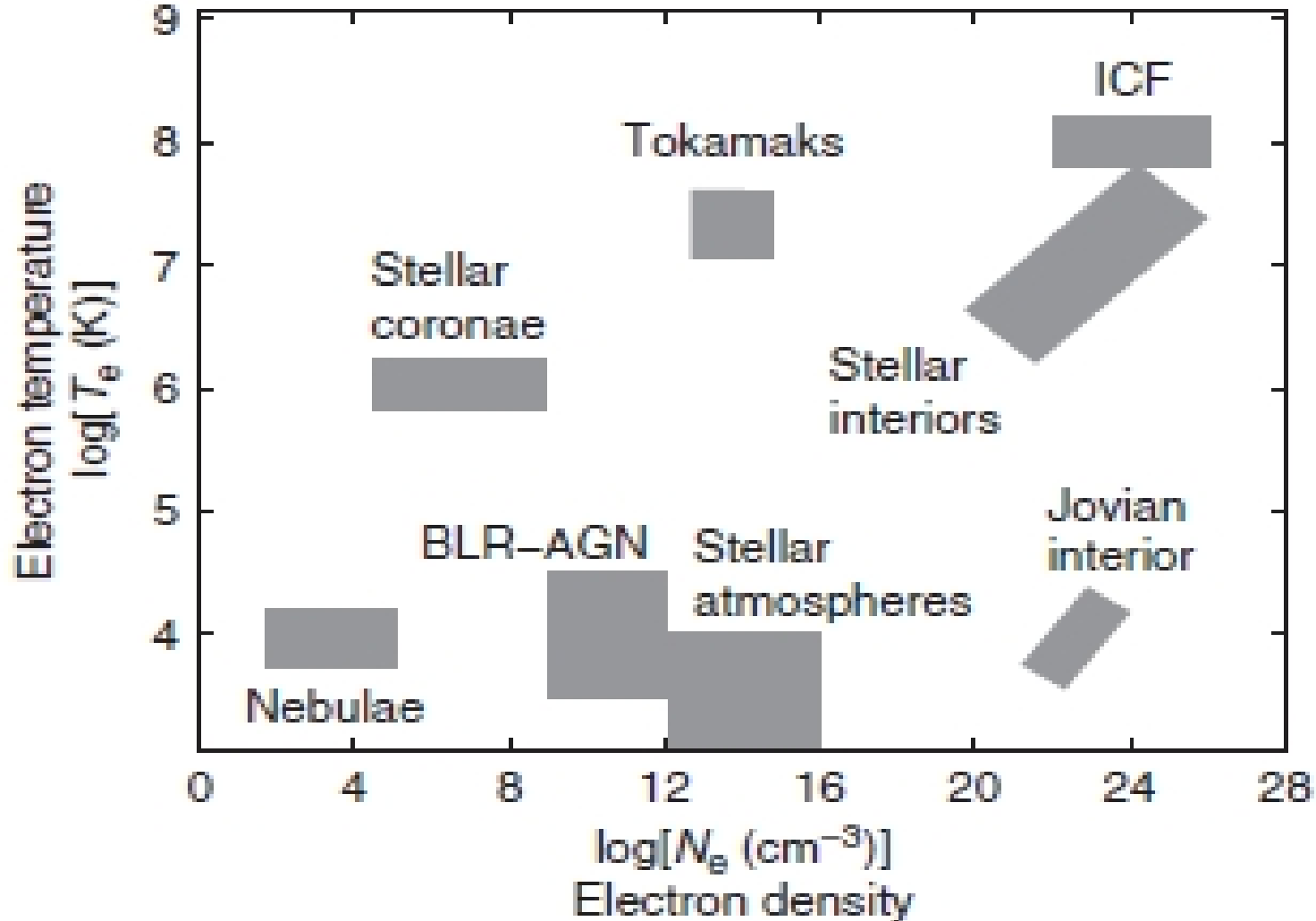


- Includes 43,000 galaxies extended over 380 million light years
- Redshifts, or measurements of galaxy distances, were added
- Missing black band in the middle because of invisibility behind our Milky Way

The MILKY WAY, Our Galaxy

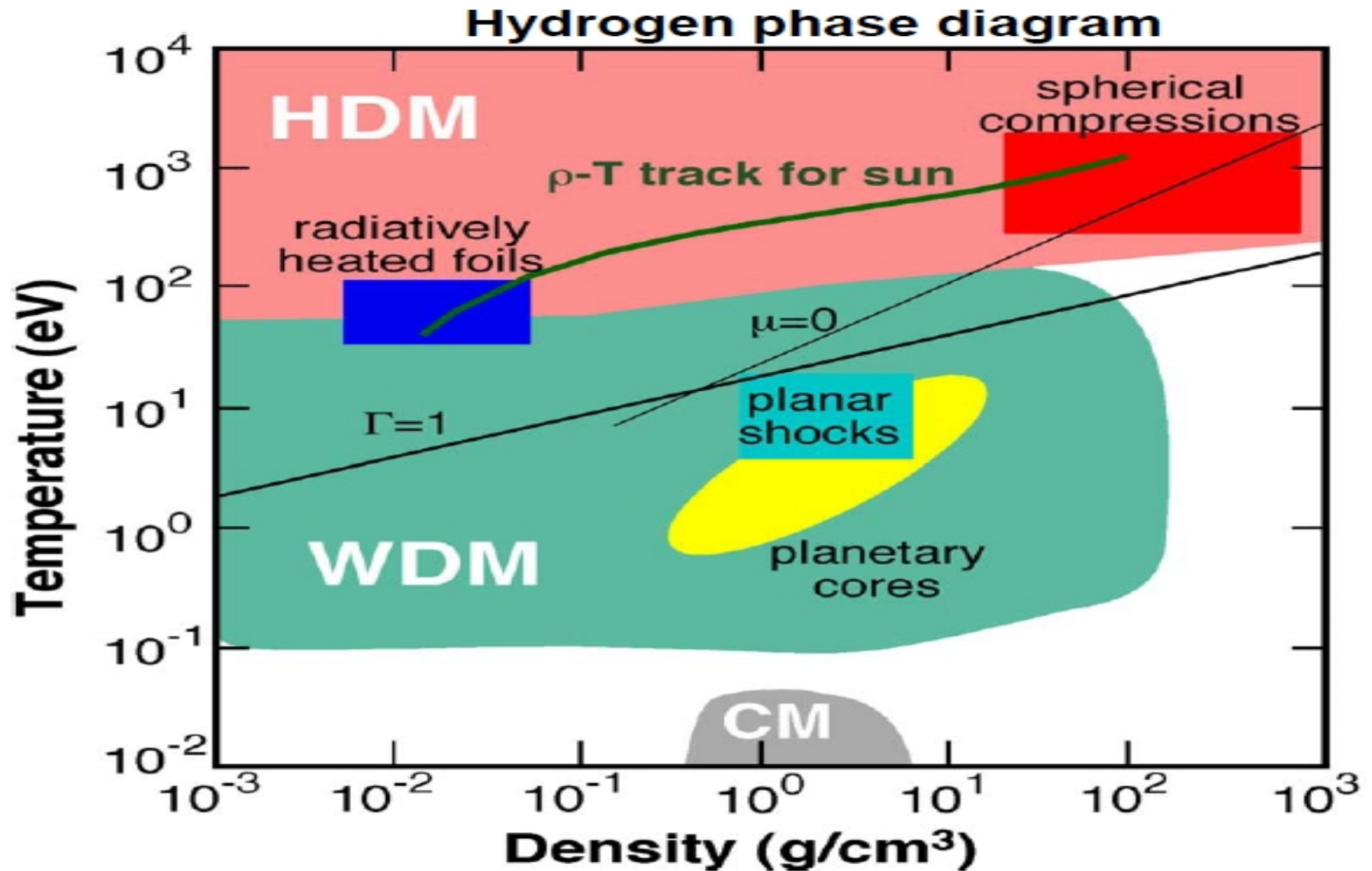


- Has 200-400 billion stars
- Astronomical Objects: Anything beyond our earth
- How do we study them? - Analyzing the light coming from them
 - Light is emitted by excited or “HOT” atoms, molecules in them



- BLR-AGN (broad-line regions in active galactic nuclei), where many spectral features are associated with the central massive black hole
- Laboratory plasmas - tokamaks (magnetic confinement fusion devices), Z-pinch machines (inertial confinement fusion (ICF) devices)

WARM & HOT DENSE MATTER (HEDLP-FESAC report)



- **Hot Dense Matter (HDM):** - Sun's ρ -T track, Supernovae, Stellar Interiors, Accretion Disks, Blackhole environments
- Lab plasmas in fusion devices: inertial confinement - laser produced (NIF) & Z pinches (e.g. Sandia), magnetic confinement (tokamaks)
- **Warm Dense Matter (WDM):** - cores of large gaseous planets

STUDYING ASTRONOMICAL OBJECTS

- 99% of known matter is plasma

ASTRONOMICAL objects are studied in three ways:

- Imaging:

- Beautiful pictures of astronomical objects, Stars, Nebulae, Active Galactic Nuclei, Blackhole Environments, etc
- Provides information of size and location of the objects

- Photometry:

