5. Atomic radiation processes

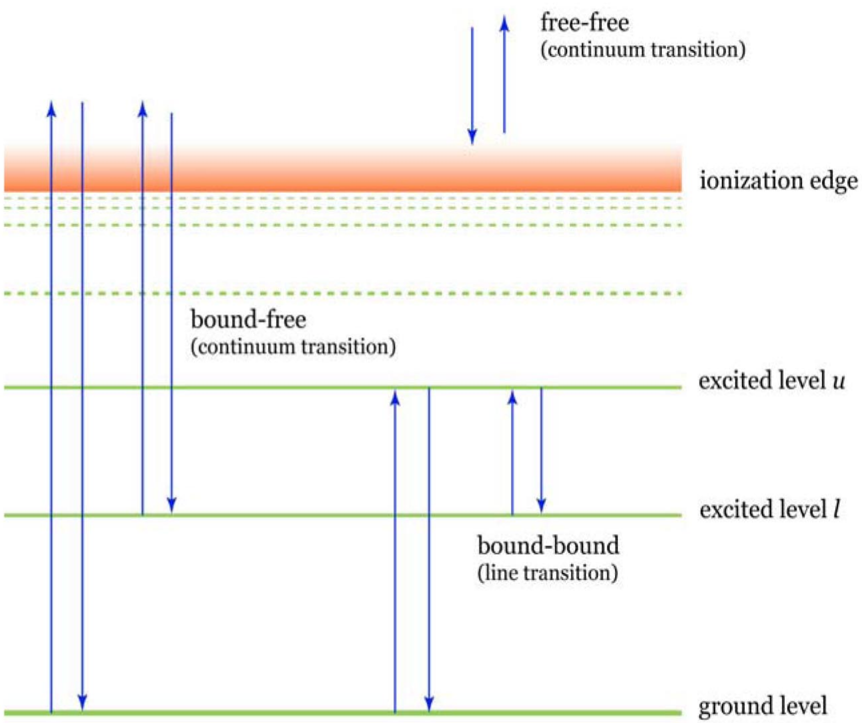
Einstein coefficients for absorption and emission

oscillator strength

line profiles: damping profile, collisional broadening, Doppler broadening

continuous absorption and scattering

Atomic transitions



absorption

$h\nu + E_l \rightarrow E_u$

emission

spontaneous $E_u \rightarrow E_l + h\nu$
(isotropic)

stimulated $h\nu + E_u \rightarrow E_l + 2h\nu$
(direction of incoming photon)

A. Line transitions

Einstein coefficients

probability that a photon in frequency interval $(\nu, \nu + d\nu)$ in the solid angle range $(\omega, \omega + d\omega)$ is <u>absorbed</u> by an atom in the energy level E_l with a resulting transition $E_l \rightarrow E_u$ per second:

$$dw^{\mathrm{abs}}(\nu, \omega, l, u) = B_{lu}\, I_\nu(\omega)\ \varphi(\nu) d\nu\, \frac{d\omega}{4\pi}$$

atomic property

~ no. of incident photons

probability for absorption of photon with $(\nu, \nu + d\nu)$ absorption profile

probability for ω with $(\omega, \omega + d\omega)$

probability for transition l → u

B_{lu}: Einstein coefficient for absorption

Einstein coefficients

similarly for stimulated emission

$$dw^{\mathrm{st}}(\nu,\omega,l,u) = B_{ul}\; I_\nu(\omega)\; \varphi(\nu) d\nu\; \frac{d\omega}{4\pi}$$

B_{ul}: Einstein coefficient for stimulated emission

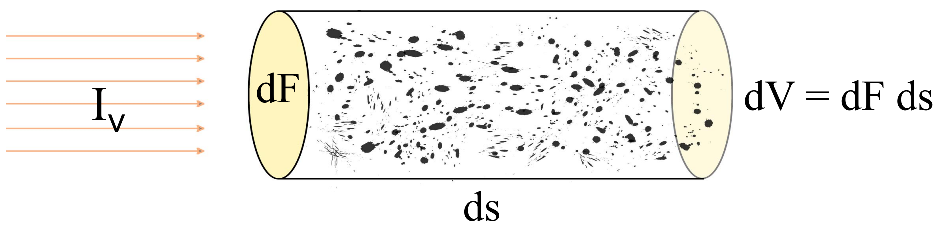
and for spontaneous emission

$$dw^{\mathrm{sp}}(\nu,\omega,l,u) = A_{ul}\; \varphi(\nu) d\nu\; \frac{d\omega}{4\pi}$$

A_{ul}: Einstein coefficient for spontaneous emission

$dw^{st}(\nu,\omega,l,u) = B_{ul}\ I_\nu(\omega)\ \varphi(\nu) d\nu\ \frac{d\omega}{4\pi}$ $\quad dw^{abs}(\nu,\omega,l,u) = B_{lu}\ I_\nu(\omega)\ \varphi(\nu) d\nu\ \frac{d\omega}{4\pi}$

Einstein coefficients, absorption and emission coefficients



Number of absorptions
& stimulated emissions
in dV per second:

$$n_l\ dw^{abs}\ dV, \quad n_u\ dw^{st}\ dV$$

absorbed energy in dV per second:

$$dE_\nu^{abs} = n_l\ h\nu\ dw^{abs}\ dV - n_u\ h\nu\ dw^{st}\ dV$$

stimulated emission counted as negative absorption

and also (using definition of intensity):

$$dE_\nu^{abs} = \kappa_\nu^L\ I_\nu\ ds\ d\omega\ d\nu\ dF$$

Absorption and emission coefficients are a function of Einstein coefficients, occupation numbers and line broadening

$$\boxed{\kappa_\nu^L = \frac{h\nu}{4\pi}\ \varphi(\nu)\ [n_l B_{lu} - n_u B_{ul}]}$$

for the spontaneously emitted energy:

$$\boxed{\epsilon_\nu^L = \frac{h\nu}{4\pi}\ n_u\ A_{ul}\ \varphi(\nu)}$$

$$\boxed{\kappa_\nu^L = \frac{h\nu}{4\pi}\,\varphi(\nu)\,[n_l B_{lu} - n_u B_{ul}]}$$

$$\boxed{\epsilon_\nu^L = \frac{h\nu}{4\pi}\,n_u\,A_{ul}\,\varphi(\nu)}$$

Relations between Einstein coefficients

Einstein coefficients are atomic properties → do not depend on thermodynamic state of matter

We can assume TE: $S_\nu = \frac{\epsilon_\nu^L}{\kappa_\nu^L} = B_\nu(T)$

$$B_\nu(T) = \frac{n_u A_{ul}}{n_l B_{lu} - n_u B_{ul}} = \frac{n_u}{n_l}\frac{A_{ul}}{B_{lu} - \frac{n_u}{n_l}B_{ul}}$$

From the Boltzmann formula: $\frac{n_u}{n_l} = \frac{g_u}{g_l}e^{-\frac{h\nu}{kT}}$

for hv/kT << 1: $\frac{n_u}{n_l} = \frac{g_u}{g_l}\left(1 - \frac{h\nu}{kT}\right)$, $B_\nu(T) = \frac{2\nu^2}{c^2}kT$

$$\frac{2\nu^2}{c^2}kT = \frac{g_u}{g_l}\left(1 - \frac{h\nu}{kT}\right)\frac{A_{ul}}{B_{lu} - \frac{g_u}{g_l}\left(1 - \frac{h\nu}{kT}\right)B_{ul}}$$

for T → ∞

0

$$\boxed{g_l B_{lu} = g_u B_{ul}}$$

$$\frac{2\nu^2}{c^2}kT = \frac{g_u}{g_l}\left(1-\frac{h\nu}{kT}\right)\frac{A_{ul}}{B_{lu}-\frac{g_u}{g_l}\left(1-\frac{h\nu}{kT}\right)B_{ul}}$$

$$\boxed{g_l B_{lu} = g_u B_{ul}}$$

Relations between Einstein coefficients

$$\frac{2\nu^2}{c^2}kT = \frac{g_u}{g_l}\left(1-\frac{h\nu}{kT}\right)\frac{A_{ul}}{B_{lu}}\frac{kT}{h\nu}$$

$$\frac{2\,h\,\nu^3}{c^2} = \frac{A_{ul}}{B_{lu}}\,\frac{g_u}{g_l}\left(1-\frac{h\nu}{kT}\right)$$

for T → ∞

$$A_{ul} = \frac{2\,h\,\nu^3}{c^2}\,\frac{g_l}{g_u}\,B_{lu}$$

$$A_{ul} = \frac{2\,h\,\nu^3}{c^2}\,B_{ul}$$

Note: Einstein coefficients atomic quantities. That means any relationship that holds in a special thermodynamic situation (such as T very large) must be generally valid.

$$\kappa_\nu^L = \frac{h\nu}{4\pi}\,\varphi(\nu)\,B_{lu}\,\left[n_l - \frac{g_l}{g_u}n_u\right]$$

$$\epsilon_\nu^L = \frac{h\nu}{4\pi}\,\varphi(\nu)\,n_u\,\frac{g_l}{g_u}\,\frac{2h\nu^3}{c^2}\,B_{lu}$$

only one Einstein coefficient needed

Oscillator strength

Quantum mechanics

The Einstein coefficients can be calculated by quantum mechanics + classical electrodynamics calculation.

Eigenvalue problem using using wave function:

$$H_{atom}\ |\psi_l >= E_l\ |\psi_l > \qquad H_{atom} = \frac{p^2}{2m} + V_{nucleus} + V_{shell}$$

Consider a time-dependent perturbation such as an external electromagnetic field (light wave) E(t) = E_0 $e^{i\omega t}$.

The potential of the time dependent perturbation on the atom is:

$$V(t) = e \sum_{i=1}^{N} \mathbf{E} \cdot \mathbf{r_i} = \mathbf{E} \cdot \mathbf{d}$$

d: dipol operator

$$[H_{atom} + V(t)]\ |\psi_l >= E_l\ |\psi_l >$$

with transition probability $\sim |<\psi_l|\mathbf{d}|\psi_u>|^2$

Oscillator strength

The result is
$$\frac{h\nu}{4\pi} B_{lu} = \boxed{\frac{\pi e^2}{m_e c}} f_{lu}$$

f_{lu}: oscillator strength (dimensionless)

classical result from electrodynamics

= 0.02654 cm^2/s

Classical electrodynamics

electron quasi-elastically bound to nucleus and oscillates within outer electric field as ***E***.
Equation of motion (damped harmonic oscillator):

$$\ddot{x} + \underbrace{\gamma}_{\text{damping constant}} \dot{x} + \underbrace{\omega_0^2}_{\text{resonant (natural) frequency}} x = \frac{e}{m_e} E$$

$$\gamma = \frac{2\,\omega_0^2 e^2}{3\,m_e c^3} = \frac{8\pi^2 e^2\,\nu_0^2}{3\,m_e c^3}$$

$$\omega_0 = 2\pi\nu_0$$

ma = damping force + restoring force + EM force

the electron oscillates preferentially at resonance (incoming radiation $\nu = \nu_0$)

The damping is caused, because the de- and accelerated electron radiates

Classical cross section and oscillator strength

Calculating the power absorbed by the oscillator, the integrated "classical" absorption coefficient and cross section, and the absorption line profile are found:

integrated over the line profile $$\int \kappa_\nu^{L,cl} d\nu = n_l \frac{\pi e^2}{m_e c} = n_l \; \sigma_{\rm tot}^{cl}$$

n_l: number density of absorbers

σ_{tot}^{cl}: classical cross section (cm^2/s)

$$\varphi(\nu) d\nu = \frac{1}{\pi} \frac{\gamma/4\pi}{(\nu-\nu_0)^2 + (\gamma/4\pi)^2} \qquad \text{[Lorentz (damping) line profile]}$$

oscillator strength f_{lu} is quantum mechanical correction to classical result

(effective number of classical oscillators, ≈ 1 for strong resonance lines)

From $\kappa_\nu^L = \frac{h\nu}{4\pi} \varphi(\nu) \; n_l B_{lu}$ (neglecting stimulated emission)

Oscillator strength

$$\frac{h\nu}{4\pi}\,\varphi(\nu)\;B_{lu} = \frac{\pi e^2}{m_e c}\,\varphi(\nu)\;f_{lu} = \sigma_{lu}(\nu)$$

absorption cross section;
dimension is cm^2

$$f_{lu} = \frac{1}{4\pi}\,\frac{m_e c}{\pi e^2}\,h\nu\;B_{lu}$$

Oscillator strength (f-value) is different for each atomic transition

Values are determined empirically in the laboratory or by elaborate numerical atomic physics calculations

Semi-analytical calculations possible in simplest cases, e.g. hydrogen

$$f_{lu} = \frac{2^5}{3^{3/2}\pi}\frac{g}{l^5u^3}\left(\frac{1}{l^2}-\frac{1}{u^2}\right)^{-3}$$

g: Gaunt factor

Hα : f=0.6407

Hβ : f=0.1193

Hγ : f=0.0447

Line profiles

line profiles contain information on physical conditions of the gas and chemical abundances

analysis of line profiles requires knowledge of distribution of opacity with frequency

several mechanisms lead to line broadening (no infinitely sharp lines)

- natural damping: finite lifetime of atomic levels
- collisional (pressure) broadening: impact vs quasi-static approximation
- Doppler broadening: convolution of velocity distribution with atomic profiles

1. Natural damping profile

finite lifetime of atomic levels → line width

NATURAL LINE BROADENING OR RADIATION DAMPING

$t = 1 / A_{ul}$ (¼ 10^{-8} s in H atom 2 → 1): finite lifetime with respect to spontaneous emission

$\Delta E\, t \geq h/2\pi$ uncertainty principle

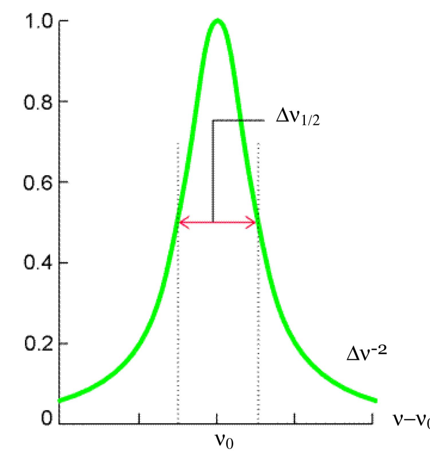
line broadening

$\Delta \nu_{1/2} = \Gamma / 2\pi$

$\Delta \lambda_{1/2} = \Delta \nu_{1/2} \lambda^2/c$

e.g. Ly α: $\Delta \lambda_{1/2} = 1.2\ 10^{-4}$ A

Hα: $\Delta \lambda_{1/2} = 4.6\ 10^{-4}$ A



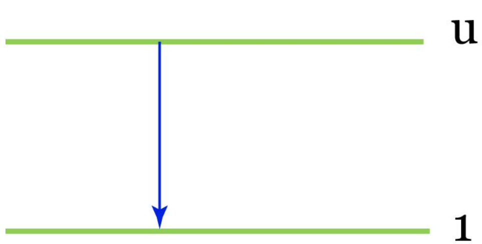
$$\boxed{\varphi(\nu) = \frac{1}{\pi} \frac{\Gamma/4\pi}{(\nu-\nu_0)^2 + (\Gamma/4\pi)^2}}$$

Lorentzian profile

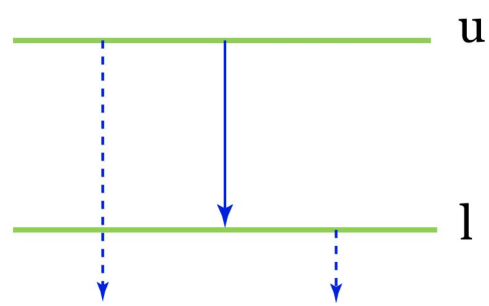
Natural damping profile

resonance line

$$\Gamma = A_{u1}$$



excited line



$$\Gamma_u = \sum_i A_{ui}$$

$$\Gamma_l = \sum_i A_{li}$$

$$\Gamma = \Gamma_u + \Gamma_l$$

natural line broadening is important for <u>strong lines</u> (resonance lines) at <u>low densities</u> (no additional broadening mechanisms)

e.g. Ly α in interstellar medium

but also in stellar atmospheres

2. Collisional broadening

radiating atoms are perturbed by the electromagnetic field of neighbour atoms, ions, electrons, molecules

energy levels are temporarily modified through the Stark - effect: perturbation is a function of separation absorber-perturber

energy levels affected → line shifts, asymmetries & **broadening**

$$\Delta E(t) = h\,\Delta\nu = C/r^n(t)$$

r: distance to perturbing atom

a) impact approximation: radiating atoms are perturbed by passing particles at distance r(t). Duration of collision << lifetime in level → lifetime shortened → line broader

in all cases a *Lorentzian profile* is obtained (but with larger total Γ than only natural damping)

b) quasi-static approximation: applied when duration of collisions >> life time in level → consider stationary distribution of perturbers

Collisional broadening

n = 2 linear Stark effect $\Delta E \sim F$

for levels with degenerate angular momentum (e.g. HI, HeII)

field strength $F \sim 1/r^2$

$\rightarrow \Delta E \sim 1/r^2$

<u>important for H I lines</u>, in particular in hot stars (high number density of free electrons and ions). However , for ion collisional broadening the quasi-static broadening is also important for strong lines (see below) $\rightarrow \Gamma_{\mathbf{e}} \sim n_e$

n = 3 resonance broadening

atom A perturbed by atom A' of same species

important in cool stars, e.g. Balmer lines in the Sun

$\rightarrow \Delta E \sim 1/r^3$ $\rightarrow \Gamma_{\mathbf{e}} \sim n_e$

Collisional broadening

n = 4 quadratic Stark effect $\Delta E \sim F^2$

field strength $F \sim 1/r^2$

$\rightarrow \Delta E \sim 1/r^4$ (no dipole moment)

important for metal ions broadened by e^- in hot stars $\rightarrow$ Lorentz profile with $\Gamma_e \sim n_e$

n = 6 van der Waals broadening

atom A perturbed by atom B

important in cool stars, e.g. Na perturbed by H in the Sun $\rightarrow \Gamma_e \sim n_e$

Quasi-static approximation

$$t_{perturbation} >> \tau = 1/A_{ul}$$

→ perturbation practically constant during emission or absorption

atom radiates in a statistically fluctuating field produced by 'quasi-static' perturbers, e.g. slow-moving ions

given a distribution of perturbers → field at location of absorbing or emitting atom

statistical frequency of particle distribution

→ probability of fields of different strength (each producing an energy shift $\Delta E = h\,\Delta\nu$)

→ field strength distribution function

→ line broadening

Linear Stark effect of H lines can be approximated to 0^{st} order in this way

Quasi-static approximation for hydrogen line broadening

Line broadening profile function determined by probability function for electric field caused by all other particles as seen by the radiating atom.

