Radiative transfer in atmospheres and introduction to NLTE

in Harrachov

2023

Peter Nemeth

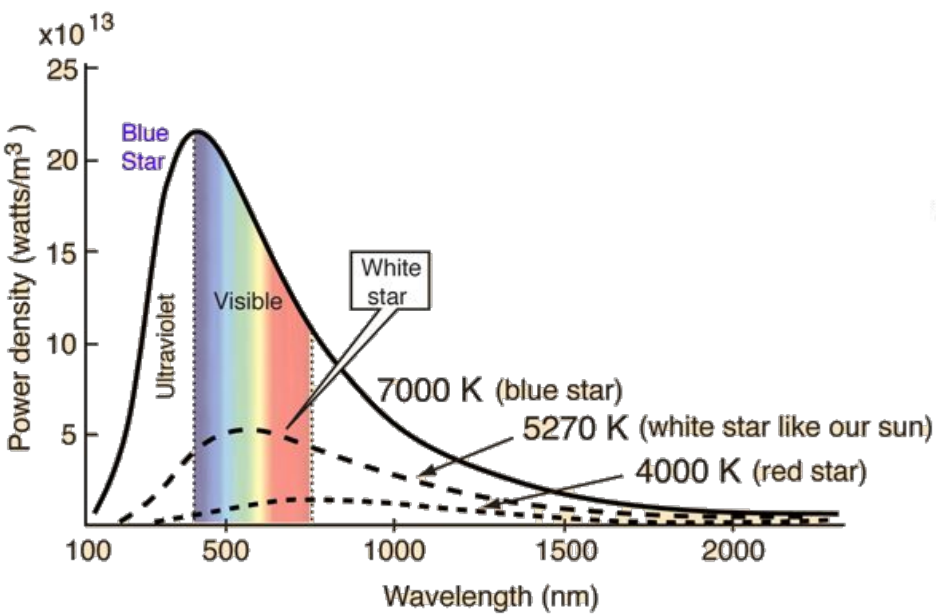
POEMS