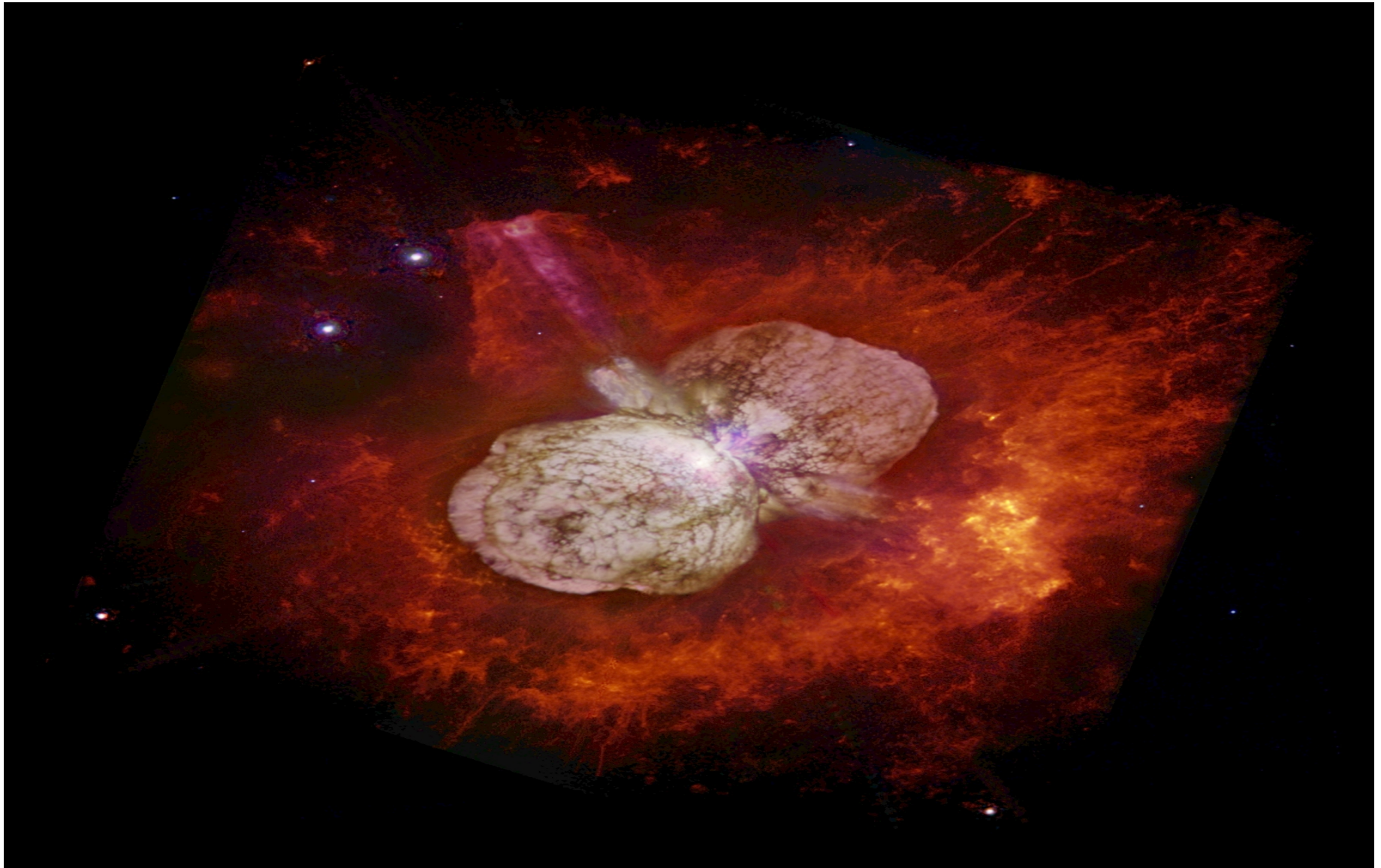
- Low resolution spectroscopy - Bands of Electromagnetic Colors ranging from X-ray to Radio waves
- macroscopic information

- Spectroscopy:

- Taken by spectrometer - Provides most of the detailed knowledge: temperature, density, extent, chemical composition, etc. of astronomical objects

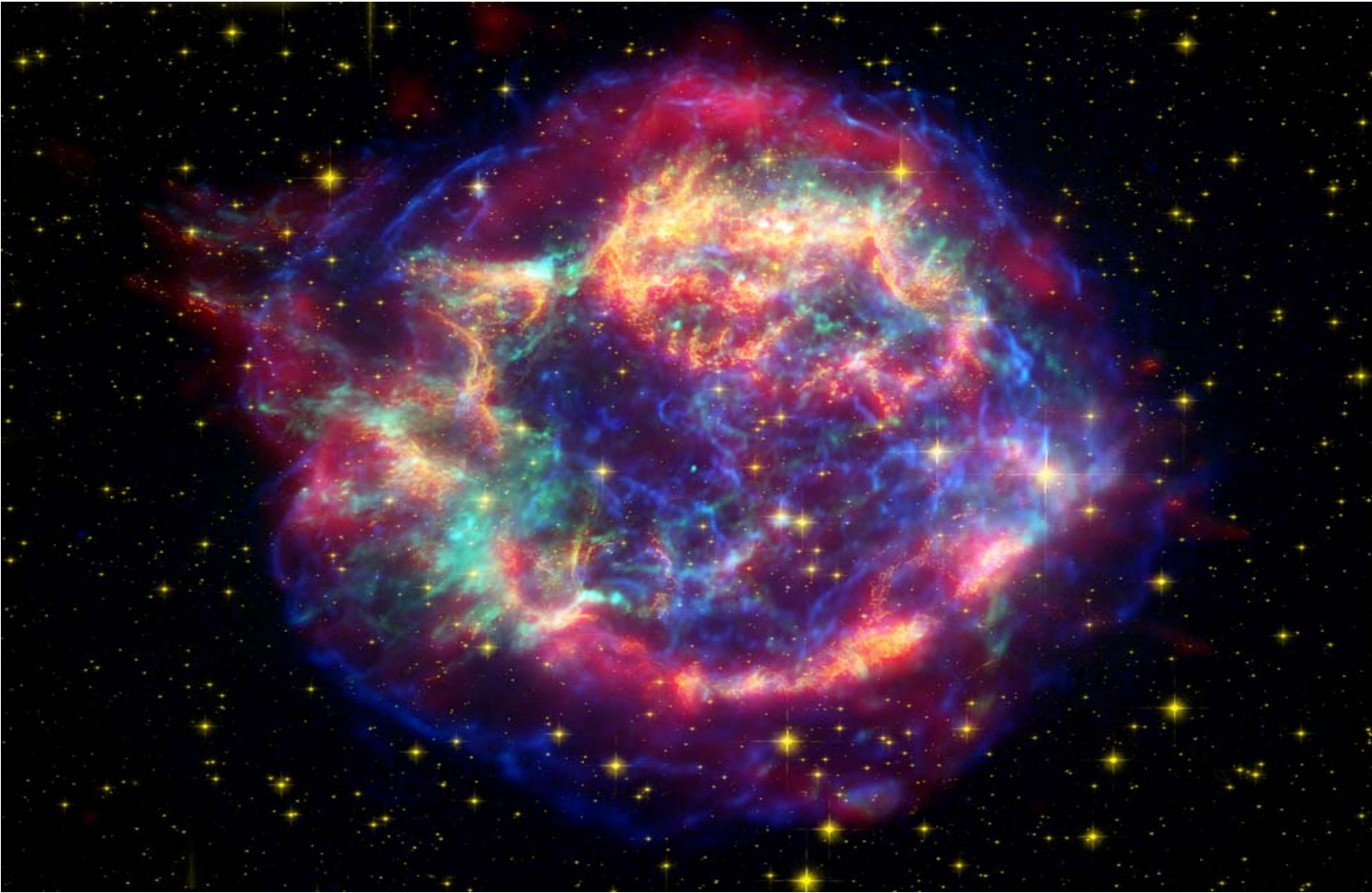
Spectroscopy is underpinned by Atomic & Molecular Physics

..ETA CARINAE: Photometric image .