W(F) dF: probability that field seen by radiating atom is F

$$\varphi(\Delta\nu)\, d\nu = W(F)\frac{dF}{d\nu}\, d\nu$$

For calculating W(F)dF we use as a first step the nearest-neighbor approximation: main effect from nearest particle

Quasi-static approximation – nearest neighbor approximation

assumption: main effect from nearest particle ($F \sim 1/r^2$)

we need to calculate the probability that nearest neighbor is in the distance range (r,r+dr) = probability that none is at distance < r and one is in (r,r+dr)

$$W(r)\,dr = [1 - \int_0^r W(x)\,dx]\,(4\pi r^2 N)\,dr$$

Integral equation for W(r) differentiating → differential equation

probability for no particle in (0,r)

relative probability for particle in shell (r,r+dr)
N: particle density

$$\frac{d}{dr}\left[\frac{W(r)}{4\pi r^2 N}\right] = -W(r) = -4\pi r^2 N\left[\frac{W(r)}{4\pi r^2 N}\right]$$

Differential equation

$$W(r) = 4\pi r^2 N e^{-\frac{4}{3}\pi r^3 N}$$

Normalized solution

Linear Stark effect: $h\Delta\nu \sim F$

$$F \sim \frac{1}{r^2}$$

Quasi-static approximation

mean interparticle distance: $r_0 = \left(\frac{4}{3}\pi N\right)^{-1/3}$ $\quad W(r)dr = e^{-\frac{r}{r_0}^3} d\{\frac{r}{r_0}\}^3$

normal field strength: $F_0 \sim \frac{1}{r_0^2}$

define: $\beta = \frac{F}{F_0} = \{\frac{r_0}{r}\}^2$

note: at high particle density → large F_0

→ stronger broadening

from W(r) dr → W(β) dβ: $W(\beta)d\beta = \frac{3}{2}\beta^{-5/2}e^{-\beta^{-3/2}}d\beta$

$$W(\beta) \sim \beta^{-5/2} \quad \text{for} \quad \beta \to \infty$$

Stark broadened line profile in the wings, not $\Delta\lambda^{-2}$ as for natural or impact broadening

$$\Delta\nu \sim \beta \qquad \phi(\Delta\nu) \sim \Delta\nu^{-5/2}$$

Quasi-static approximation – advanced theory

complete treatment of an ensemble of particles: Holtsmark theory

+ interaction among perturbers (Debye shielding of the potential at distances > Debye length)

Holtsmark (1919),

Chandrasekhar (1943, Phys. Rev. 15, 1)

$$W(\beta) = \frac{2\beta}{\pi} \int_0^\infty e^{-y^{3/2}} y \; sin(\beta y) dy$$

Ecker (1957, Zeitschrift f. Physik, 148, 593 & 149,245)

$$W(\beta) = \frac{2\beta\delta^{4/3}}{\pi} \int_0^\infty e^{-\delta g(y)} y \; sin(\delta^{2/3}\beta y) dy$$

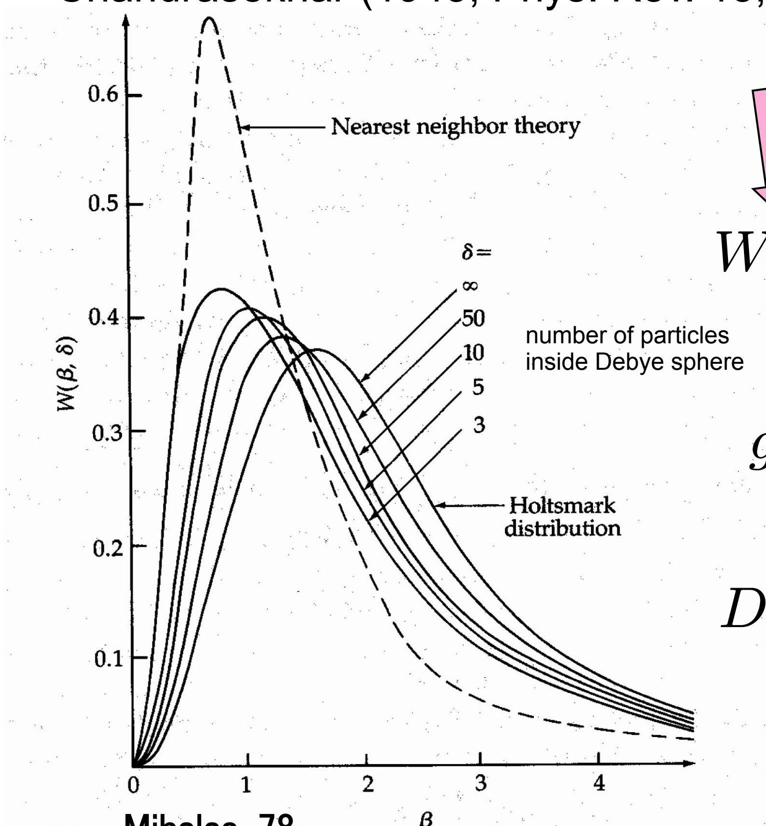
$$g(y) = \frac{2}{3} y^{3/2} \int_y^\infty (1 - z^{-1} sinz) z^{-5/2} dz$$

$$D = 4.8 \frac{T}{n_e}^{1/2} cm$$

Debye length, field of ion vanishes beyond D

$$\delta = \frac{4\pi}{3} D^3 N$$

number of particles inside Debye sphere



Mihalas, 78

3. Doppler broadening

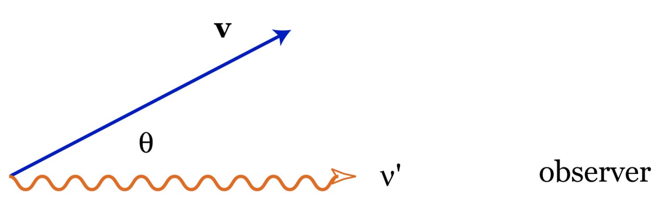
radiating atoms have thermal velocity

Maxwellian distribution:

$$P(v_x, v_y, v_z)\, dv_x dv_y dv_z = \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{m}{2kT}(v_x^2+v_y^2+v_z^2)}\, dv_x dv_y dv_z$$

Doppler effect: atom with velocity v emitting at frequency ν', observed at frequency ν :

$$\nu' = \nu - \nu\frac{v\cos\theta}{c}$$



$$\Delta\nu_D = \nu_0 \frac{\xi_0}{c}$$

Doppler broadening

Define the velocity component along the line of sight: ξ

The Maxwellian distribution for this component is:

$$P(\xi)\, d\xi = \frac{1}{\pi^{1/2}\xi_0} e^{-\left(\frac{\xi}{\xi_0}\right)^2}\, d\xi$$

$$\xi_0 = (2kT/m)^{1/2}$$ thermal velocity

→ $$\nu' = \nu - \nu\frac{\xi}{c}$$

if we observe at ν, an atom with velocity component ξ absorbs at ν' in its frame

if v/c <<1 → $(\nu' - \nu)/\nu \ll 1$

line center

$$\Delta\nu = \nu' - \nu = -\nu\frac{\xi}{c} = -[(\nu - \nu_0) + \nu_0]\,\frac{\xi}{c} \approx -\nu_0\,\frac{\xi}{c}$$

$$P(\xi)\, d\xi = \frac{1}{\pi^{1/2}\xi_0} e^{-\left(\frac{\xi}{\xi_0}\right)^2} d\xi$$

$$\xi_0 = (2kT/m)^{1/2}$$

Doppler broadening

line profile for v = 0 → profile for v ≠ 0 $\nu \to \nu'$

$$\varphi^R(\nu - \nu_0) \implies \varphi^R(\nu' - \nu_0) = \varphi(\nu - \nu_0 - \nu_0 \frac{\xi}{c})$$

New line profile: convolution

$$\varphi^{\text{new}}(\nu - \nu_0) = \int_{-\infty}^{\infty} \varphi(\nu - \nu_0 - \nu_0 \frac{\xi}{c})\, P(\xi)\, d\xi$$

profile function in rest frame

velocity distribution function

$$P(\xi)\,d\xi = \frac{1}{\pi^{1/2}\xi_0} e^{-\left(\frac{\xi}{\xi_0}\right)^2}\,d\xi$$

$$\Delta\nu_D = \nu_0 \frac{\xi_0}{c}$$

$$\xi_0 = (2kT/m)^{1/2}$$

Doppler broadening: sharp line approximation

$$\Rightarrow \quad \varphi^{\mathrm{new}}(\nu-\nu_0) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \varphi\left(\nu-\nu_0-\nu_0\frac{\xi_0}{c}\frac{\xi}{\xi_0}\right) e^{-\left(\frac{\xi}{\xi_0}\right)^2} \frac{d\xi}{\xi_0}$$

$\Delta\nu_D$: Doppler width of the line

$$\Delta\nu_D = 4.301 \times 10^{-7}\nu(T/\mu)^{1/2}$$
$$\Delta\lambda_D = 4.301 \times 10^{-7}\lambda(T/\mu)^{1/2}$$

$\xi_0 = (2kT/m)^{1/2}$ thermal velocity

Approximation 1: assume a sharp line – half width of profile function << $\Delta\nu_D$

$\Rightarrow$ $\varphi(\nu-\nu_0) \approx \delta(\nu-\nu_0)$ delta function

$$\Delta\nu_D = \nu_0 \frac{\xi_0}{c}$$

Doppler broadening: sharp line approximation

$$\varphi^{\mathrm{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \delta(\nu - \nu_0 - \Delta\nu_D \frac{\xi}{\xi_0})\, e^{-\left(\frac{\xi}{\xi_0}\right)^2} \frac{d\xi}{\xi_0}$$

$$\delta(a\, x) = \frac{1}{a}\, \delta(x)$$

$$\varphi^{\mathrm{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \delta\left(\frac{\nu - \nu_0}{\Delta\nu_D} - \frac{\xi}{\xi_0}\right) e^{-\left(\frac{\xi}{\xi_0}\right)^2} \frac{d\xi}{\Delta\nu_D\, \xi_0}$$

$$\boxed{\varphi^{\mathrm{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2}\, \Delta\nu_D} e^{-\left(\frac{\nu - \nu_0}{\Delta\nu_D}\right)^2}}$$

Gaussian profile – valid in the line core

$$\varphi^{\text{new}}(\nu - \nu_0) = \int_{-\infty}^{\infty} \varphi(\nu - \nu_0 - \nu_0 \frac{\xi}{c})\; P(\xi)\; d\xi$$

Doppler broadening: Voigt function

Approximation 2: assume a Lorentzian profile – half width of profile function > $\Delta\nu_D$

$$\varphi(\nu) = \frac{1}{\pi} \frac{\Gamma/4\pi}{(\nu - \nu_0)^2 + (\Gamma/4\pi)^2}$$

$$\Rightarrow \quad \varphi^{\text{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2}\, \Delta\nu_D} \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{\left(\frac{\Delta\nu}{\Delta\nu_D} - y\right)^2 + a^2}\, dy \qquad a = \frac{\Gamma}{4\pi \Delta\nu_D}$$

$$\boxed{\varphi^{\text{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2}\, \Delta\nu_D}\; H\left(a, \frac{\nu - \nu_0}{\Delta\nu_D}\right)}$$

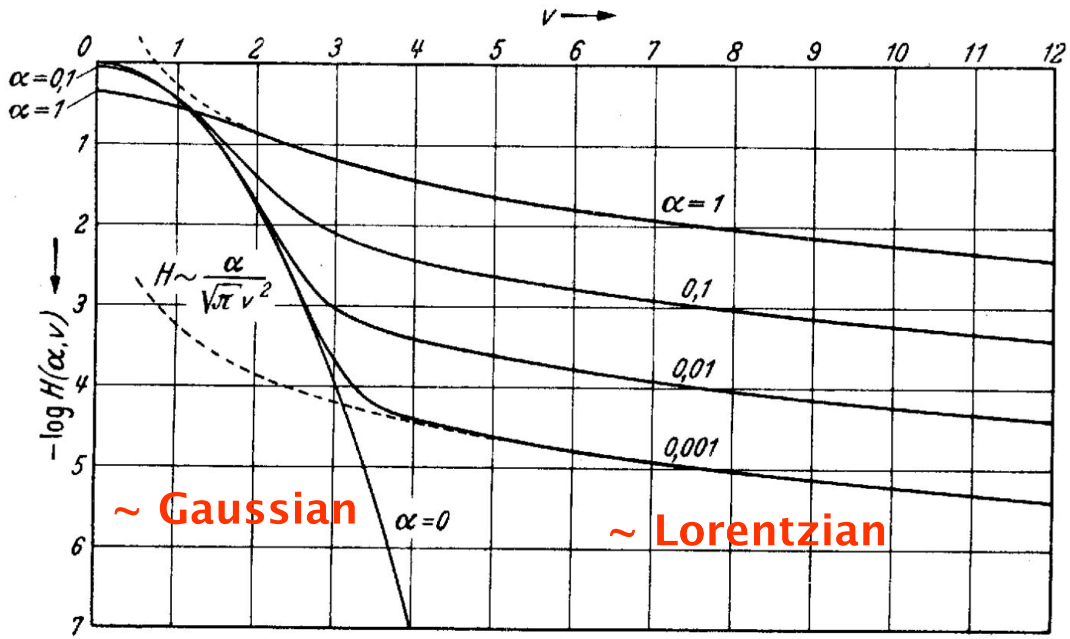
$\downarrow$

Voigt function (Lorentzian * Gaussian):
calculated numerically

$$\varphi^{\mathrm{new}}(\nu-\nu_0) = \frac{1}{\pi^{1/2}\,\Delta\nu_D}\,\frac{a}{\pi}\int_{-\infty}^{\infty}\frac{e^{-y^2}}{\left(\frac{\Delta\nu}{\Delta\nu_D}-y\right)^2+a^2}\,dy \qquad a=\frac{\Gamma}{4\pi\Delta\nu_D}$$

Voigt function: core Gaussian, wings Lorentzian

normalization: $$\int_{-\infty}^{\infty} H(a,v)\,dv = \sqrt{\pi}$$



usually α <<1

max at v=0:

H(α,v=0) ≈ 1-α

Unsoeld, 68

Doppler broadening: Voigt function

Approximate representation of Voigt function:

$$H\left(a, \frac{\nu-\nu_0}{\Delta\nu_D}\right) \approx e^{-\left(\frac{\nu-\nu_0}{\Delta\nu_D}\right)^2}$$

line core: Doppler broadening

$$\approx \frac{a}{\pi^{1/2}\left(\frac{\nu-\nu_0}{\Delta\nu_D}\right)^2}$$

line wings: damping profile
only visible for strong lines

General case: for any intrinsic profile function (Lorentz, or Holtsmark, etc.) – the observed profile is obtained from numerical convolution with the different broadening functions and finally with Doppler broadening

General case: two broadening mechanisms

$\varphi_1(\Delta\lambda)$ two broadening functions representing

$\varphi_2(\Delta\lambda)$ two broadening mechanisms

$$\varphi^{\text{new}}(\Delta\lambda) = \int_{-\infty}^{\infty} \varphi_1(\Delta\lambda - \overline{\Delta\lambda})\varphi_2(\overline{\Delta\lambda})d\overline{\Delta\lambda}$$

Resulting broadening function is convolution of the two individual broadening functions

$$\varphi^{\text{new}} = \varphi_1 \otimes \varphi_2$$

4. Microturbulence broadening

In addition to thermal velocity: Macroscopic turbulent motion of stellar atmosphere gas within optically thin volume elements. This is approximated by an additional Maxwellian velocity distribution.