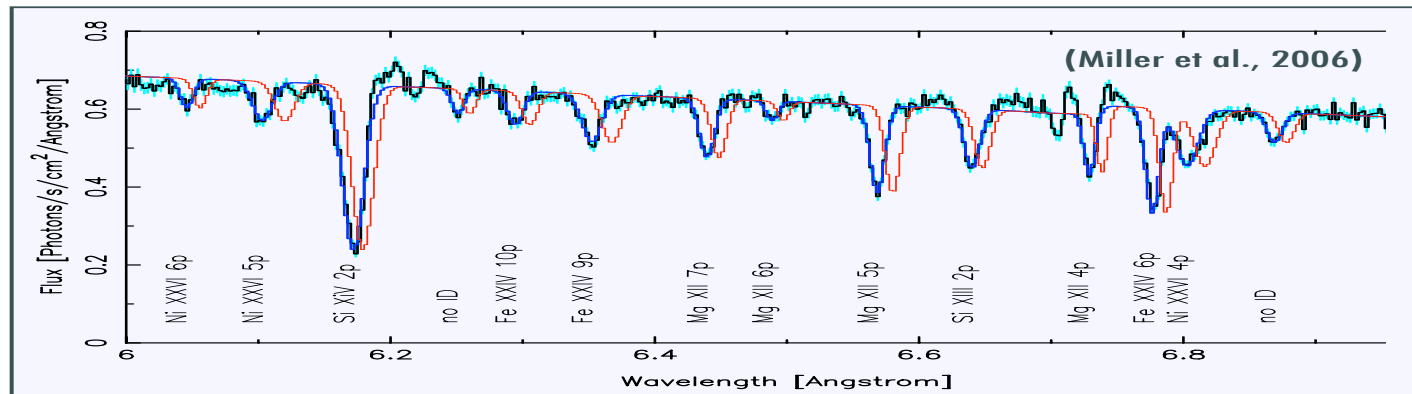
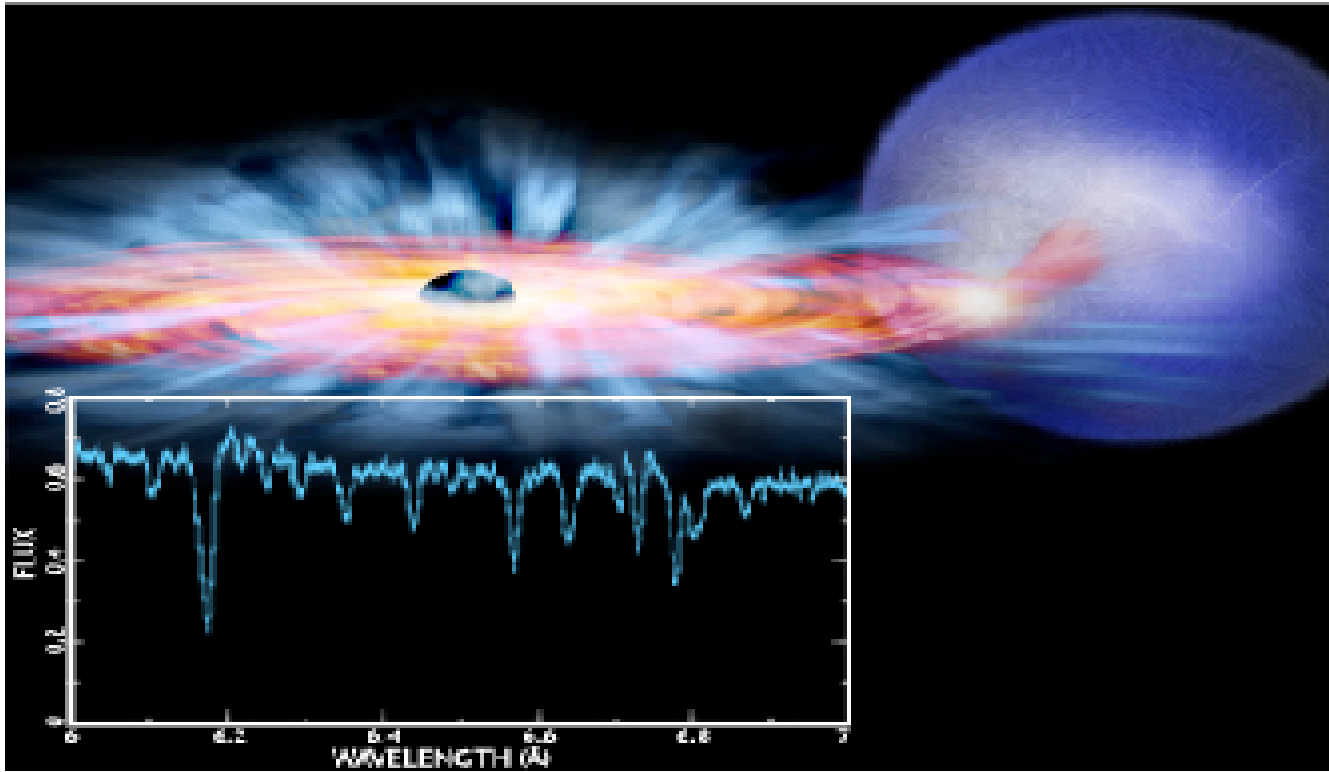
- ...● Consists of 2 massive bright (5M times the sun) stars, heavier one went under a near supernova explosion
- Explosion produced two polar lobes, and a large but thin equatorial disk, all moving outward at 670 km/s. Mass indicates future eruptions
- ..● HST image shows the bipolar Homunculus Nebula surrounds it ..

Photometry - Low resolution analysis: Supernova Remnant CASSIOPIA A



- Photometric Observation: Spitzer (Infrared - red), Hubble (Visible - yellow), Chandra (X-ray - green & blue)
- Heavier elements - Supernova explosion, Kilonova (recent finding)
- Solar system made from debris of supernova explosions

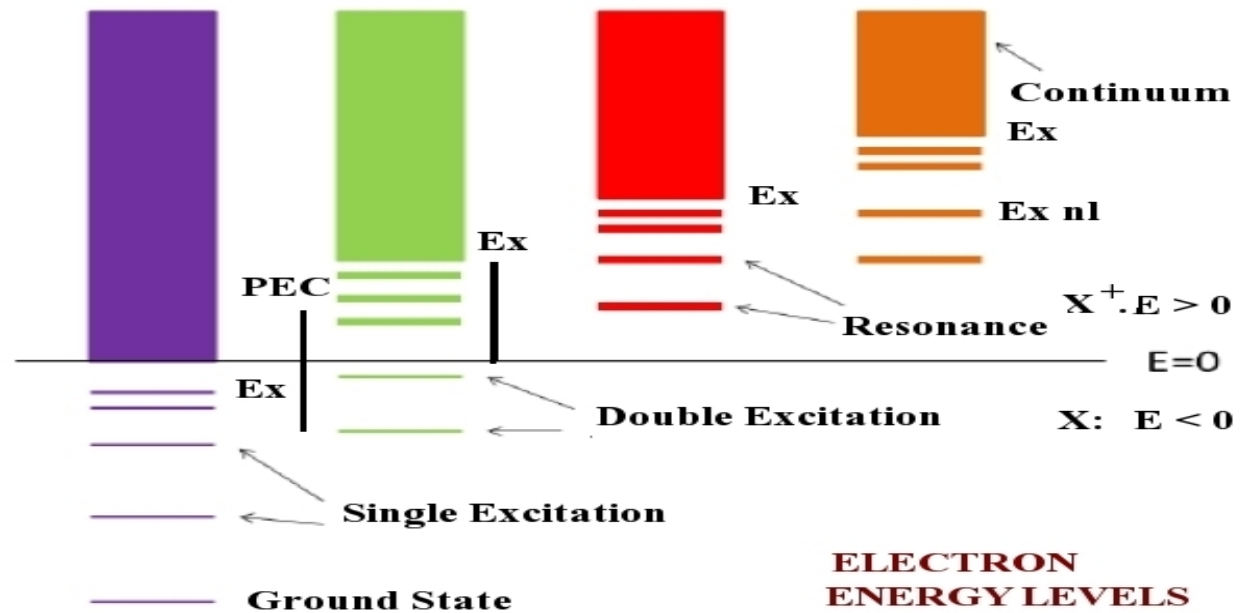
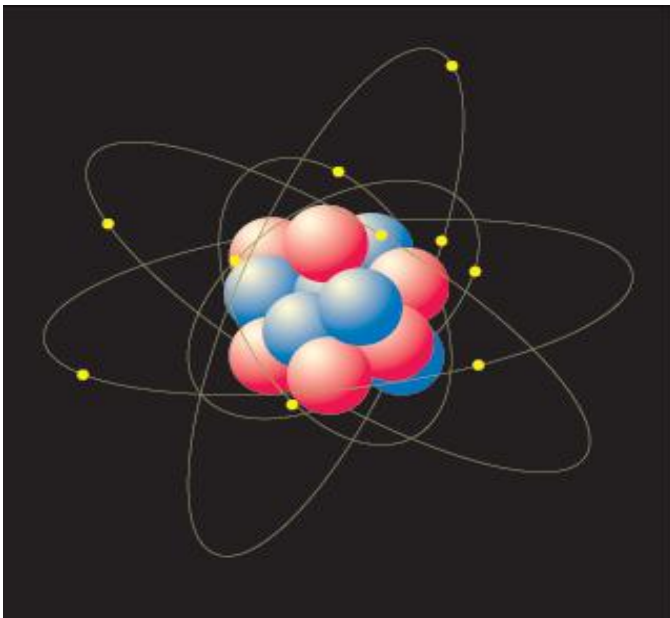
SPECTRUM of the Wind of Black hole: GRO J1655-40 Binary Star System



- Materials from the large star is sucked into companion black hole - form wind as they spiral to it. Spectrum of the wind (BLUE):
- Highly charged Mg, Si, Fe, Ni lines. RED: Elements in natural widths
- Doppler Blue Shift - Wind is blowing toward us
- Information from analysis of light produced from atomic transitions