Additional Gaussian broadening function in absorption coefficient

$$\boxed{\varphi^{\mathrm{micro}}(\nu - \nu_0) = \frac{1}{\pi^{1/2}\,\Delta\nu_{micro}} e^{-\left(\frac{\nu-\nu_0}{\Delta\nu_{micro}}\right)^2}}$$

$$\boxed{\Delta\nu_{micro} = \nu_0 \frac{v_{micro}}{c}}$$

$$\Delta\lambda = \frac{v_{rot} sini}{c}\frac{x}{R}$$

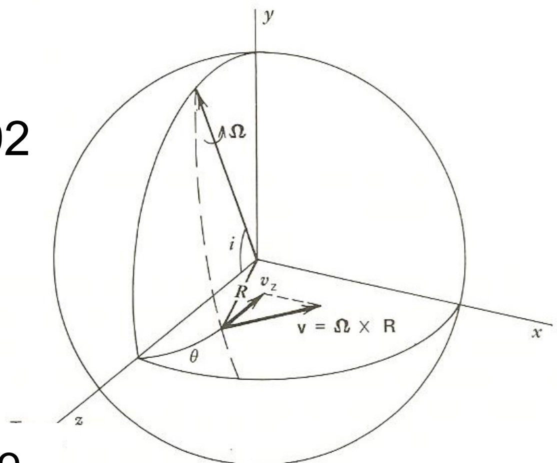
blueshift

If the star rotates, some surface elements move towards the observer and some away

redshift

5. Rotational broadening

Gray, 1992



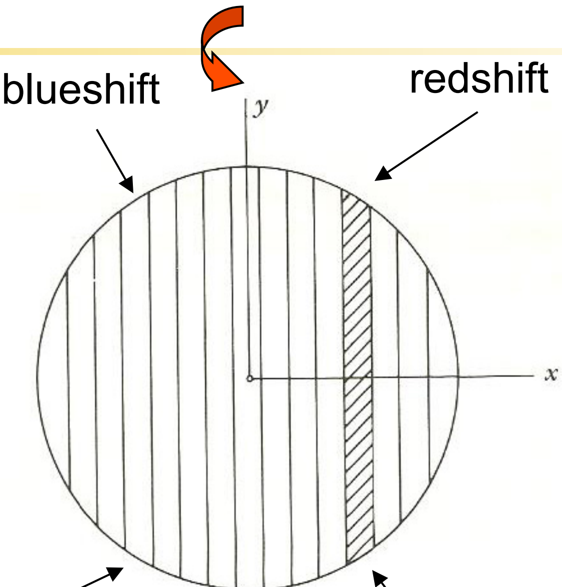
to observer

Rotational velocity at equator: $v_{rot} = \Omega \cdot R$

Observer sees v_{rot} sini

blueshift

redshift



$$\frac{\Delta\lambda}{\lambda} = -\frac{v_{rot} sin(i)}{c}\frac{x}{R}$$

$$\frac{\Delta\lambda}{\lambda} = +\frac{v_{rot} sin(i)}{c}\frac{x}{R}$$

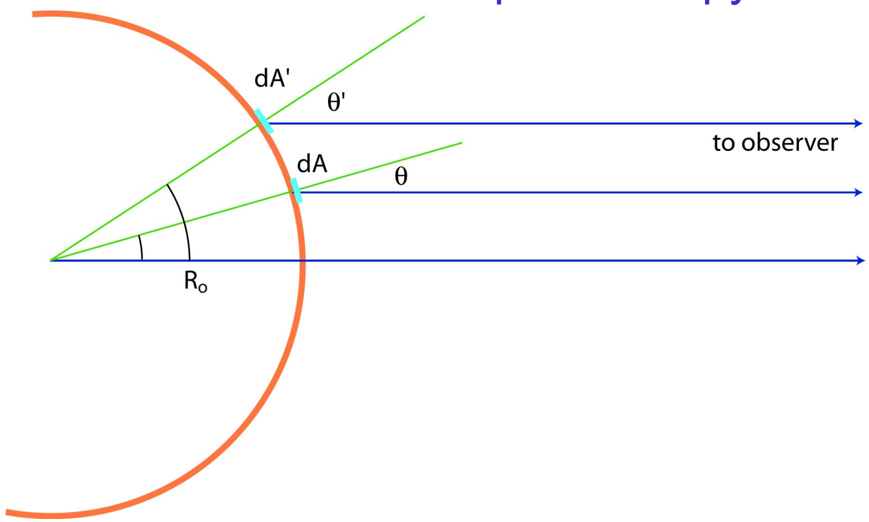
stripes of constant wavelength shift

$$I(\lambda) \rightarrow I(\lambda + \Delta\lambda)$$

Intensity shifts in wavelength along stripe

Rotation and observed line profile

stellar spectroscopy uses mostly normalized spectra → F_λ / $F^{continuum}$



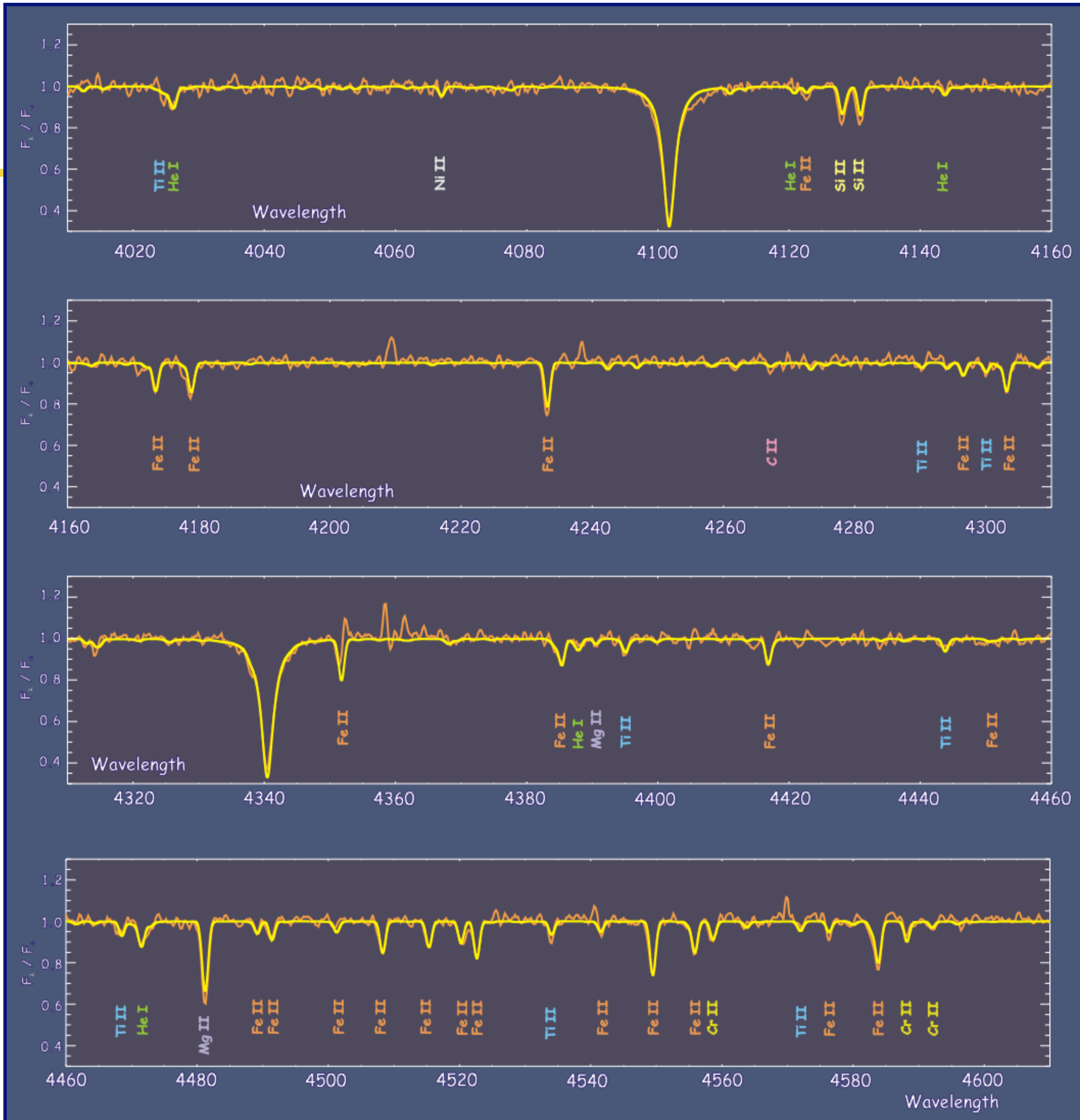
$$\pi F(\lambda) = \int I(\lambda, cos\theta) cos\theta \frac{dA}{R^2}$$

integral over stellar disk towards observer, also integral over all solid angles for one surface element

$$P(\lambda) = F(\lambda)/F^c$$

observed stellar line profile

$F_\lambda / F_{continuum}$



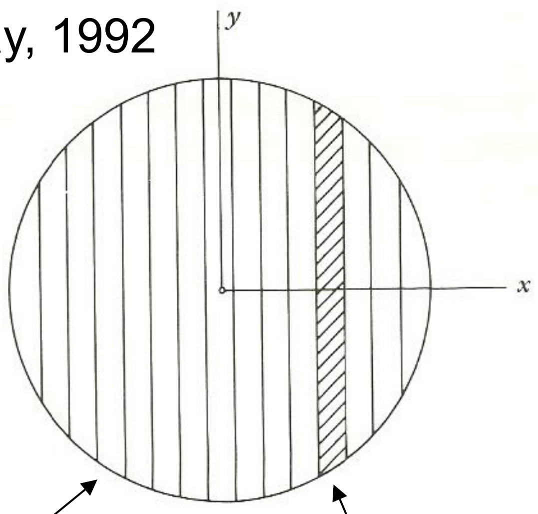
M33 A supergiant
Keck (ESI)

U, Urbaneja, Kudritzki, 2009, ApJ 740, 1120

Rotation changes integral over stellar surface

stellar spectroscopy uses mostly normalized spectra → F_λ / $F^{continuum}$

Gray, 1992



$$\frac{\Delta\lambda}{\lambda} = -\frac{v_{rot} sin(i)}{c}\frac{x}{R} \qquad \frac{\Delta\lambda}{\lambda} = +\frac{v_{rot} sin(i)}{c}\frac{x}{R}$$

$$\pi F(\lambda) = \int I(\lambda - \Delta\lambda, cos\theta) cos\theta \frac{dA}{R^2}$$

integral over stellar disk towards observer

$$P(\lambda) = F(\lambda)/F^c(\lambda)$$

observed stellar line profile

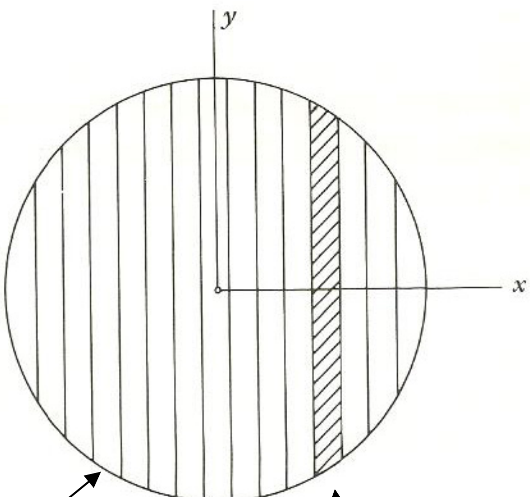
Correct treatment by numerical integral over stellar surface with intensity calculated by model atmosphere

$$\pi F(\lambda) = \int I(\lambda - \Delta\lambda, cos\theta) cos\theta \frac{dA}{R^2} \qquad P(\lambda) = I(\lambda, cos\theta)/I_c(\lambda, cos\theta)$$

Approximation: assume intrinsic P_λ const. over surface independent of cosθ

$$\pi F(\lambda) = \int P(\lambda - \Delta\lambda) I^c(cos\theta) cos\theta \frac{dA}{R^2}$$

integral of Doppler shifted profile over stellar disk and weighted by continuum intensity towards obs.



$$dA = \frac{1}{cos\theta} dxdy \qquad \pi F(\lambda) = \int\int P(\lambda - \Delta\lambda) I^c(cos\theta) \frac{dxdy}{R^2}$$

$$\frac{\Delta\lambda}{\lambda} = \frac{v_{rot} sin(i)}{c} \frac{x}{R} \qquad \frac{x}{R} = \frac{\Delta\lambda}{\Delta\lambda_{rot}} = \tilde{x} \qquad \frac{y}{R} = \tilde{y}$$

$$\pi F(\lambda) = 2 \int_{-1}^{1} P(\lambda - \Delta\lambda) \int_0^{\sqrt{1-\tilde{x}^2}} I^c(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x}$$

$$I^c = I_0(1 + \beta cos\theta)$$
$$cos\theta = \sqrt{1 - (\tilde{x}^2 + \tilde{y}2}$$

continuum limb darkening

$$\frac{\Delta\lambda}{\lambda} = -\frac{v_{rot} sin(i)}{c} \frac{x}{R}$$

$$\frac{\Delta\lambda}{\lambda} = +\frac{v_{rot} sin(i)}{c} \frac{x}{R}$$

$$\pi F(\lambda) = 2I_0 \int_{-1}^{1} P(\lambda - \Delta\lambda) \int_0^{\sqrt{1-\tilde{x}^2}} (1 + \beta\sqrt{1 - (\tilde{x}^2 + \tilde{y}^2)}) d\tilde{y} d\tilde{x}$$

$$\pi F^c = 2I_0 \int_{-1}^{1} \int_0^{\sqrt{1-\tilde{x}^2}} (1 + \beta\sqrt{1 - (\tilde{x}^2 + \tilde{y}^2)}) d\tilde{y} d\tilde{x}$$

$$\pi F(\lambda) = 2I_0 \int_{-1}^{1} P(\lambda - \Delta\lambda) \int_0^{\sqrt{1-\tilde{x}^2}} (1 + \beta\sqrt{1 - (\tilde{x}^2 + \tilde{y}^2)})d\tilde{y}d\tilde{x}$$

$$\pi F^c = 2I_0 \int_{-1}^{1} \int_0^{\sqrt{1-\tilde{x}^2}} (1 + \beta\sqrt{1 - (\tilde{x}^2 + \tilde{y}^2)})d\tilde{y}d\tilde{x}$$

$$P_{rot}(\lambda) = \frac{F(\lambda)}{F_c}$$

$$P_{rot}(\lambda) = \frac{\int_{-1}^{1} P[\lambda - \Delta\lambda(\tilde{x})]A(\tilde{x})d\tilde{x}}{\int_{-1}^{1} A(\tilde{x})d\tilde{x}} \qquad A(\tilde{x}) = \int_0^{\sqrt{1-\tilde{x}^2}} (1 + \beta\sqrt{1 - \tilde{x}^2 + \tilde{y}^2})d\tilde{y}$$

$$P_{rot}(\lambda) = \int_{-1}^{1} P[\lambda - \Delta\lambda(\tilde{x})]G[\Delta\lambda(\tilde{x})]d\tilde{x}$$

using

$$\int \sqrt{a^2 - x^2}dx = \frac{1}{2}(x\sqrt{a^2 - x^2} + a^2 arcsin\frac{x}{a})$$

and normalization →

$$G[\Delta\lambda(\tilde{x}] = \frac{\frac{2}{\pi}\sqrt{1 - \tilde{x}^2} + \frac{\beta}{2}(1 - \tilde{x}^2)}{1 + \frac{2}{3}\beta}$$

rotational line broadening

profile function

Rotational line broadening

$$\tilde{x} = \frac{\Delta\lambda}{\Delta\lambda_{rot}}$$

$$G[\Delta\lambda(\tilde{x})] = \frac{\frac{2}{\pi}\sqrt{1-\tilde{x}^2} + \frac{\beta}{2}(1-\tilde{x}^2)}{1+\frac{2}{3}\beta}$$

$$\Delta\lambda = \lambda \frac{v_{rot} sin(i)}{c} \frac{x}{R}$$

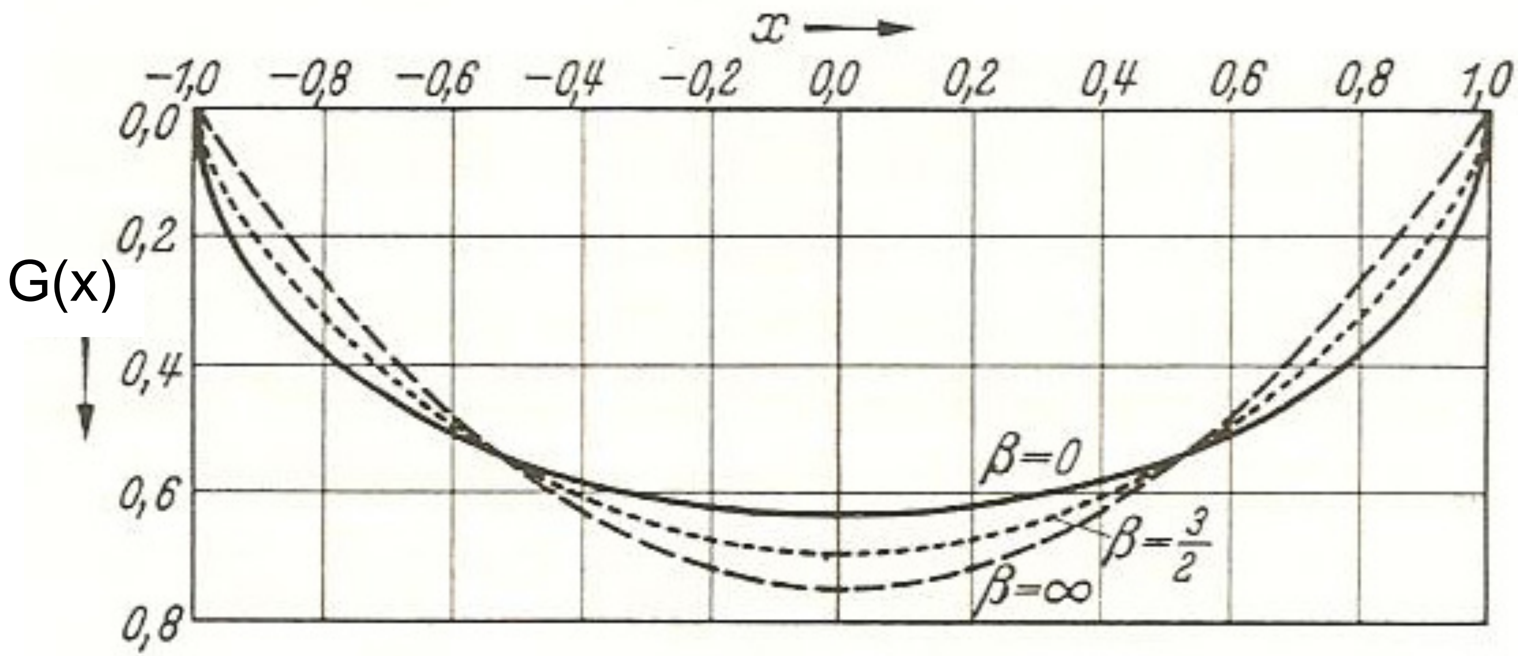
$$P_{rot}(\lambda) = \int_{-\Delta\lambda_{rot}}^{\Delta\lambda_{rot}} P(\lambda - \Delta\lambda) G(\Delta\lambda) d\Delta\lambda$$