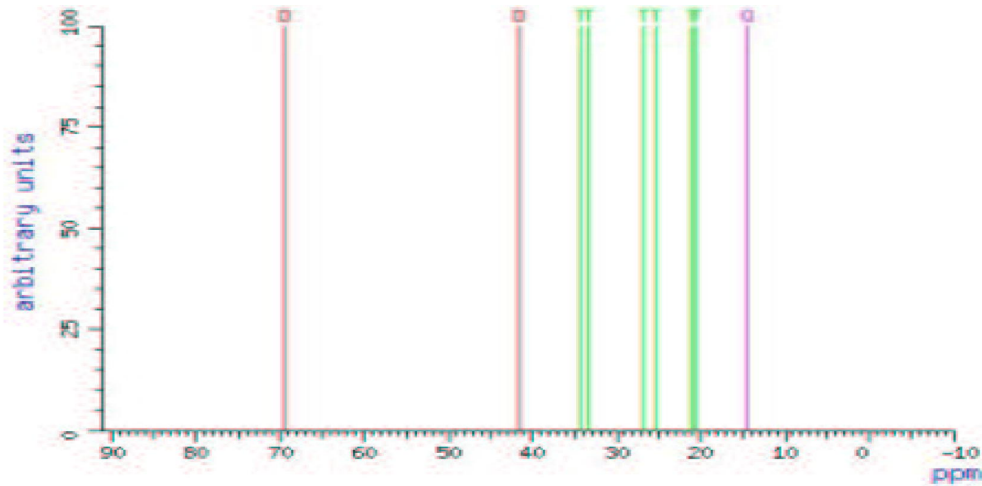
ATOMIC STRUCTURE

- Atomic structure - i) Organization of electrons in various shells and subshells, ii) Determinations of electron energies and wave functions → transition probabilities
- Fermions, unlike Bosons, e.g. electrons form *structured* orbital arrangements, known as **configuration**, bound by the attractive nuclear potential. Li configuration: $1s^2 2s$
- Electrons move in quantized orbitals with orbital L and spin S angular momenta. L and S give rise to various atomic states. Transitions among those states involve photons which are seen as lines in observed spectra



SPECTRUM

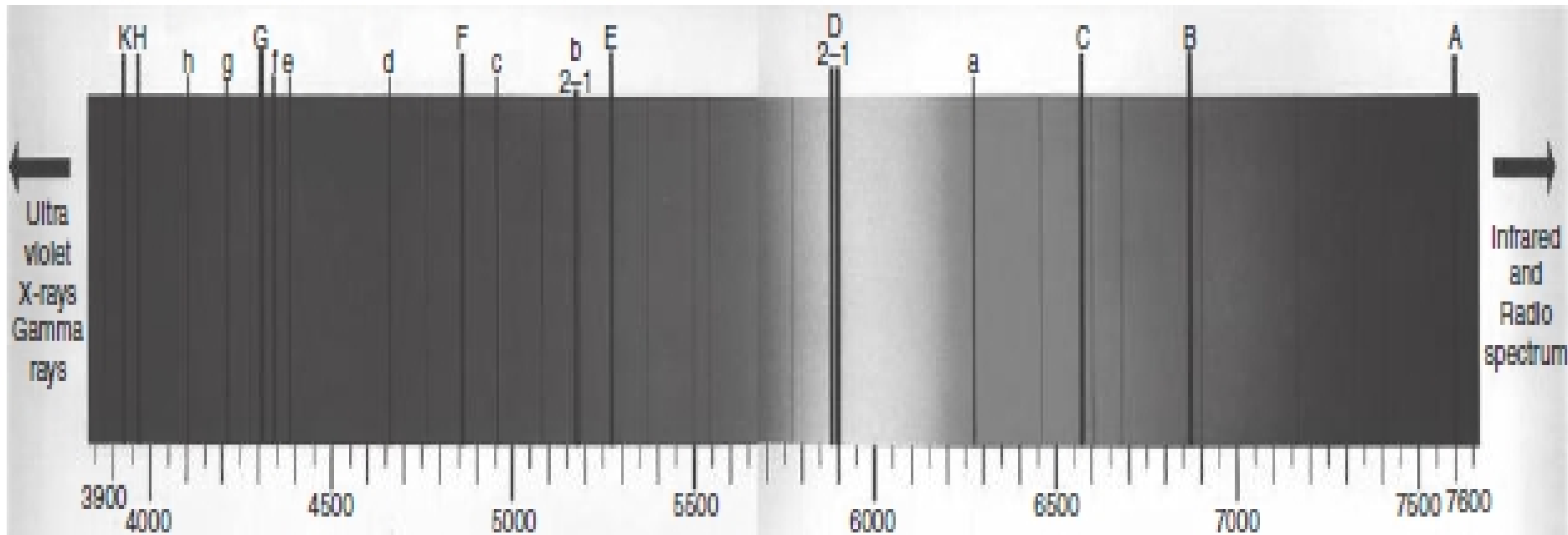
- The combination of orbital angular momentum L and spin angular momentum S follow strict coupling rules, known as selection rules
- Each atom gives out its own set of photons or colors
- Spectrum is the lines of colors,



- Left: Carbon spectrum, Right: Rainbow: Solar spectrum
- Light is a mixture of colors - Spectrum: splitting of colors
 - We study the dynamic state of an atom by Schrodinger equation - quantum equivalence of classical Newton's eq
 - The solution for Schrodinger equation is exact only for **HYDROGEN ATOM**
 - **Approximation begins from 2-electrons systems**

SOLAR SPECTRA: ABSORPTION & EMISSION LINES

- Absorption line - forms as an electron absorbs a photon to jump to a higher energy level
- Emission line - forms as a photon is emitted due to the electron dropping to a lower energy level
- For the same transition levels, both lines form at the same energy position



- Fraunhofer (1815) observed lines in the solar spectrum & used alphabet for designation
- Later, following Russel and Saunders (1925) LS coupling designation, spectroscopy with quantum mechanics identified them: A (7594 Å, O), B (6867 Å, O) (air), C (6563 Å H), D1 & D2 (5896, 5890 Å Na, yellow sun), E (5270 Å, Fe I), F (4861 Å, H), G (4300 Å, CH), H & K (3968, 3934 Å, Ca II)

HYDROGEN ATOM

Schrodinger equation of hydrogen, with $\text{KE} = \mathbf{P}^2/(2m)$ and nuclear potential energy $V(\mathbf{r})$, is

$$\left[-\frac{\hbar^2}{2m} (\nabla^2) + V(r) \right] \Psi = E \Psi \quad (1)$$

or,

$$\left[-\frac{\hbar^2}{2m} (\nabla_r^2 + \nabla_{\perp}^2) + V(r) \right] \Psi = E \Psi$$
$$V(r) = -\frac{Ze^2}{r} = -\frac{2Z}{r/a_0} \text{Ry}$$

In spherical coordinates

$$\nabla_{\mathbf{r}}^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \quad (2)$$
$$\nabla_{\perp}^2 = \frac{1}{r^2 \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial}{\partial \vartheta} \right) + \frac{1}{r^2 \sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2}$$

The solution or wavefunction has independent variables r , θ , ϕ , each will correspond to a quantum number,

$$\Psi(\mathbf{r}, \vartheta, \varphi) = R(r) Y(\vartheta, \varphi)$$

HYDROGEN WAVEFUNCTION WITH QUANTUM NUMBERS

- With quantum numbers n, l, m , the complete solution for the bound states of hydrogen may be written as

$$\langle |nlm\rangle \equiv \psi_{nlm}(\mathbf{r}, \vartheta, \varphi) = \mathbf{R}_{nl}(\mathbf{r}) \mathbf{Y}_{lm}(\vartheta, \varphi) = \frac{1}{r} \mathbf{P}_{nl}(\mathbf{r}) \mathbf{Y}_{lm}(\vartheta, \varphi) \quad (3)$$

The radial function is

$$\mathbf{P}_{nl}(\mathbf{r}) = \sqrt{\frac{(n-l-1)!Z}{n^2[(n+l)!]^3 a_0}} \left[\frac{2Zr}{na_0} \right]^{l+1} e^{\frac{-Zr}{na_0}} \times L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right),$$

where the Laguerre polynomial is

$$L_{n+l}^{2l+1}(\rho) = \sum_{k=0}^{n-l-1} \frac{(-1)^{k+2l+1} [(n+l)!]^2 \rho^k}{(n-l-1-k)! (2l+1+k)! k!}. \quad (4)$$

The angular solution of normalized spherical harmonic:

$$\mathbf{Y}_{lm}(\vartheta, \varphi) = \mathbf{N}_{lm} P_l^m(\cos \vartheta) e^{im\varphi} \quad (5)$$

where

$$\mathbf{N}_{lm} = \epsilon \left[\frac{2l+1}{4\pi} \frac{(1-|m|)!}{(1+|m|)!} \right]^{1/2}, \quad (6)$$

HYDROGEN WAVEFUNCTION WITH QUANTUM NUMBERS

$\epsilon = (-1)^m$ for $m > 0$ and $\epsilon = 1$ for $m \leq 0$. The solutions are associated Legendre polynomials of order l and m ,

$$P_l^m(w) = (1 - w^2)^{|m|/2} \frac{d^{|m|}}{dw^{|m|}} P_l(w), \quad (7)$$

$m = l, l - 1, \dots - l$. $m = 0 \rightarrow P_l(w) =$ Legendre polynomial of order l .

The energies E are given by,

$$E = -\frac{Z^2}{n^2} \times \text{Ry}; = -\frac{Z^2}{2n^2} \times (\text{a.u.}) E = -(Z^2/n^2) \times \text{Ry}; \quad (8)$$

n is a positive integer & defined as the *principal quantum number*. The energy difference between two levels gives the spectral line and is given by Rydberg formula as.

$$\Delta \mathcal{E}_{n,n'} = \mathcal{R}_H \left[\frac{1}{n^2} - \frac{1}{n'^2} \right] \quad (n' > n), \quad (9)$$

where $\mathcal{R}_H = 109,677.576 / \text{cm} = 1/911.76 \text{ \AA}$ is

QUANTUM DESIGNATION OF A STATE

- Atomic Shells: $n = 1, 2, 3, 4 \dots = K, L, M, N$
- No of electrons = $2n^2$ - Closed shell, $< 2n^2$ - Open Shell
- Orbital angular momentum: $l = 0, 1, 2, 3, 4 \dots (n-1) = s, p, d, f, \dots$
- Total Angular Momentum: $L = 0, 1, 2, 3, 4, \dots$, = S, P, D, F, ..
- No of nodes in a wavefunction = $n - l - 1$
- Magnetic angular momentum: $m_l = 0, \pm 1, \pm 2, \pm 3, 4 \dots \pm l$
($2l + 1$) values - angular multiplicity
- Spin angular momentum S was introduced due to electron spin. It is inherent in Dirac equation. $S = \text{integer or } 1/2$
integer depending on number of electrons with spin $s = 1/2$
- Spin magnetic angular momentum = $m_s = \pm S$ - ($2S + 1$)
values - spin multiplicity
- Spin multiplicity = 1, 2, 3, .. = singlet, doublet, triplet ..
- Total angular momentum: $J = |L \pm S|$, $J_M = 0, \pm 1, \pm 2, \pm 3, 4 \dots \pm J$,
 J multiplicity = $2J + 1$
- Parity (introduced from wavefunction) = $\pi = (-1)^l = +1$
(even) or -1 (odd)
- Symmetry of a state: $(2S + 1)L^\pi$ (LS), $(2S + 1)L_J^\pi$ (LSJ)

MULTI-ELECTRON ATOM

A many-electron system requires to sum over (i) all one-electron operators, that is KE & attractive nuclear Z/r potential, (ii) two-electron Coulomb repulsion potentials

$$\mathbf{H}\Psi = [H_0 + H_1]\Psi, \quad (10)$$

$$H_0 = \sum_{i=1}^N \left[-\nabla_i^2 - \frac{2Z}{r_i} \right], H_1 = \sum_{j<i} \frac{2}{r_{ij}} \quad (11)$$

$$H = \sum_i f_i + \sum_{j \neq i} g_{ij} \equiv F + G \quad (12)$$

- H_0 : one-body term, stronger, H_1 : two-body term, weaker, can be treated perturbatively
- Start with a trial wave function Ψ^t in some parametric form, Slater Type Orbitals

$$\mathbf{P}_{nl}^{\text{STO}}(\mathbf{r}) = r^{l+1} e^{-ar}$$

- A trial function should satisfy variational principle that through optimization an upper bound of energy eigenvalue is obtained in the Schrödinger equation.

HARTREE-FOCK EQUATION (Book AAS)

- The N -electron wavefunction in the determinantal representation

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(1) & \psi_1(2) & \dots & \psi_1(N) \\ \psi_2(1) & \psi_2(2) & \dots & \psi_2(N) \\ \dots & \dots & \dots & \dots \\ \psi_N(1) & \psi_N(2) & \dots & \psi_N(N) \end{vmatrix} \quad (13)$$

This is called the *Slater determinant*. Ψ vanishes if coordinates of two electrons are the same. Substitution in Schrodinger equation results in Hartree-Fock equation. Simplification gives set of one-electron radial equations,

$$\left[-\nabla_i^2 - \frac{2Z}{r_i} \right] u_k(r_i) + \left[\sum_l \int u_l^*(r_j) \frac{2}{r_{ij}} u_l(r_j) dr_j \right] u_k(r_i) - \sum_l \delta_{m_L^k, m_L^l} \left[\int u_l^*(r_j) \frac{2}{r_{ij}} u_k(r_j) dr_j \right] u_l(r_i) = E_k u_k(r_i).$$

1st term= 1-body term, 2nd term= Direct term, 3rd term= Exchange term. • The total energy is given by

$$E[\Psi] = \sum_i I_i + \frac{1}{2} \sum_i \sum_j [J_{ij} - K_{ij}]. \quad (14)$$

Central Field Approximation for a Multi-Electron System

- H_1 consists of non-central forces between electrons which contains a large spherically symmetric component
- We assume that each electron is acted upon by the averaged charge distribution of all the other electrons and construct a potential energy function $V(r_i)$ with one-electron operator. When summed over all electrons, this charge distribution is spherically symmetric and is a good approximation to actual potential. Neglecting non-radial part,

$$H = - \sum_{i=1}^N \frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}).$$

where

$$V(\mathbf{r}) = - \sum_{i=1}^N \frac{e^2 Z}{r_i} + \left\langle \sum_{i \neq j}^N \frac{e^2}{r_{ij}} \right\rangle. \quad (15)$$

- $V(\mathbf{r})$ is the *central-field potential* with boundary conditions

$$V(\mathbf{r}) = -\frac{Z}{r} \quad \text{if } r \rightarrow 0, \quad = -\frac{Z}{r} \quad \text{if } \mathbf{r} \rightarrow \infty \quad (16)$$

THOMAS-FERMI-DIRAC-AMALDI (TFDA) APPROXIMATION

- One most useful procedure (implemented in program SS):
- Treats electrons as Fermi sea: Electrons, constrained by Pauli exclusion principle, fill in cells up to a highest Fermi level of momentum $p = p_F$ at $T=0$
- As T rises, electrons are excited out of the Fermi sea close to the 'surface' levels & approach a Maxwellian distribution
→ spatial density of electrons:

$$\rho = \frac{(4/3)\pi p_F^3}{h^3/2}$$

- Based on quantum statistics, the TFDA model gives a continuous function $\phi(x)$ such that the potential is

$$V(\mathbf{r}) = \frac{Z_{\text{eff}}(\lambda_{\text{nl}}, \mathbf{r})}{r} = -\frac{Z}{r}\phi(\mathbf{x}),$$

where

$$\phi(\mathbf{x}) = e^{-Zr/2} + \lambda_{\text{nl}}(1 - e^{-Zr/2}), \quad \mathbf{x} = \frac{\mathbf{r}}{\mu},$$

$$\mu = 0.8853 \left(\frac{N}{N-1} \right)^{2/3} Z^{-1/3} = \text{constant}.$$

THOMAS-FERMI-DIRAC-AMALDI (TFDA) APPROXIMATION

- The function $\phi(x)$ is a solution of the potential equation

$$\frac{d^2\phi(x)}{dx^2} = \frac{1}{\sqrt{x}}\phi(x)^{\frac{3}{2}}$$

- The boundary conditions on $\phi(x)$ are

$$\phi(0) = 1, \quad \phi(\infty) = -\frac{Z - N + 1}{Z}.$$

- The one-electron orbitals $P_{nl}(r)$ can be obtained by solving the wave equation

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

- This is similar to the radial equation for the hydrogenic case, with the same boundary conditions on $P_{nl}(r)$ as $r \rightarrow 0$ and $r \rightarrow \infty$, and $(n - l + 1)$ nodes.

- The second order radial is solved numerically since, unlike the hydrogenic case, there is no general analytic solution.

- It may be solved using an exponentially decaying function appropriate for a bound state, e.g. Whittaker function

THOMAS-FERMI-DIRAC-AMALDI (TFDA) APPROXIMATION

- The solution is normalized Whittaker function

$$\mathbf{W}(\mathbf{r}) = e^{-z\mathbf{r}/\nu} \left(\frac{2z\mathbf{r}}{\nu} \right) \left(1 + \sum_{\mathbf{k}=1}^{\infty} \frac{\mathbf{a}_{\mathbf{k}}}{\mathbf{r}^{\mathbf{k}}} \right) \mathcal{N}$$

where $\nu = z/\sqrt{\epsilon}$ is the effective quantum number and ϵ is the eigenvalue. The coefficients are

$$\mathbf{a}_1 = \nu \{1(1+1) - \nu(\nu-1)\} \frac{1}{2z}$$

$$\mathbf{a}_{\mathbf{k}} = \mathbf{a}_{\mathbf{k}-1} \nu \{1(1+1) - (\nu-\mathbf{k})(\nu-\mathbf{k}+1)\} \frac{1}{2\mathbf{k}z}$$

and the normalization factor is

$$\mathcal{N} = \left\{ \frac{\nu^2}{z} \Gamma(\nu+1+1) \Gamma(\nu-1) \right\}^{-1/2}$$

The one-electron spin orbital functions then assume the familiar hydrogenic form

$$\psi_{\mathbf{n},\ell,\mathbf{m}_{\ell},\mathbf{m}_s}(\mathbf{r}, \theta, \phi, \mathbf{m}_s) = \phi(r, \theta, \phi) \zeta_{\mathbf{m}_s}$$

THOMAS-FERMI-DIRAC-AMALDI (TFDA) APPROXIMATION

- TFDA orbitals are based on a statistical treatment of the free electron gas, & hence neglect the shell-structure
- However, in practice configuration interaction accounts for much of the discrepancy that might otherwise result.
- Configuration interaction - when wavefunction includes more than one configuration

CONFIGURATION INTERACTION

- A multi-electron system is described by its configuration and a defined spectroscopic state.
- All states of the same $SL\pi$, with different configurations, interact with one another - configuration interaction. Hence the wavefunction of the $SL\pi$ may be represented by a linear combination of configurations giving the state.
- Example, the ground state of Boron is $1s^2 2s^2 2p$ ($^2P^0$). $^2P^0$ state can also form from $2s^2 3p$ ($^2P^0$), $2s 2p 3d$ (\dots , $^2P^0$), $2p^3$ ($^2P^0$) and so on. These 4 configurations contribute with different amplitudes or mixing coefficients (a_i) to form the four state vectors $^2P^0$ of a 4×4 Hamiltonian matrix.