Rotationally broadened line profile

$$P_{rot} = P \otimes G$$

convolution of original profile with rotational broadening function

Rotational broadening profile function

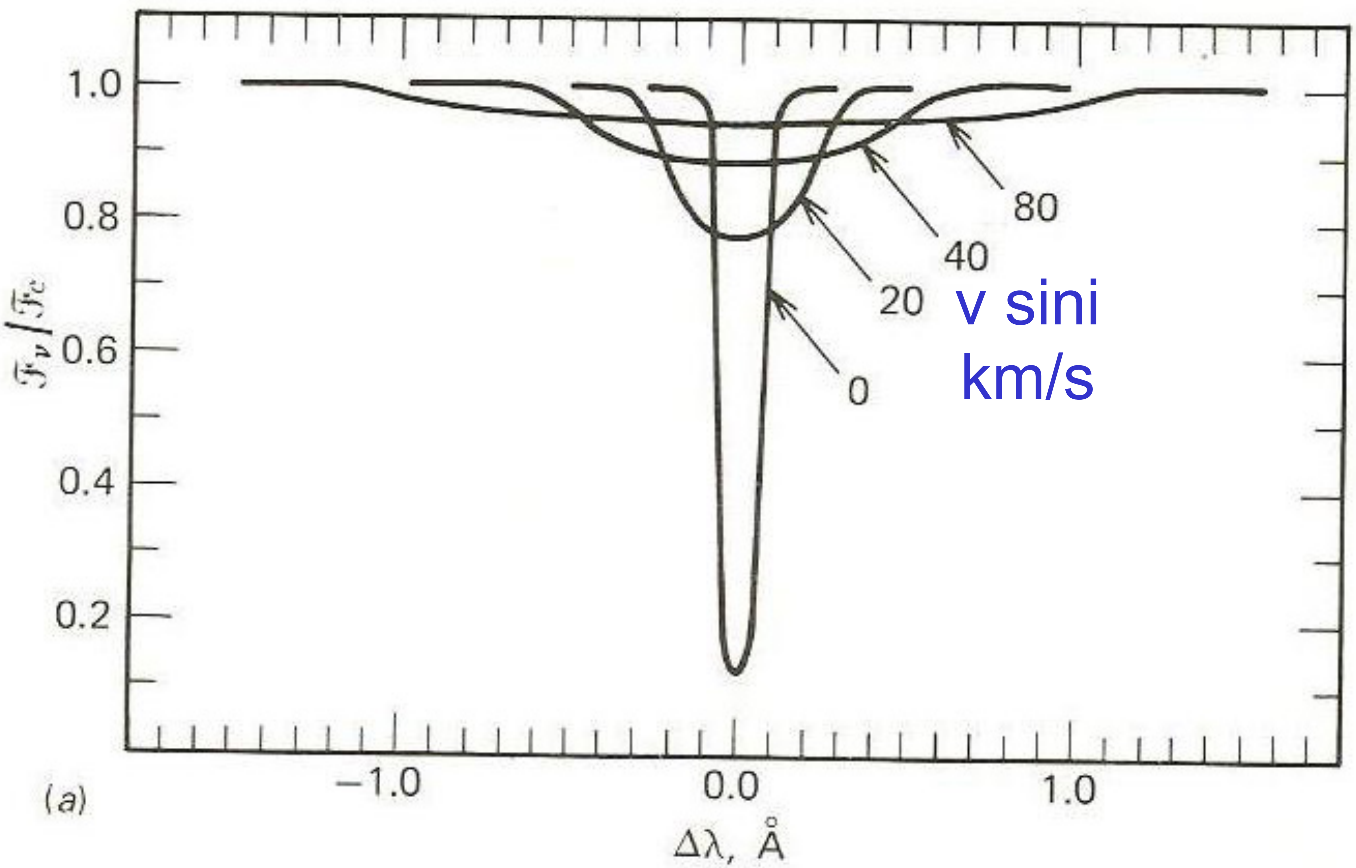


$$x = \frac{\Delta\lambda}{\Delta\lambda_{rot}}$$

Unsoeld, 1968

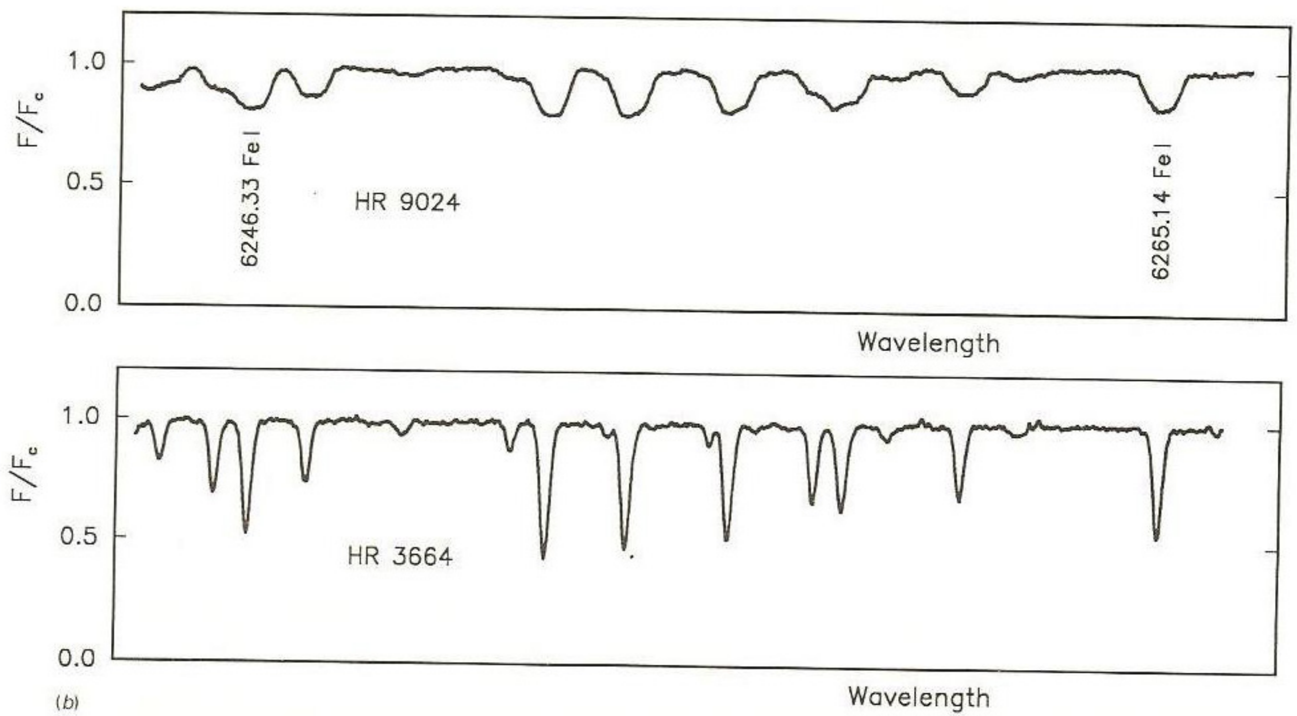
Note: rotation does not change equivalent width!!!

Rotationally broadened line profiles



Gray, 1992

observed stellar line profiles



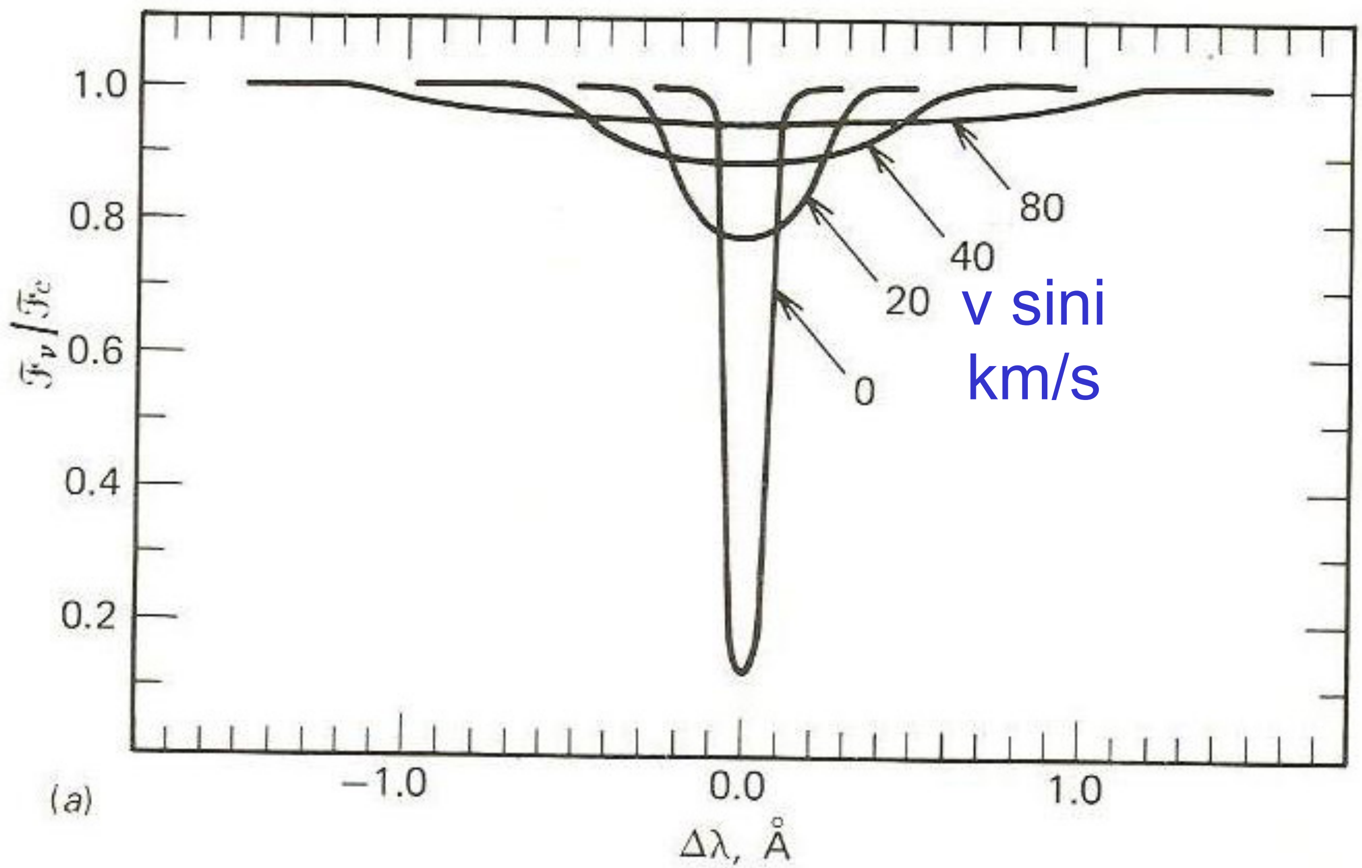
v sini large

v sini small

Gray, 1992

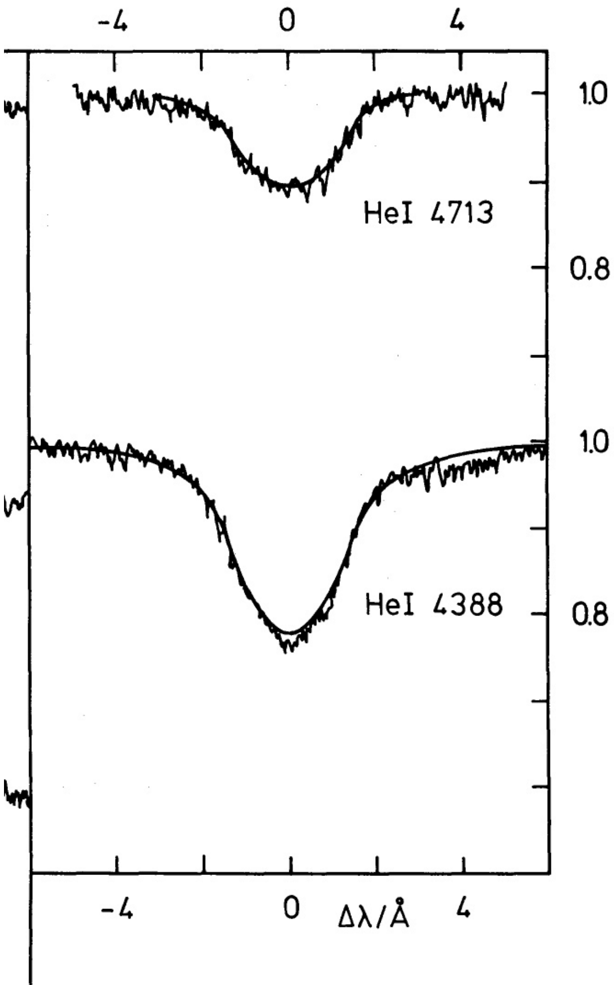
Note: rotation does not change equivalent width!!!