THOMAS-FERMI-DIRAC-AMALDI (TFDA) APPROXIMATION

Hence for the optimized energy and wavefunction for each $^2\text{P}^0$ state all 4 configurations should be included,

$$\Psi(^2\text{P}^0) = \sum_{i=1}^4 a_i \psi[C_i(^2\text{P}^0)] = [a_1 \psi(2s^2 2p) + a_2 \psi(2s^2 3p) + a_3 \psi(2p^3) + a_4 \psi(2s 2p 3d)]$$

- The wave function will result in 4 energies. Each energy level will be designated by the configuration for which the mixing coefficients a_i has the highest value.
- When we calculate the transition matrix for the electron going from one state to another state, these configurations interfere and impact on the results.
- Typically the more configurations we have for a multi-electron system, the more accurate wave function and energies we get, and the more accurate transition parameters are obtained.

RYDBERG FORMULA FOR ENERGIES & QUANTUM DEFECT

- General Rydberg formula is similar to that of H-like ions, but accounts for the screening effect on the valence electron by the core electrons
- The outer/interacting electron experiences an *effective charge* $z = Z - N + 1$, $N =$ no of electrons
- Departure from a pure Coulomb form effectively *reduces* the principal quantum numbers n in Rydberg formula as

$$E(nl) = \frac{z^2}{(n - \mu)^2} = \frac{z^2}{\nu^2}$$

where $\mu \geq 0 =$ *quantum defect*, $\nu = n - \mu =$ *effective quantum number*. While n is an integer and changes by 1, ν is a fractional number and changes ~ 1

- The amount of screening (μ) depends on the orbital angular momentum ℓ such that $\mu_s > \mu_p > \mu_d \dots$ & μ is a constant for each ℓ . We can write,

$$E(nl) = \frac{z^2}{(n - \mu_\ell)^2} = \frac{z^2}{\nu_\ell^2}$$

- Energy levels from Rydberg formula \rightarrow “Rydberg levels”

Relativistic Breit-Pauli Approximation (Textbook AAS)

For a multi-electron atom, the relativistic Breit-Pauli Hamiltonian is:

$$\mathbf{H}_{\text{BP}} = \mathbf{H}_{\text{NR}} + \mathbf{H}_{\text{mass}} + \mathbf{H}_{\text{Dar}} + \mathbf{H}_{\text{so}} + \frac{1}{2} \sum_{i \neq j}^N [\mathbf{g}_{ij}(\mathbf{so} + \mathbf{so}') + \mathbf{g}_{ij}(\mathbf{ss}') + \mathbf{g}_{ij}(\mathbf{css}') + \mathbf{g}_{ij}(\mathbf{d}) + \mathbf{g}_{ij}(\mathbf{oo}')]]$$

where the non-relativistic Hamiltonian is

$$\mathbf{H}_{\text{NR}} = \left[\sum_{i=1}^N \left\{ -\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^N \frac{2}{r_{ij}} \right\} \right]$$

and one-body correction terms are

$$\mathbf{H}_{\text{mass}} = -\frac{\alpha^2}{4} \sum_i \mathbf{p}_i^4, \quad \mathbf{H}_{\text{Dar}} = \frac{\alpha^2}{4} \sum_i \nabla^2 \left(\frac{Z}{r_i} \right), \quad \mathbf{H}_{\text{so}} = \frac{Ze^2 \hbar^2}{2m^2 c^2 r^3} \mathbf{L} \cdot \mathbf{S}$$

and the Breit interaction is

$$\mathbf{H}_{\text{B}} = \sum_{i>j} [\mathbf{g}_{ij}(\mathbf{so} + \mathbf{so}') + \mathbf{g}_{ij}(\mathbf{ss}')]]$$

SS includes all these terms and partial contributions from the last 3 terms. Wave functions and energies are obtained solving

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

- The accuracy is comparable to that of Dirac-Fock approximation for most ions

ANGULAR MOMENTA COUPLINGS

- Total L and S angular momenta may couple differently for the total angular momentum J - depends on Z
- Multi-electron elements may be divided as, 'light' ($Z \leq 18$) and 'heavy' ($Z > 18$) (although not precise)
- **LS coupling** (typically $Z \leq 18$): Vector summation of orbital and spin angular momenta is done separately
 $L = |L_2 - L_1|, \dots, |L_2 + L_1|$, L Multiplicity = $2L+1$
 $S = |S_2 - S_1|, \dots, |S_2 + S_1|$, S Multiplicity = $2S+1$
Then the *total angular momentum quantum numbers*:
 $J = |L - S|, \dots, |L + S|$, J Multiplicity = $2J+1$
- The J -values \rightarrow finestructure levels. Each LS can correspond to several finestructure J levels
- The symmetry of a state is $J\pi$ or $(2S+1)L_J^\pi$
- Coulomb force between an electron and nucleus becomes stronger for large Z and highly charged ions and can increase the velocity of the electron to relativistic level. Angular coupling changes
- **Intermediate or LSJ coupling** (typically $19 \leq Z \leq 40$): Consideration of full relativistic effects is not necessary

ANGULAR MOMENTA COUPLINGS

- For the total angular momentum J , the angular momenta l and $s = 1/2$ of an interacting electron are added to the total orbital & spin angular momenta, J_1 of all other electrons, as:

$$J_1 = \sum_i l_i + \sum_i s_i, \quad K = J_1 + l, \quad J = K + s,$$

- ***jj* coupling** (typically for $Z > 40$): When relativistic effect is more prominent, the total J is obtained from sum of individual electron total angular momentum j_i from its angular & spin angular momenta:

$$j_i = l_i + s_i, \quad J = \sum_i j_i, \quad (17)$$

For any 2 electrons, J ranges from $|j_1 + j_2|$ to $|j_1 - j_2|$

- States designation = $(j_1 j_2)_J$ Ex; (*pd*) configuration- $j_1(1 \pm 1/2) = 1/2, 3/2$, and $j_2(2 \pm 1/2) = 3/2, 5/2$. The states are:
 $(1/2 \ 3/2)_{2,1}$, $(1/2 \ 5/2)_{3,2}$, $(3/2 \ 3/2)_{3,2,1,0}$, $(3/2 \ 5/2)_{4,3,2,1}$

NON-EQUIVALENT & EQUIVALENT ELECTRON STATES

- **Equivalent electron state** → Number of valence electrons in the outer orbit: > 1

Non-equivalent electron state → 1 valence electron

- Non-equivalent electron states: All possible states allowed by the vectorial sum. Ex. Find $(2S+1)L_J^\pi$ states of a 3-electron configuration: $nsn'pn''d$ (different orbitals):

Total S: For $nsn'p$: $|1/2 \pm 1/2| = [0,1]$. Add $1/2$ of $n''d$ to them → $(1/2, 3/2, 1/2) \rightarrow 2S+1 = 2, 4, 2$

Total L: For $nsn'p$, $|0 \pm 1| = 1$, Add 2 for $n''d$: $|1 \pm 2| = 1, 2, 3$

Net parity π : $(-1)^{\sum_i l_i} = (-1)^{0+1+2} = -1$ (odd parity)

Total J: $|L \pm S$; Ex: $|1 \pm 1/2| = 1/2, 3/2$

$ns n'p (^1P^o) n''d \rightarrow ^2P^o, ^2D^o, ^2F^o$ - 3 states

$ns n'p (^3P^o) n''d \rightarrow (^{2,4})(P, D, F)^o$ - 6 states.

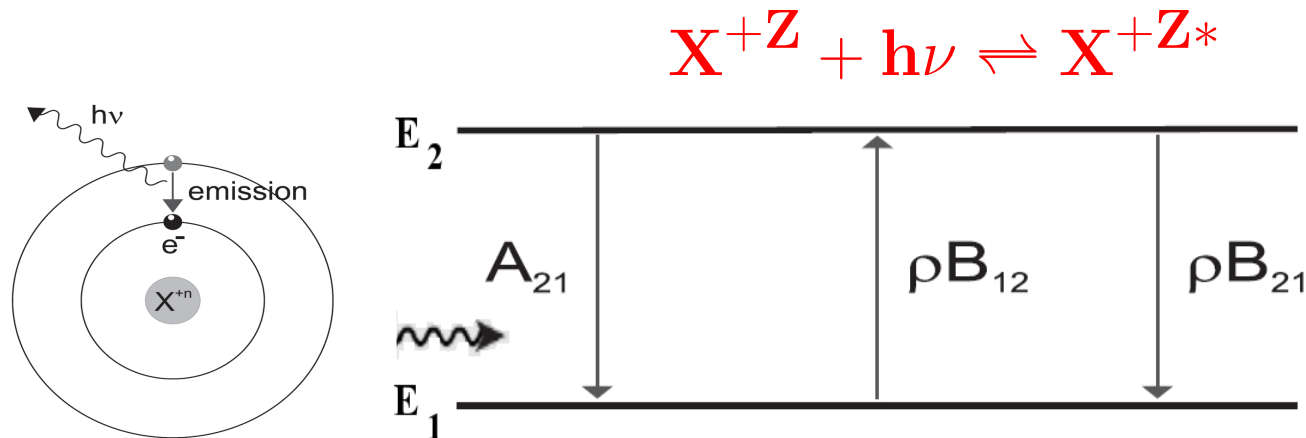
Ex: $(2S+1)L_J^\pi = ^2P_{1/2}^o, ^2P_{3/2}^o$

- Equivalent electron state: Less number of LS states.