Rotationally broadened line profiles



Gray, 1992

observed stellar line profiles



θ Car, B0V
vsini~250 km/s

Schoenberner, Kudritzki et al. 1988

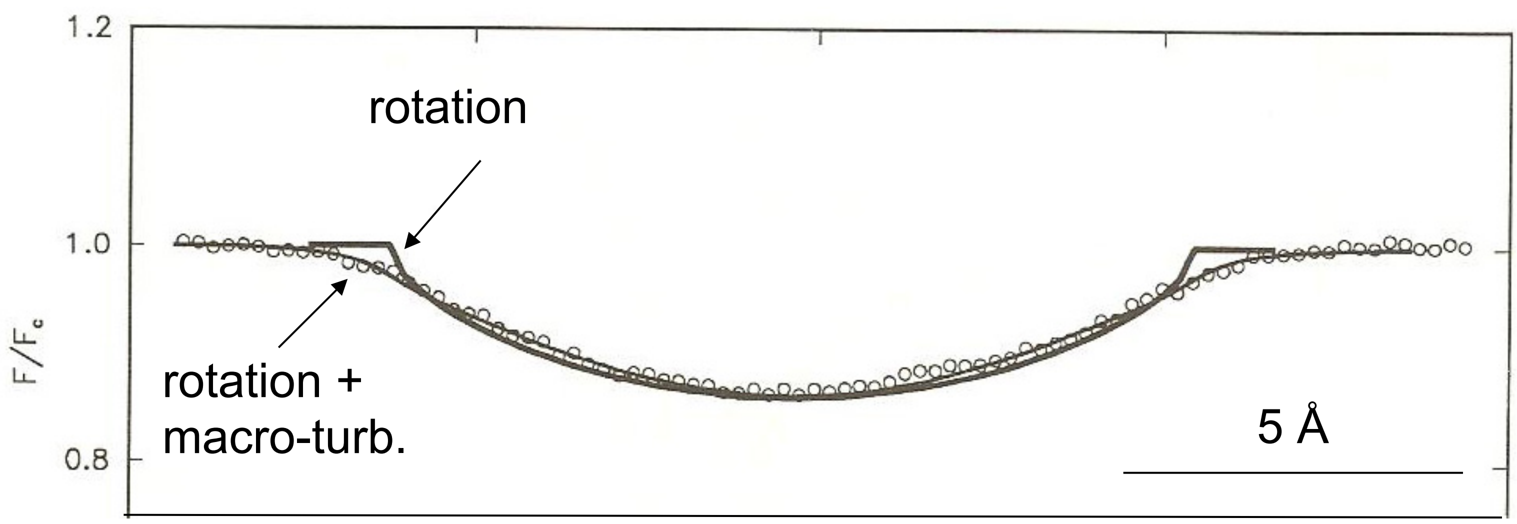
6. Macro-turbulence

The macroscopic motion of optically thick surface volume elements is approximated by a Maxwellian velocity distribution. This broadens the emergent line profiles in addition to rotation

$$\Phi^{\mathrm{macro}}(\lambda - \lambda_0) = \frac{1}{\pi^{1/2}\,\Delta\lambda_{macro}} e^{-\left(\frac{\lambda-\lambda_0}{\Delta\lambda_{macro}}\right)^2} \qquad \Delta\lambda_{micro} = \lambda_0 \frac{v_{macro}}{c}$$

$$\boxed{P_{observed} = P \otimes G^{rot} \otimes \Phi^{macro}}$$

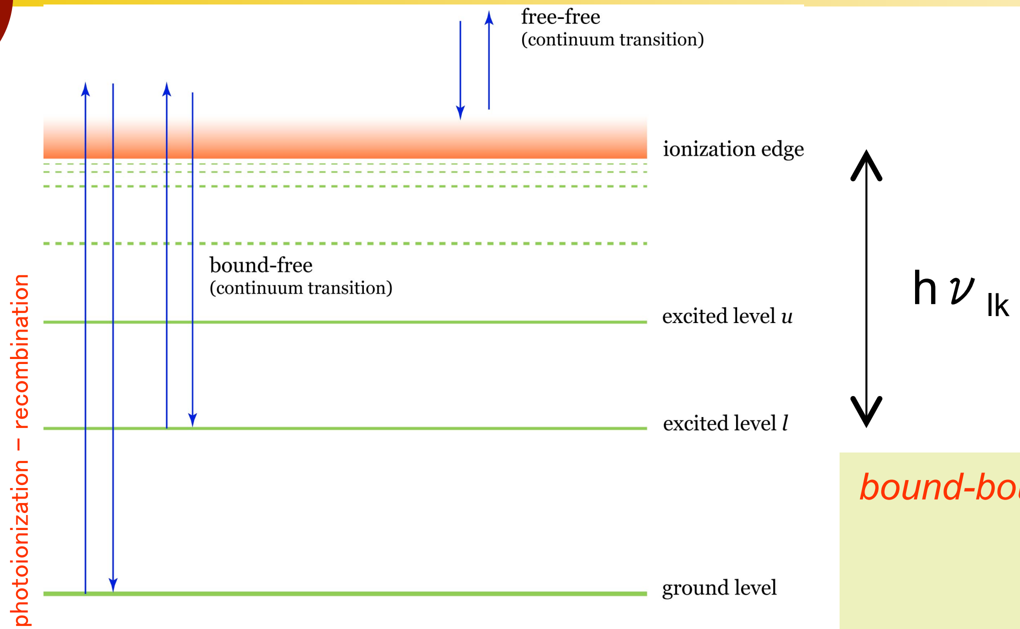
Rotation and macro-turbulence



Gray, 1992

B. Continuous transitions

1. Bound-free and free-free processes



absorption

$h\nu + E_l \rightarrow E_u$

emission

spontaneous (isotropic) $E_u \rightarrow E_l + h\nu$

stimulated (non-isotropic) $h\nu + E_u \rightarrow E_l + 2h\nu$

bound-bound: spectral lines

bound-free

free-free

κ_ν^{cont}

consider photon $h\nu \geq h\nu_{lk}$ (energy > threshold): extra-energy to free electron

e.g. **Hydrogen**

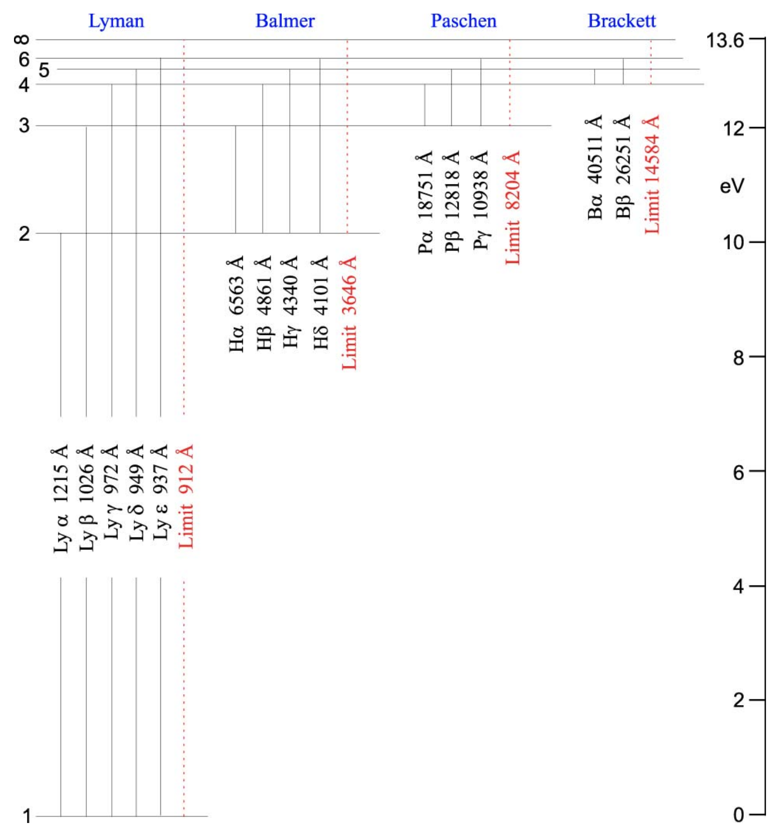
$$\frac{1}{2}mv^2 = h\nu - hc\frac{R}{n^2}$$

R = Rydberg constant = 1.0968 10^5 cm^{-1}

b-f and f-f processes

Hydrogen

l → continuum	Wavelength (A)	Edge
1 → continuum	912	Lyman
2 → continuum	3646	Balmer
3 → continuum	8204	Paschen
4 → continuum	14584	Brackett
5 → continuum	22790	Pfund



b-f and f-f processes

- for a single transition $$\kappa_\nu^{\mathrm{b-f}} = n_l\ \sigma_{lk}(\nu)$$

- for all transitions: $$\kappa_\nu^{\mathrm{b-f}} = \sum_{\substack{elements,\\ ions}} \sum_l n_l\ \sigma_{lk}(\nu)$$

Gaunt factor ≈ 1

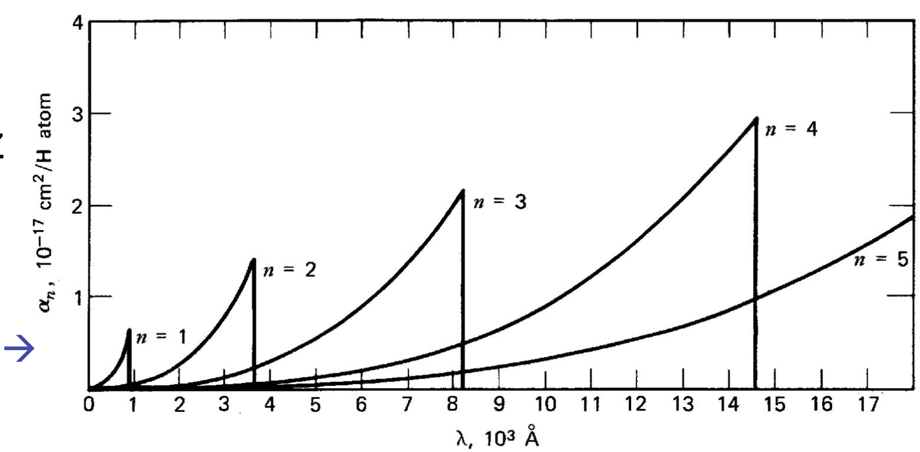
for hydrogenic ions $$\sigma_{lk}(\nu) = \sigma_0(n) \left(\frac{\nu_l}{\nu}\right)^3\ g_{\mathrm{bf}}(\nu)$$ Kramers 1923

Gray, 92

for H: σ_0 = 7.9 10^{-18} n cm^2

ν_l = 3.29 10^{15} / n^2 Hz

absorption per particle →



b-f and f-f processes

Gray, 92

$$\sigma_n^{\mathrm{b\text{-}f}}(\nu) = 2.815 \times 10^{29} \frac{Z^4}{n^5 \nu^3} g_{\mathrm{bf}}(\nu)$$

peaks increase with *n:*

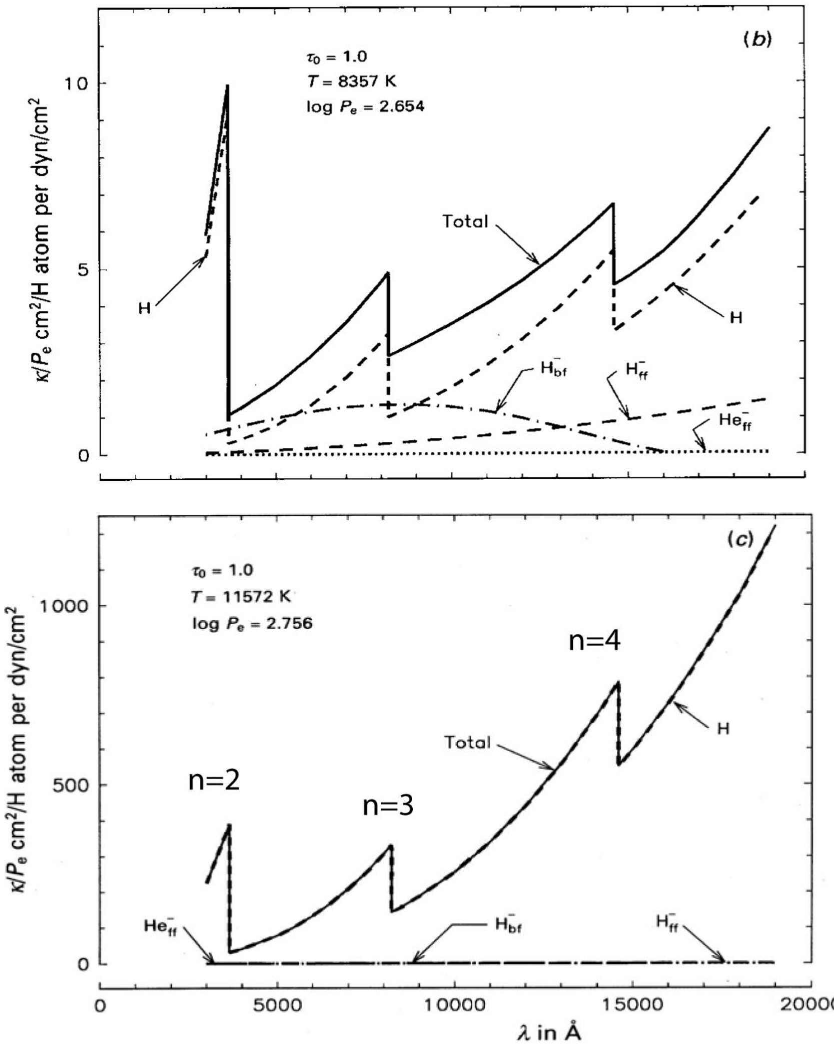
$$h\nu_n = E_\infty - E_n = 13.6/n^2 \mathrm{eV}$$

$$\Longrightarrow \nu^{-3} \rightarrow n^6$$

for non-H-like atoms no ν^{-3} dependence

peaks at resonant frequencies

free-free absorption much smaller



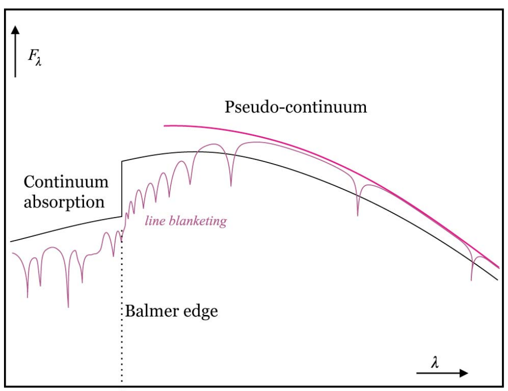
late A

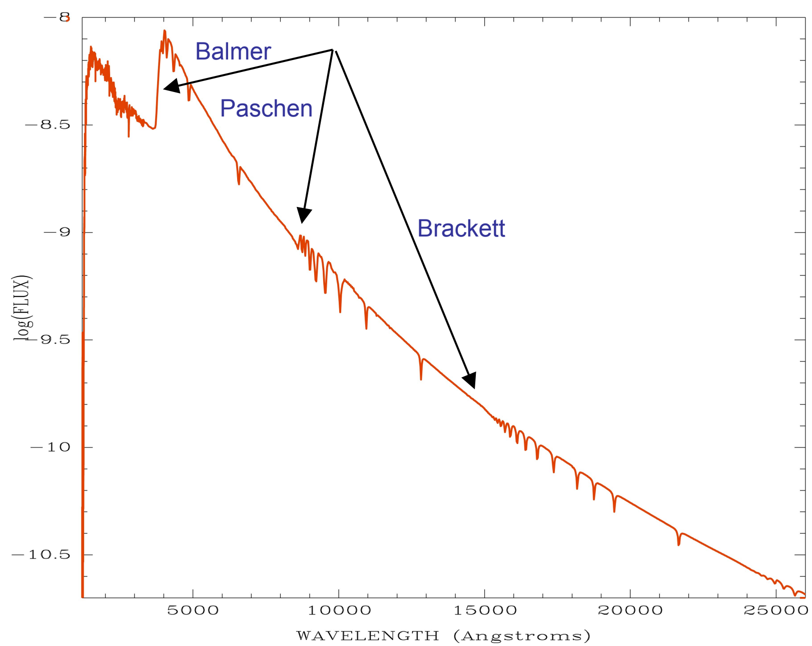
late B

b-f and f-f processes

Hydrogen dominant continuous absorber in B, A & F stars (later stars H^-)

Energy distribution strongly modulated at the edges:





Vega

b-f and f-f processes : Einstein-Milne relations

Generalize Einstein relations to bound-free processes relating photoionizations and radiative recombinations

<u>line transitions</u>

$$\sigma_{lu}(\nu) = \frac{h\nu}{4\pi}\,\varphi(\nu)\;B_{lu} \qquad g_l B_{lu} = g_u B_{ul}$$

$$A_{ul} = \frac{2\,h\,\nu^3}{c^2}\;B_{ul}$$

<u>b-f transitions</u>

$$\kappa_\nu^{\mathrm{b-f}} = \sum_{\substack{elements,\\ ions}} \sum_i \sigma_{ik}(\nu) \left[n_i - \overbrace{\underbrace{n_e n_1^{\mathrm{Ion}} \frac{g_i}{2g_1} \left(\frac{h^2}{2\pi m k T}\right)^{3/2} e^{E^i_{\mathrm{Ion}}/kT}}_{n_i^* \quad \text{LTE occupation number}} \; e^{-h\nu/kT}}^{\text{stimulated b-f emission}} \right]$$

2. Scattering

In scattering events photons are not destroyed, but redirected and perhaps shifted in frequency. In <u>free-free</u> process photon interacts with electron in the presence of ion's potential. For <u>scattering</u> there is no influence of ion's presence.

in general: $\kappa^{sc} = n_e \, \sigma_e$

Calculation of cross sections for scattering by free electrons:

- very high energy (several MeV's): *<u>Klein-Nishina</u>* formula (Q.E.D.)
- high energy photons (electrons): *<u>Compton (inverse Compton)</u>* scattering
- low energy (< 12.4 kEV ' 1 Angstrom): *<u>Thomson</u>* scattering

Thomson scattering

THOMSON SCATTERING: important source of opacity in hot OB stars

$$\boxed{\sigma_e = \frac{8\pi}{3}\, r_0^2 = \frac{8\pi}{3}\, \frac{e^4}{m_e^2\, c^4} = 6.65 \times 10^{-25}\, cm^2}$$

independent of frequency, isotropic

Approximations:

- angle averaging done, in reality: $\sigma_e \rightarrow \sigma_e (1+\cos^2 \theta)$ for single scattering
- neglected velocity distribution and Doppler shift (frequency-dependency)