Ex: configuration, np^2 . For different orbitals, $n p n' p \rightarrow ^1, ^3S, ^1, ^3P, ^1, ^3D$ (6 states). For $n=n'$, Pauli exclusion principle eliminates some -reducing 6 to 3 states, $^1S, ^3P, ^1D$,

1. "PHOTO-EXCITATION"

Photo-Excitation & De-excitation:



- Atomic quantities

B_{12} - Photo-excitation, Oscillator Strength (f)

A_{21} - Spontaneous Decay, - Radiative Decay Rate (A -value)

B_{21} - Stimulated Decay with a radiation field

- P_{ij} , transition probability,

$$P_{ij} = 2\pi \frac{c^2}{h^2 \nu_{ji}^2} \left| \langle j | \frac{e}{mc} \hat{e} \cdot p e^{i\mathbf{k} \cdot \mathbf{r}} | i \rangle \right|^2 \rho(\nu_{ji}). \quad (18)$$

$$e^{i\mathbf{k} \cdot \mathbf{r}} = 1 + i\mathbf{k} \cdot \mathbf{r} + [i\mathbf{k} \cdot \mathbf{r}]^2 / 2! + \dots,$$

- Various terms in $e^{i\mathbf{k} \cdot \mathbf{r}} \rightarrow$ various transitions 1st term E1, 2nd term E2 and M1, ...

ALLOWED & FORBIDDEN TRANSITIONS

Determined by angular momentum selection rules

i) Allowed: Electric Dipole (E1) transitions - same-spin & intercombination (different spin) transition
($\Delta J = 0, \pm 1, \Delta L = 0, \pm 1, \pm 2$; parity changes)

Forbidden:

ii) Electric quadrupole (E2) transitions
($\Delta J = 0, \pm 1, \pm 2$, parity does not change)

iii) Magnetic dipole (M1) transitions
($\Delta J = 0, \pm 1$, parity does not change)

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

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

Allowed transitions are much stronger than Forbidden transitions

Transition Matrix elements with a Photon

- 1st term: **Dipole operator: $D = \sum_i \mathbf{r}_i$:**
- **Transition matrix for Photo-excitation & Deexcitation:**

$$\langle \Psi_B || D || \Psi_{B'} \rangle$$

Matrix element is reduced to generalized line strength (length form):

$$S = \left| \left\langle \Psi_f \left| \sum_{j=1}^{N+1} \mathbf{r}_j \right| \Psi_i \right\rangle \right|^2 \quad (19)$$

- There are also "Velocity" & "Acceleration" forms

Allowed electric dipole (E1) transitions

The oscillator strength (f_{ij}) and radiative decay rate (A_{ji}) for the bound-bound transition are

$$f_{ij} = \left[\frac{E_{ji}}{3g_i} \right] S,$$

$$A_{ji}(\text{sec}^{-1}) = \left[0.8032 \times 10^{10} \frac{E_{ji}^3}{3g_j} \right] S$$

FORBIDDEN TRANSITIONS

i) Electric quadrupole (E2) transitions ($\Delta J = 0, \pm 1, \pm 2, \pi$ - same)

$$A_{ji}^{E2} = 2.6733 \times 10^3 \frac{E_{ij}^5}{g_j} S^{E2}(i, j) \text{ s}^{-1}, \quad (20)$$

ii) Magnetic dipole (M1) transitions ($\Delta J = 0, \pm 1, \pi$ - same)

$$A_{ji}^{M1} = 3.5644 \times 10^4 \frac{E_{ij}^3}{g_j} S^{M1}(i, j) \text{ s}^{-1}, \quad (21)$$

iii) Electric octupole (E3) transitions ($\Delta J = \pm 2, \pm 3, \pi$ changes)

$$A_{ji}^{E3} = 1.2050 \times 10^{-3} \frac{E_{ij}^7}{g_j} S^{E3}(i, j) \text{ s}^{-1}, \quad (22)$$

iv) Magnetic quadrupole (M2) transitions ($\Delta J = \pm 2, \pi$ changes)

$$A_{ji}^{M2} = 2.3727 \times 10^{-2} \text{ s}^{-1} \frac{E_{ij}^5}{g_j} S^{M2}(i, j). \quad (23)$$

LIFETIME:

$$\tau_{\mathbf{k}}(\text{s}) = \frac{1}{\sum_{\mathbf{i}} A_{\mathbf{ki}}(\text{s}^{-1})}. \quad (24)$$

EX: ALLOWED & FORBIDDEN TRANSITIONS

Diagnostic Lines of He-like Ions: w,x,y,z

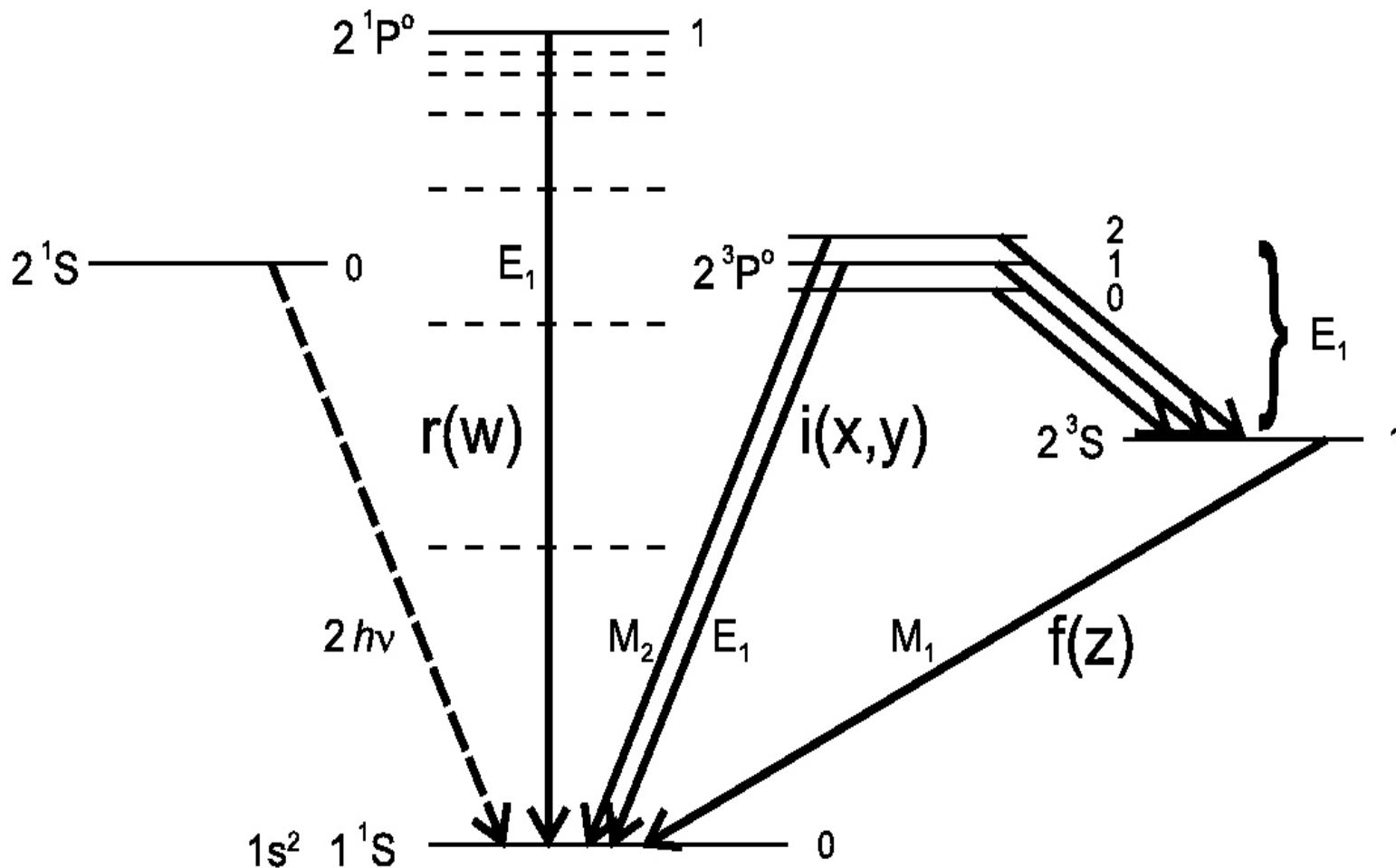
w(E1) : $1s2p(^1P_1^o) - 1s^2(^1S_0)$ (Allowed Resonant)

x(M2) : $1s2p(^3P_2^o) - 1s^2(^1S_0)$ (Forbidden)

y(E1) : $1s2p(^3P_1^o) - 1s^2(^1S_0)$ (Intercombination)

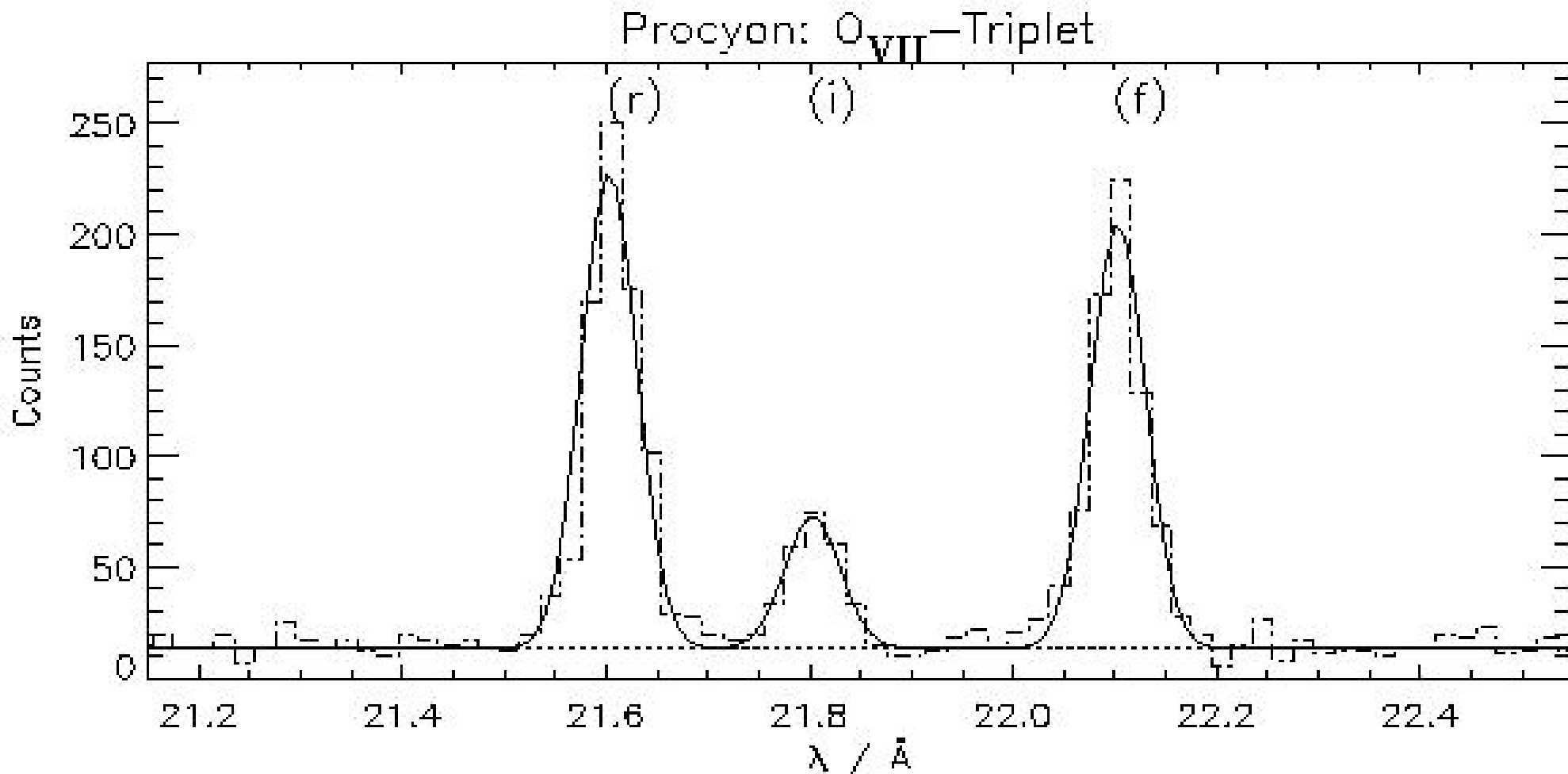
z(M1) : $1s2s(^3S_1) - 1s^2(^1S_0)$ (Forbidden)

NOTE: 1s-2p are the K_α transitions

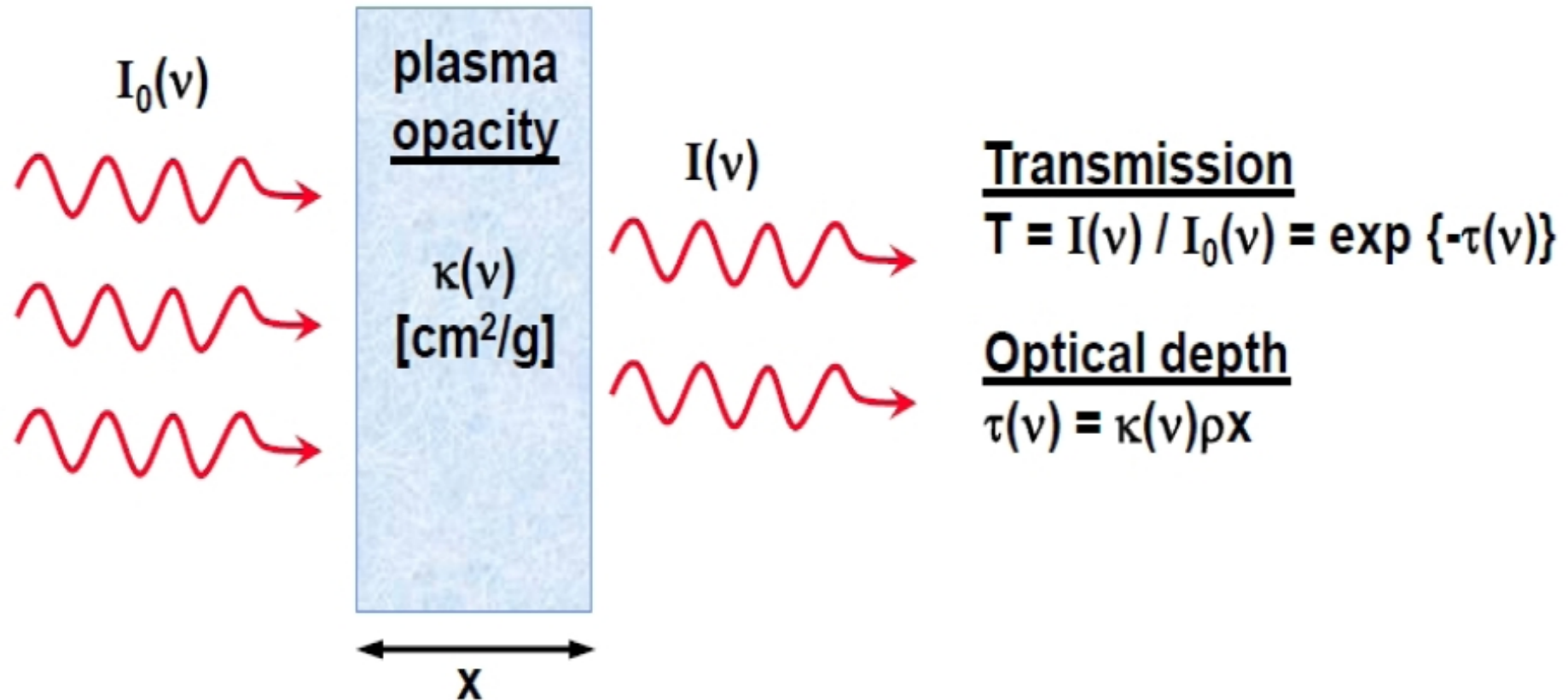


PROCYON: w,x,y,z DIAGNOSTIC LINES

Procyon, a star similar to the Sun, is a binary with a white dwarf companion. Figure shows w, i(x,y), z lines of He-like oxygen O VII in the spectrum of Procyon corona. ('Triplet' for 3 observed lines nor spin multiplicity). Here 'i' corresponds to overlapped x,y lines. All these lines are the primary diagnostics for density, temperature, and ionization balance in high temperature.



Atomic transitions in PLASMA OPACITY



- Opacity is a fundamental quantity for radiation transfer in plasmas. It is caused by repeated absorption and emission of the propagating radiation by the constituent plasma elements.

1. Photoexcitation: Atomic parameter - Oscillator Strength (f_{ij})

$$\kappa_{\nu}(\mathbf{i} \rightarrow \mathbf{j}) = \frac{\pi e^2}{mc} N_i f_{ij} \phi_{\nu}$$

N_i = ion density in state i , ϕ_{ν} = profile factor (Gaussian, Lorentzian, or combination of both)

- Total monochromatic κ_{ν} is obtained from summed contributions of all possible transitions

Monochromatic Opacities κ_ν of Fe II on Sun's Surface

- Monochromatic opacity (κ_ν) depends on f_{ij}

$$\kappa_\nu(\mathbf{i} \rightarrow \mathbf{j}) = \frac{\pi e^2}{mc} N_i f_{ij} \phi_\nu$$

- Increased opacity over 3000\AA explains missing radiation from solar surface **TOP: κ_ν of Fe II (Nahar & Pradhan 1993)**. **BOTTOM: solar black body radiation in $2 - 3.5 \times 10^3\text{\AA}$.**