Simple example: hot star -pure hydrogen atmosphere total opacity

Total opacity

$$\kappa_\nu = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sigma_{ij}^{\text{line}}(\nu) \left(n_i - \frac{g_i}{g_j} n_j \right)$$

line absorption

$$+ \sum_{i=1}^{N} \sigma_{ik}(\nu) \left(n_i - n_i^* e^{-h\nu/kT} \right)$$

bound-free

$$+ n_e n_p \sigma_{kk}(\nu, T) \left(1 - e^{-h\nu/kT} \right)$$

free-free

$$+ n_e \sigma_e$$

Thomson scattering

Simple example: hot star -pure hydrogen atmosphere total emissivity

Total emissivity

$$\epsilon_\nu = \frac{2h\nu^3}{c^2}\sum_{i=1}^{N}\sum_{j=i+1}^{N}\sigma_{ij}^{\rm line}(\nu)\frac{g_i}{g_j}n_j$$

line emission

$$+\frac{2h\nu^3}{c^2}\sum_{i=1}^{N} n_i^*\sigma_{ik}(\nu)e^{-h\nu/kT}$$

bound-free

$$+\frac{2h\nu^3}{c^2}n_e n_p \sigma_{kk}(\nu,T)e^{-h\nu/kT}$$

free-free

$$+n_e\sigma_e\, J_\nu$$

Thomson scattering

Rayleigh scattering – important in cool stars

RAYLEIGH SCATTERING: line absorption/emission of atoms and molecules far from resonance frequency: $\nu << \nu_0$

from classical expression of cross section for oscillators:

$$\sigma(\omega) = f_{ij}\sigma_{kl}(\omega) = f_{ij}\ \sigma_e\ \frac{\omega^4}{(\omega^2 - \omega_{ij}^2)^2 + \omega^2\gamma^2}$$

$$\text{for}\ \ \omega << \omega_{ij} \qquad \sigma(\omega) \approx f_{ij}\ \sigma_e\ \frac{\omega^4}{\omega_{ij}^4 + \omega^2\gamma^2}$$

$$\text{for}\ \ \gamma << \omega_{ij} \qquad \sigma(\omega) \approx f_{ij}\ \sigma_e\ \frac{\omega^4}{\omega_{ij}^4}$$

$$\boxed{\sigma(\omega) \sim \omega^4 \sim \lambda^{-4}}$$

important in cool G-K stars

for strong lines (e.g. Lyman series when H is neutral) the λ^{-4} decrease in the far wings can be important in the optical

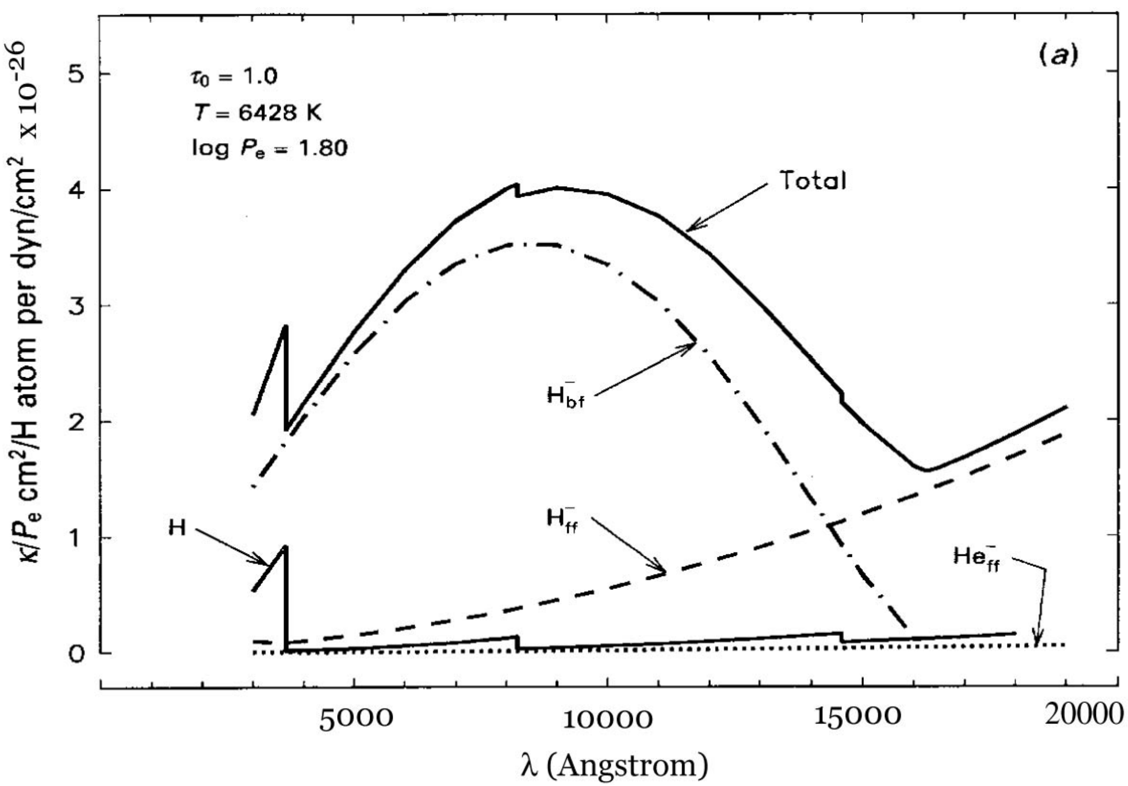
What are the dominant elements for the continuum opacity?

- *hot stars (B,A,F)* : H, He I, He II

- *cool stars (G,K)*: the bound state of the H^- ion (1 proton + 2 electrons)

only way to explain solar continuum (Wildt 1939)

The H^- ion - important in cool stars



Gray, 92

ionization potential = 0.754 eV

→ λ_{ion} = 16550 Angstroms

H^- b-f peaks around 8500 A

H^- f-f ~ λ^3 (IR important)

He^- b-f negligible,

He^- f-f can be important

in cool stars in IR

requires metals to provide

source of electrons

dominant source of

b-f opacity in the Sun

Additional absorbers

Hydrogen molecules in cool stars

H_2 molecules more numerous than atomic H in M stars

H_2^+ absorption in UV

H_2^- f-f absorption in IR

Helium molecules

He^- f-f absorption for cool stars

Metal atoms in cool and hot stars (lines and b-f)

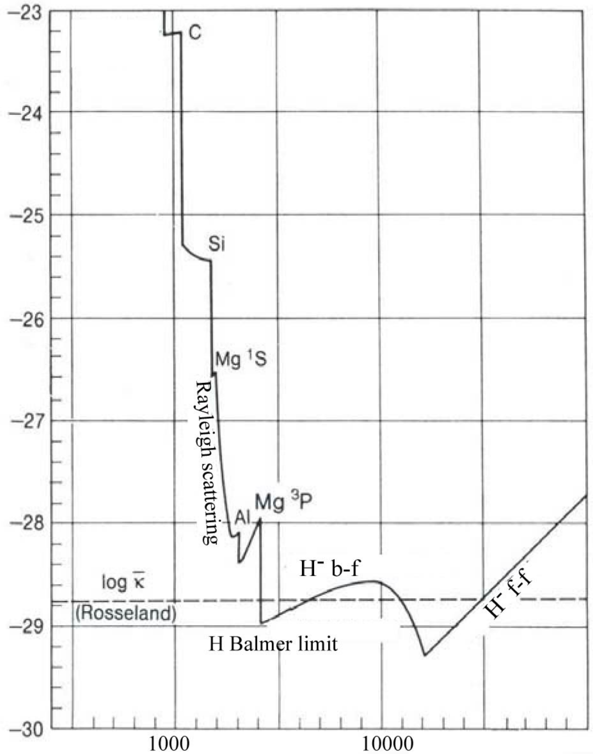
C,N,O, Si, Al, Mg, Fe, Ti, ….

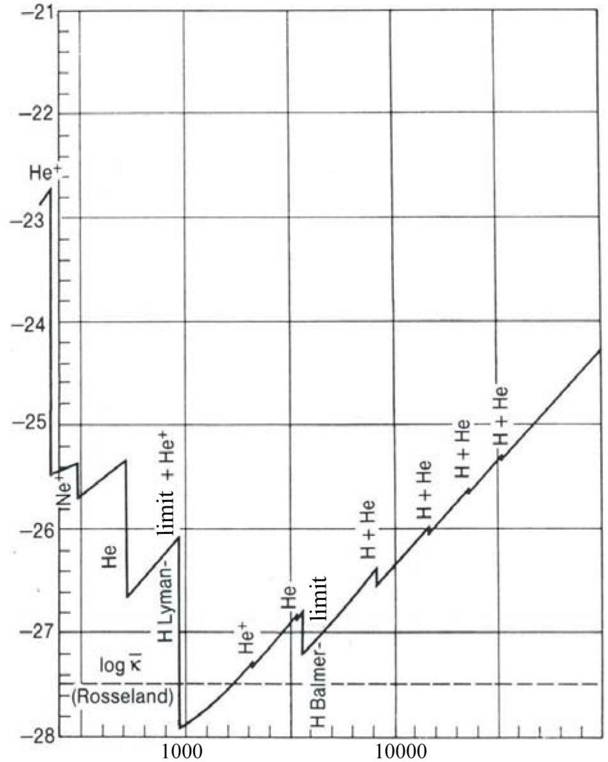
Molecules in cool stars

TiO, CO, H_2O, FeH, CH_4, NH_3,…

Examples of continuous absorption coefficients

Unsoeld, 68





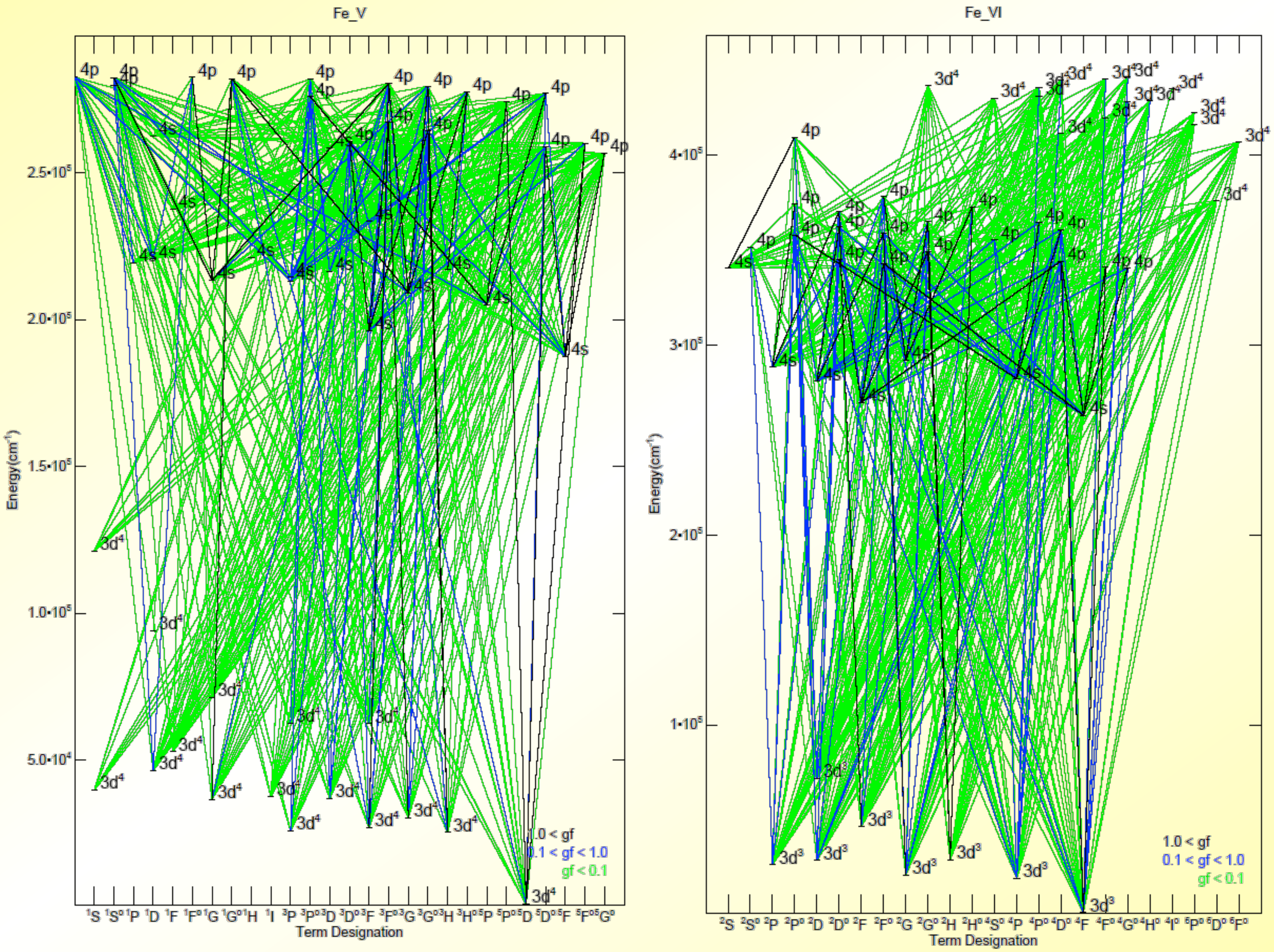
T_{eff} = 5040 K

B0: T_{eff} = 28,000 K

Modern model atmospheres include

- millions of spectral lines (atoms and ions)
- all bf- and ff-transitions of hydrogen helium and metals
- contributions of all important negative ions
- molecular opacities (lines and continua)

complex atomic models for O-stars (Pauldrach et al., 2001)



NLTE Atomic Models in modern model atmosphere codes

lines, collisions, ionization, recombination

Essential for occupation numbers, line blocking, line force

Accurate atomic models have been included

26	**elements**
149	**ionization stages**
5,000	**levels (+** 100,000 **)**
20,000	**diel. rec. transitions**
4 10^6	**b-b line transitions**
	Auger-ionization

recently improved models are based on Superstructure

Eisner et al., 1974, CPC 8,270

	I	II	III	IV	V	VI	VII	VIII
1	H_I							
2	He_I	He_II						
6	C_I	C_II	C_III	C_IV	C_V			
7	N_I	N_II	N_III	N_IV	N_V	N_VI		
8	O_I	O_II	O_III	O_IV	O_V	O_VI		
9	F_I	F_II	F_III	F_IV	F_V	F_VI		
10	Ne_I	Ne_II	Ne_III	Ne_IV	Ne_V	Ne_VI		
11	Na_I	Na_II	Na_III	Na_IV	Na_V	Na_VI		
12	Mg_I	Mg_II	Mg_III	Mg_IV	Mg_V	Mg_VI		
13	Al_I	Al_II	Al_III	Al_IV	Al_V	Al_VI		
14	Si_I	Si_II	Si_III	Si_IV	Si_V	Si_VI		
15	P_I	P_II	P_III	P_IV	P_V	P_VI		
16	S_I	S_II	S_III	S_IV	S_V	S_VI	S_VII	
17	Cl_I	Cl_II	Cl_III	Cl_IV	Cl_V	Cl_VI		
18	Ar_I	Ar_II	Ar_III	Ar_IV	Ar_V	Ar_VI	Ar_VII	ArVIII
19	K_I	K_II	K_III	K_IV	K_V	K_VI		
20	Ca_I	Ca_II	Ca_III	Ca_IV	Ca_V	Ca_VI		
22	Ti_I	Ti_II	Ti_III	Ti_IV	Ti_V			
23	V_I	V_II	V_III	V_IV	V_V			
24	Cr_I	Cr_II	Cr_III	Cr_IV	Cr_V	Cr_VI		
25	Mn_I	Mn_II	Mn_III	Mn_IV	Mn_V	Mn_VI		
26	Fe_I	Fe_II	Fe_III	Fe_IV	Fe_V	Fe_VI	Fe_VII	FeVIII
27	Co_I	Co_II	Co_III	Co_IV	Co_V	Co_VI	Co_VII	
28	Ni_I	Ni_II	Ni_III	Ni_IV	Ni_V	Ni_VI	Ni_VII	NiVIII
29	Cu_I	Cu_II	Cu_III	Cu_IV	Cu_V	Cu_VI		
30	Zn_I	Zn_II	Zn_III					

atomic data status:

excellent	good	poor	bad

Recent Improvements on Atomic Data

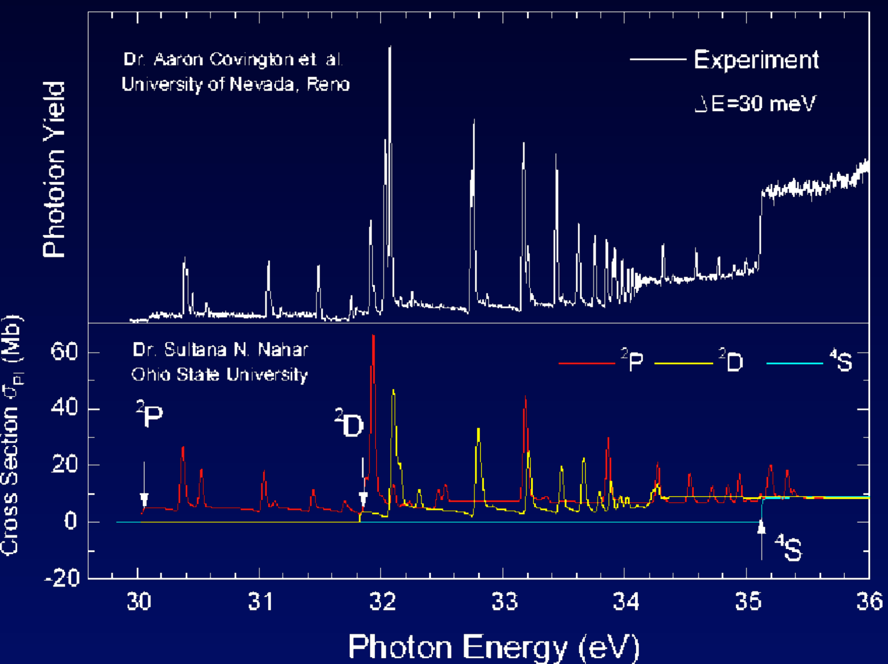
- requires solution of Schrödinger equation
  for N-electron system
- efficient technique:
  R-matrix method in CC approximation
- Opacity Project   Seaton et al. 1994, MNRAS, 266, 805
- IRON Project   Hummer et al. 1993, A&A, 279, 298

accurate radiative/collisional data
to 10% on the mean

Confrontation with Reality

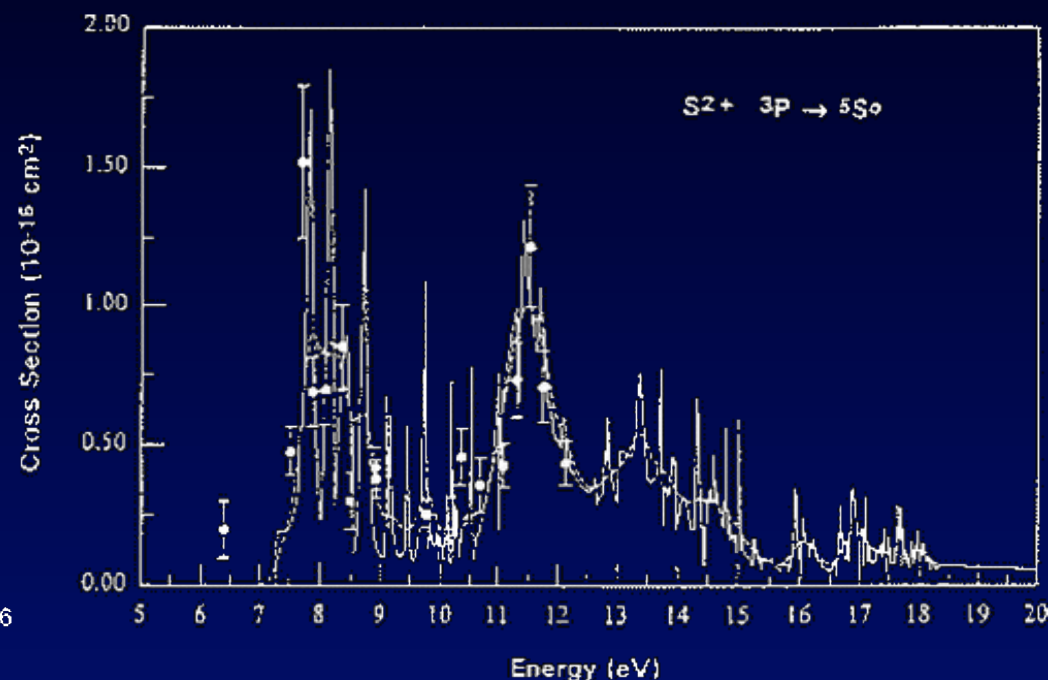
Photoionization

$h\nu + O^{+} \quad O^{2+} + e^{-}$



Nahar 2003, ASP Conf. Proc.Ser. 288, in press

Electron Collision

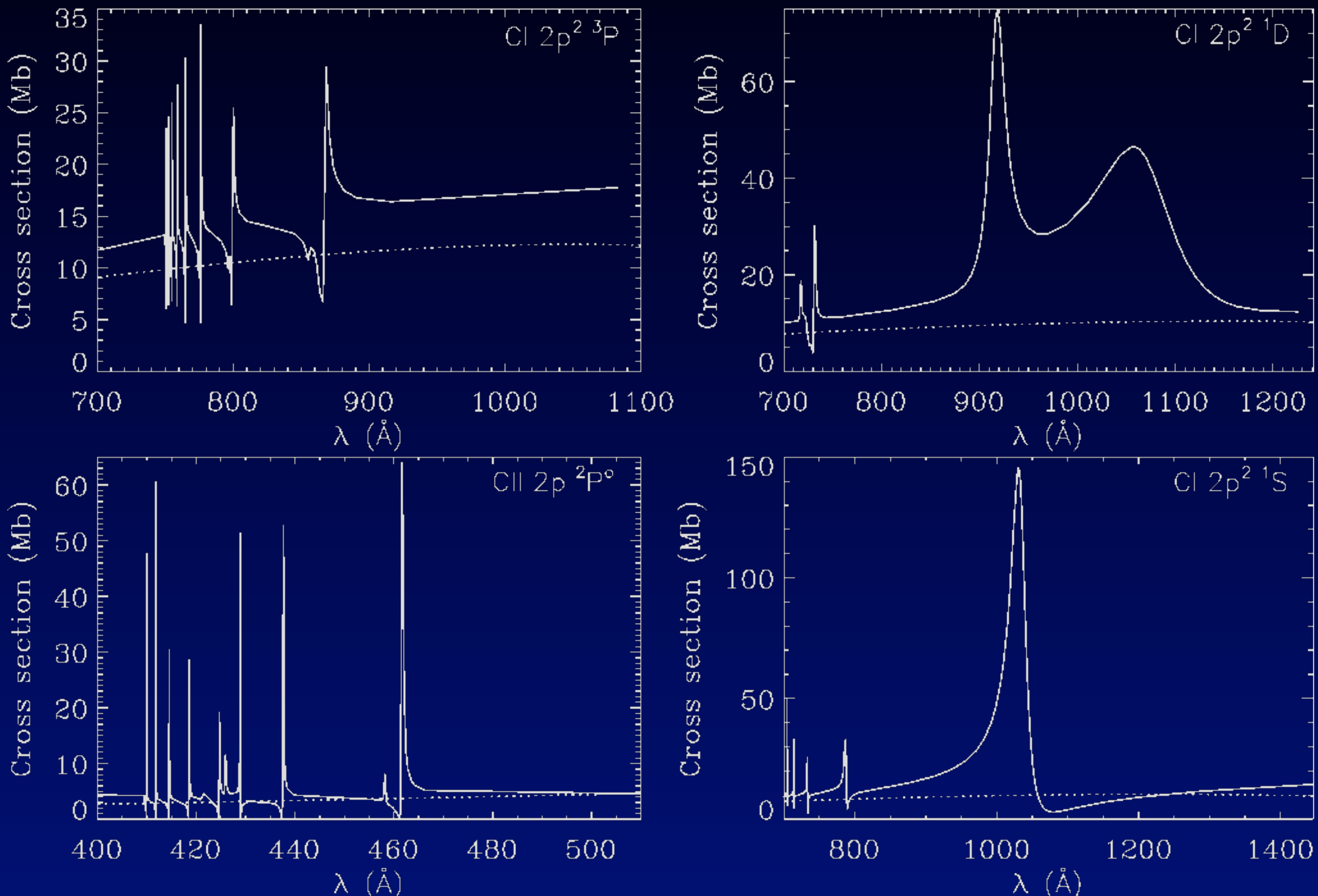


Williams 1999, Rep. Prog. Phys., 62, 1431

✓ high-precision atomic data ✓

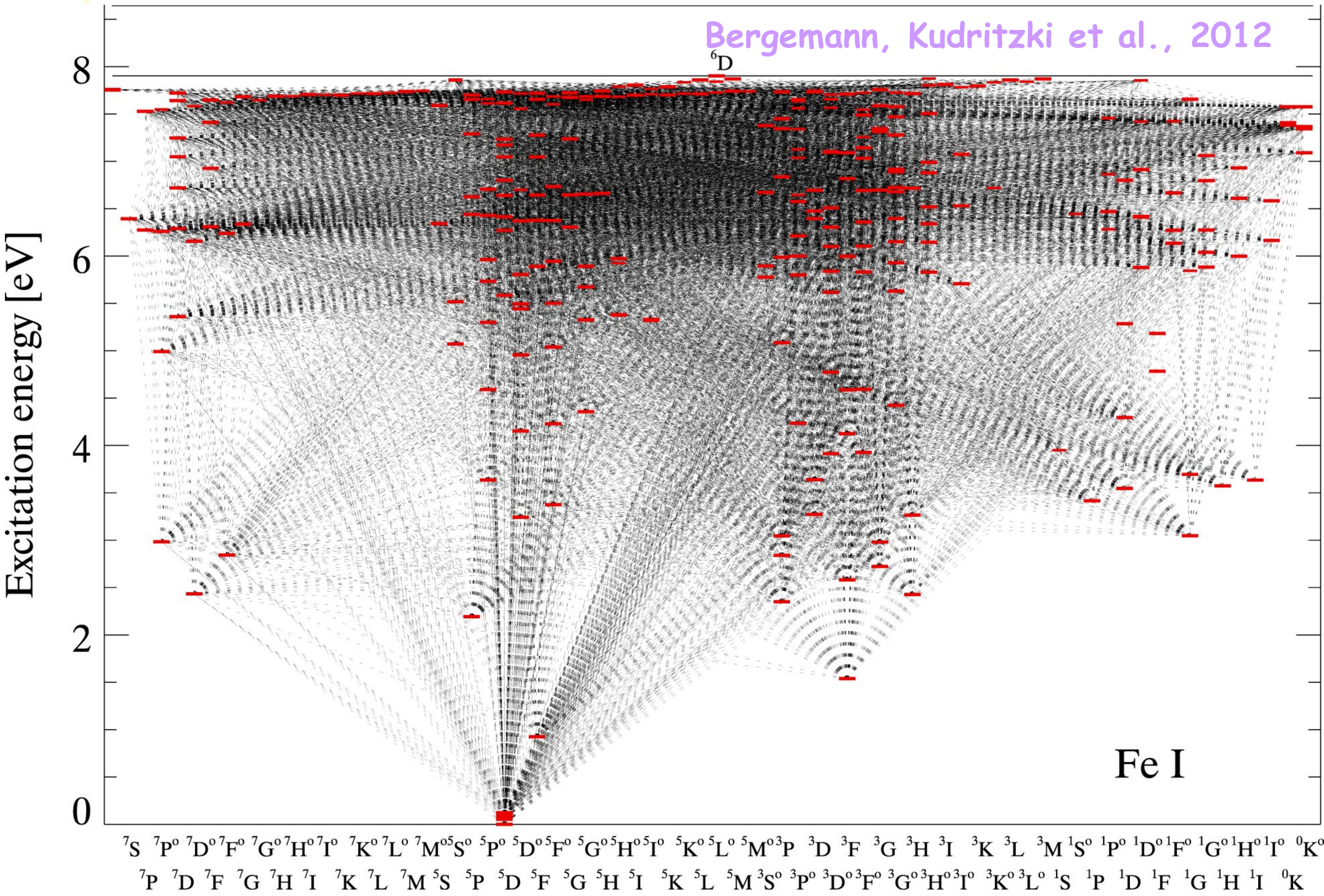
Improved Modelling for Astrophysics

e.g. photoionization cross-sections for carbon model atom

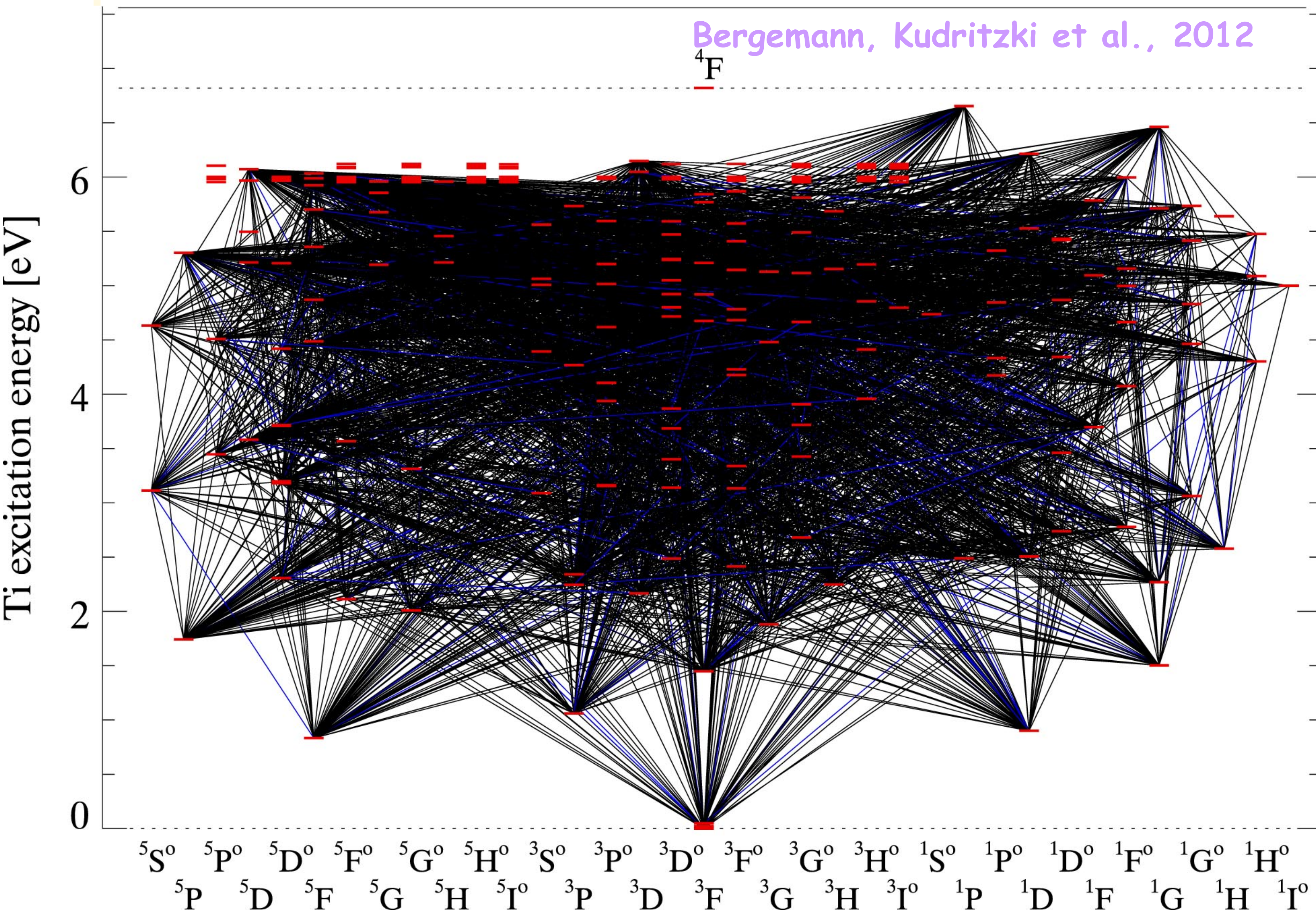


Przybilla, Butler & Kudritzki 2001b, A&A, 379, 936

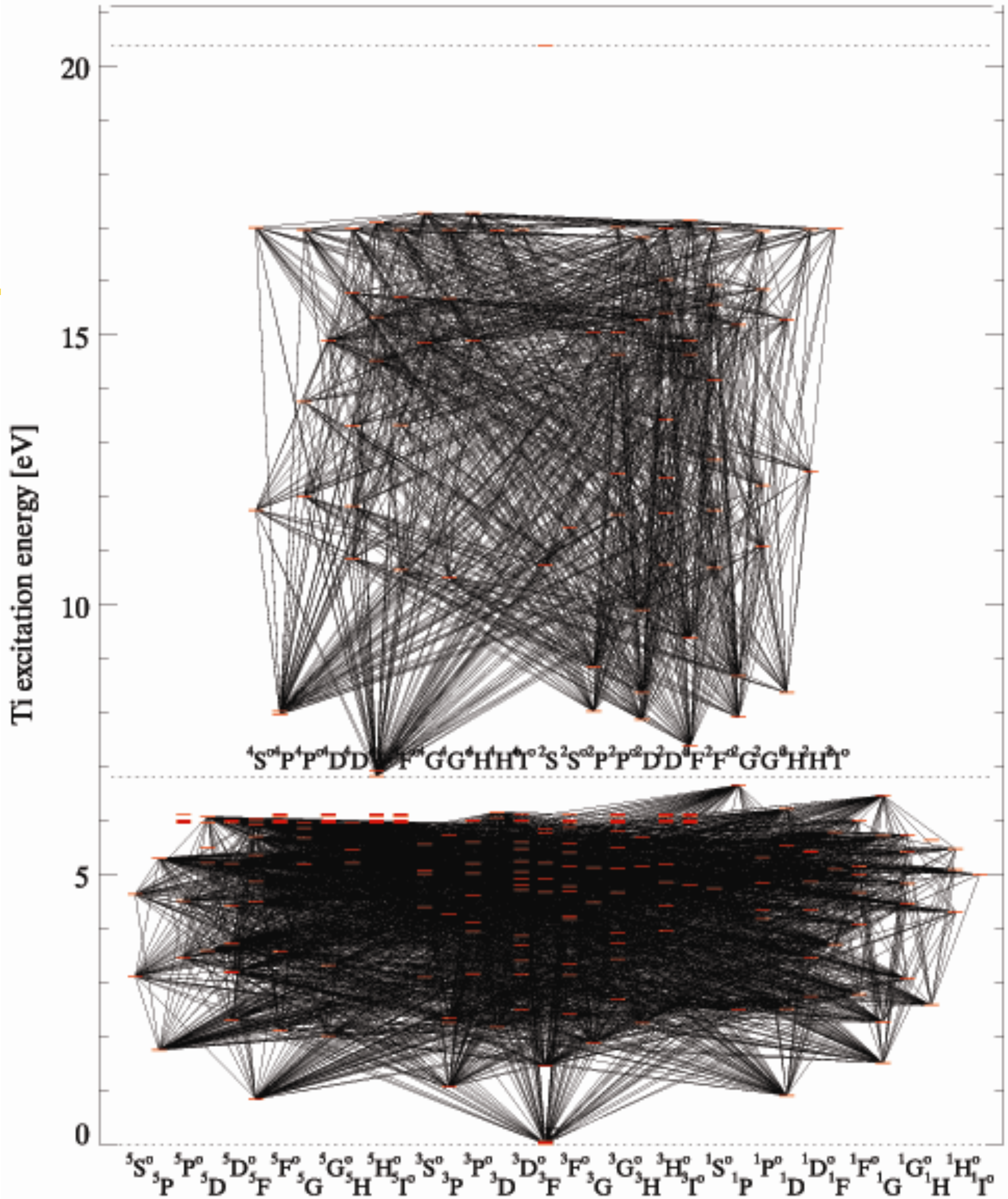
Red supergiants, NLTE model atom for FeI



Red supergiants, NLTE model atom for TiI



Bergemann,
Kudritzki et al., 2012

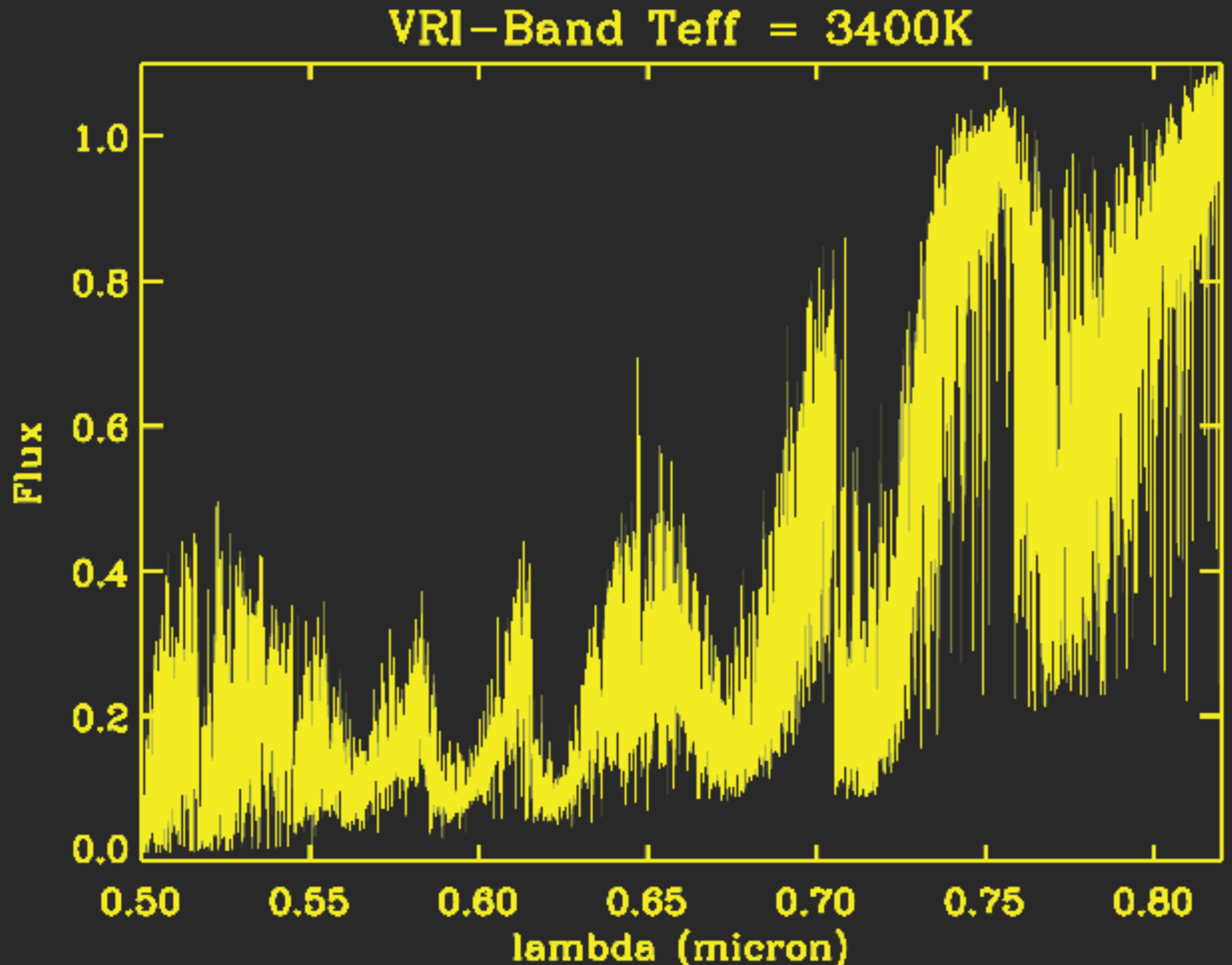


TiII

TiI

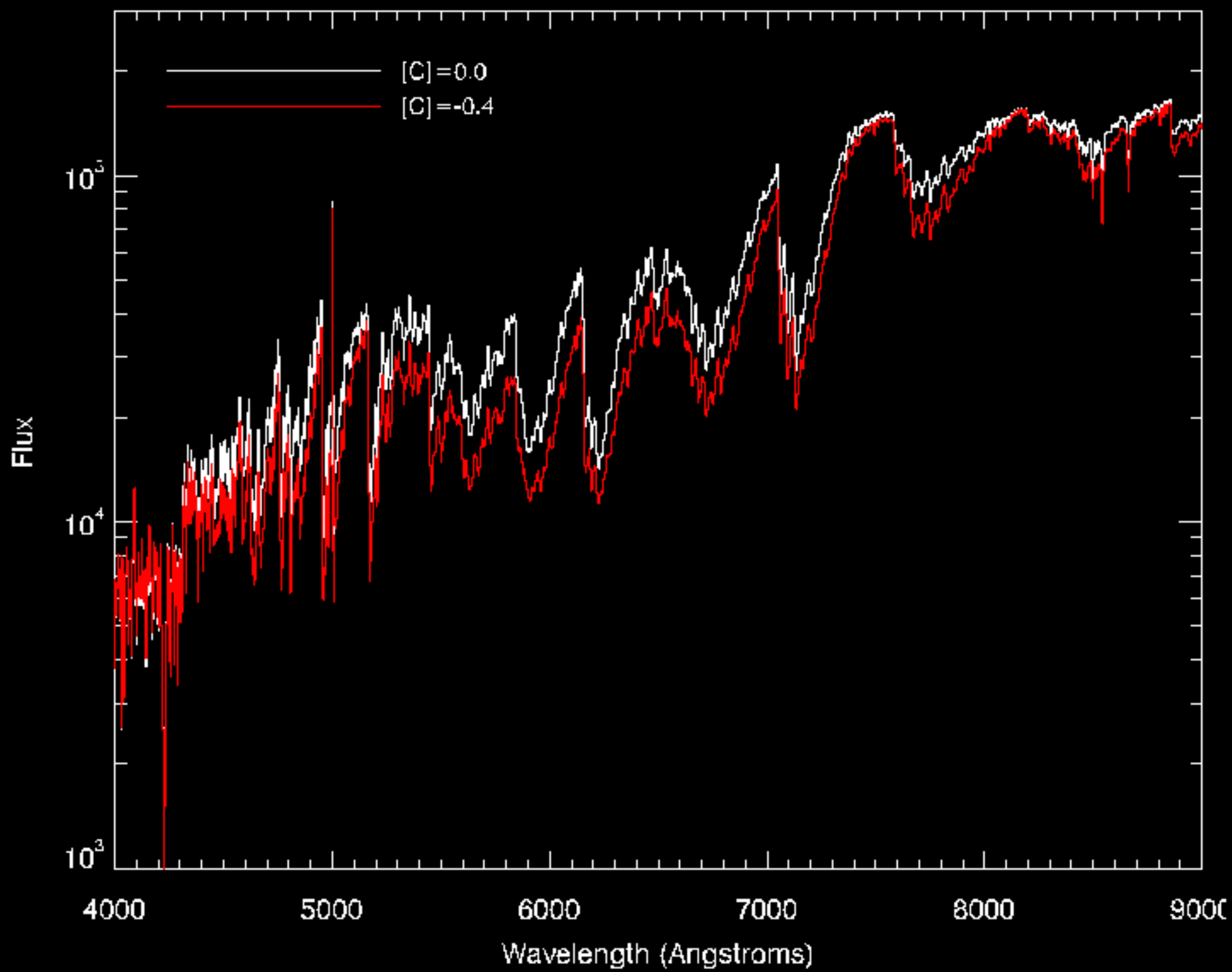
TiO in red supergiants

MARCS model atmospheres, Gustafsson et al., 2009



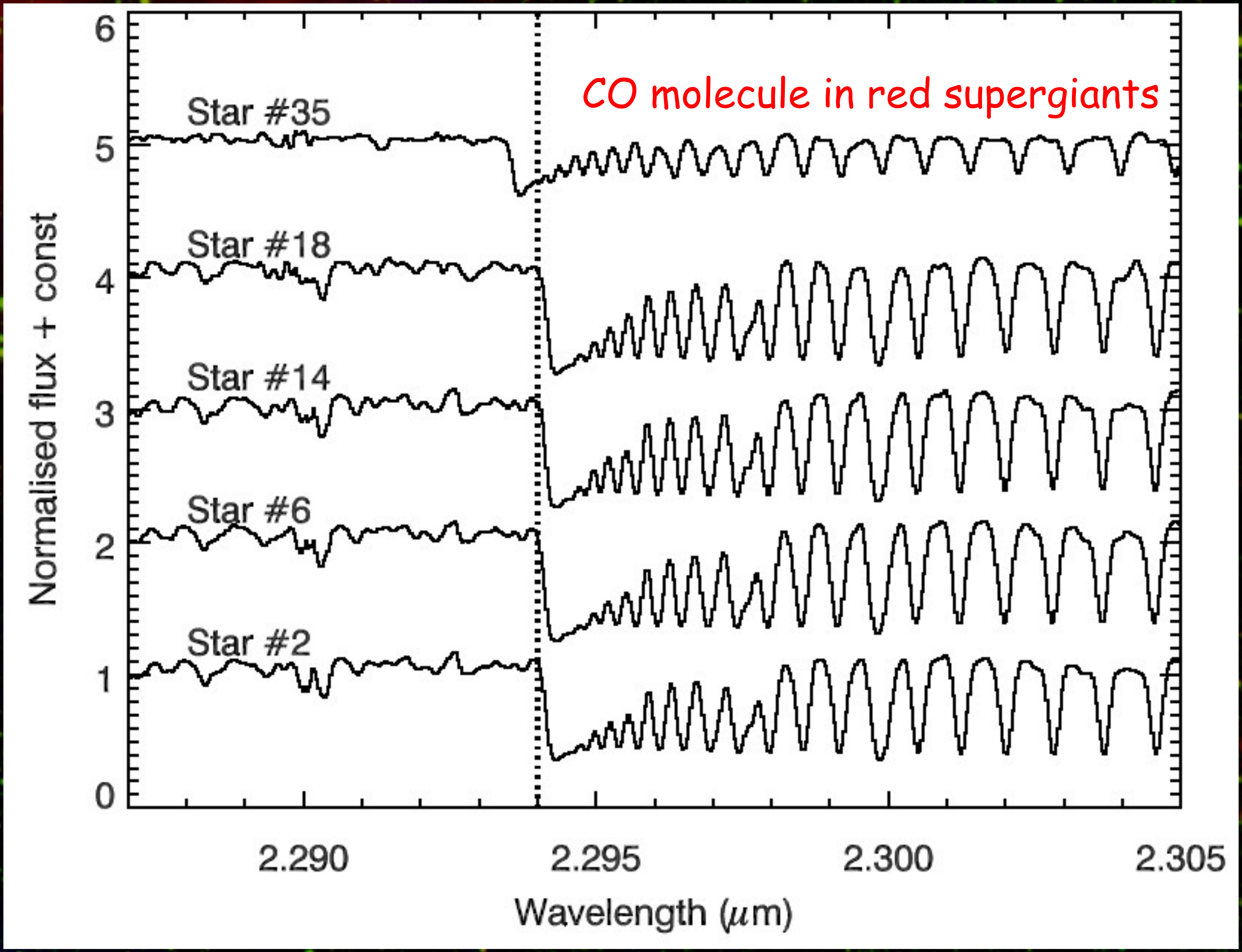
USM 2011

TiO in red supergiants



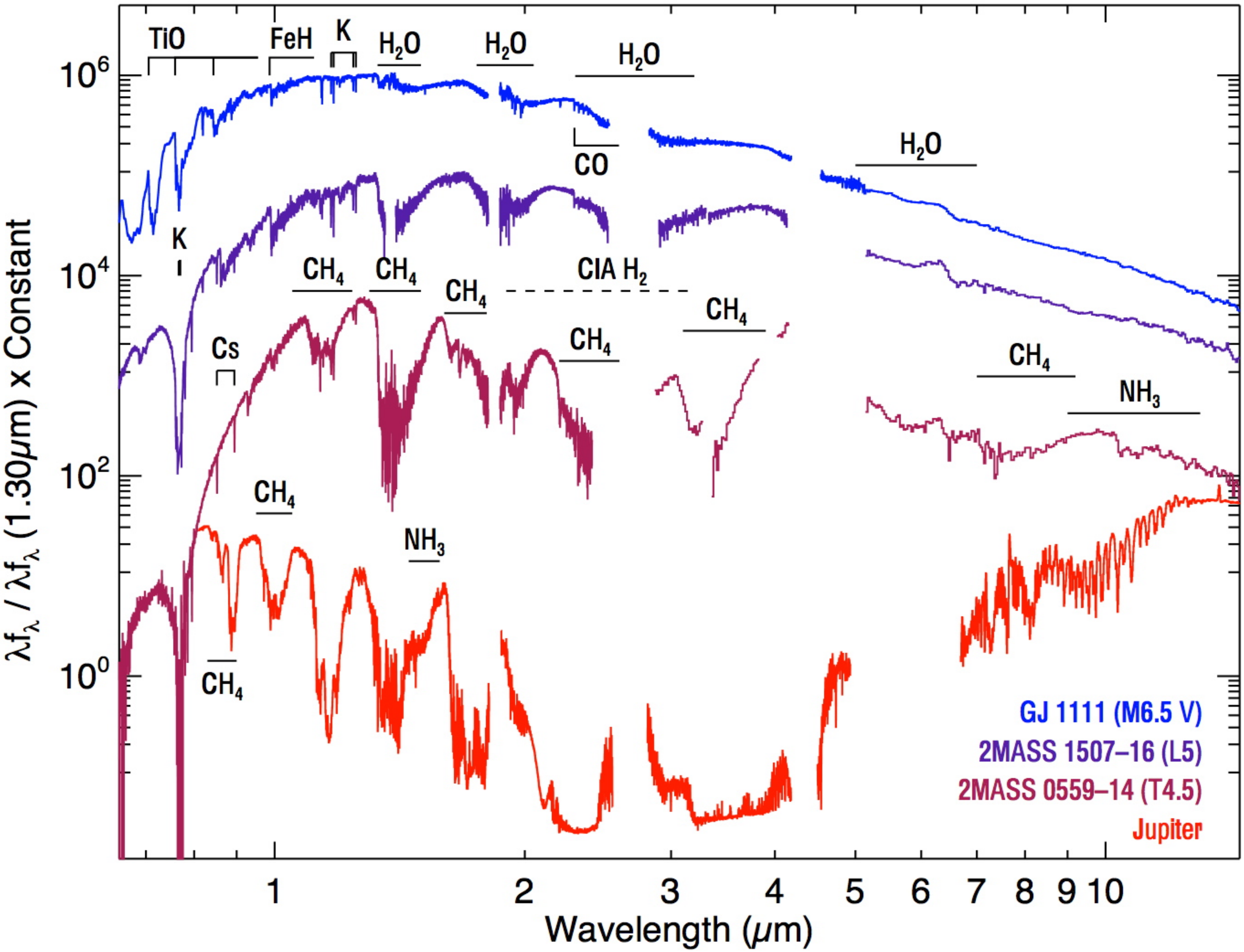
A small change in carbon abundances…

MARCS model atmospheres



Davies, Origilia, Kudritzki et al., 2009

Rayner, Cushing, Vacca, 2009: molecules in Brown Dwarfs



Exploring the substellar temperature regime down to ~550K
Burningham et al. (2009)