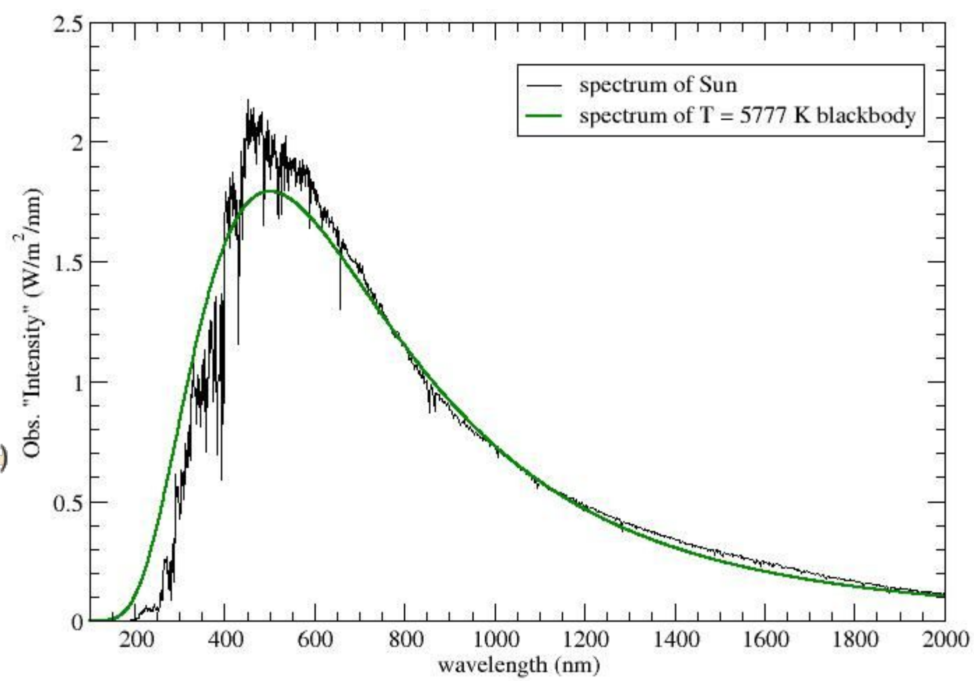
Physics of Extreme Massive Stars

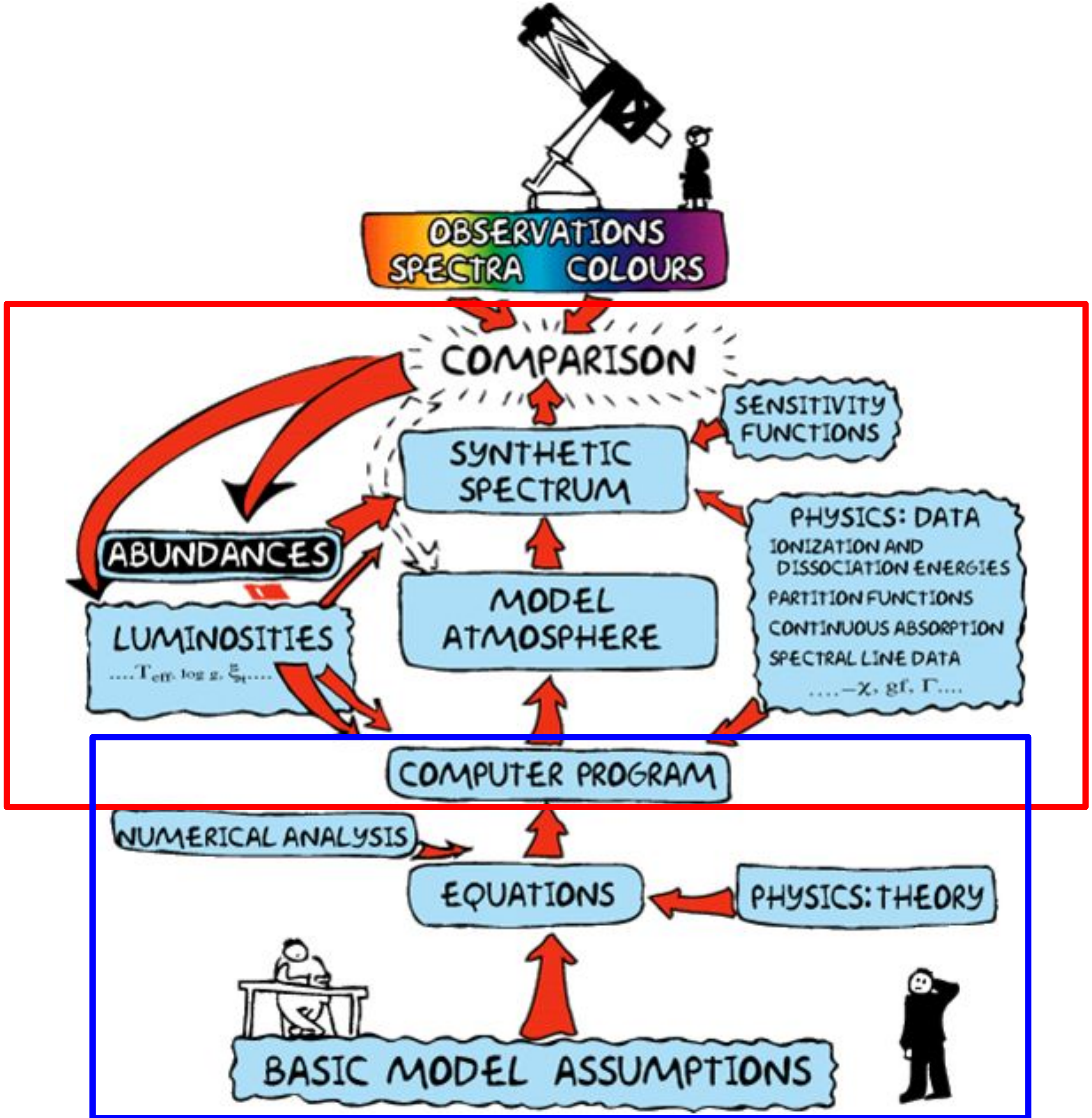
Marie-Curie-RISE project
funded by the European Union

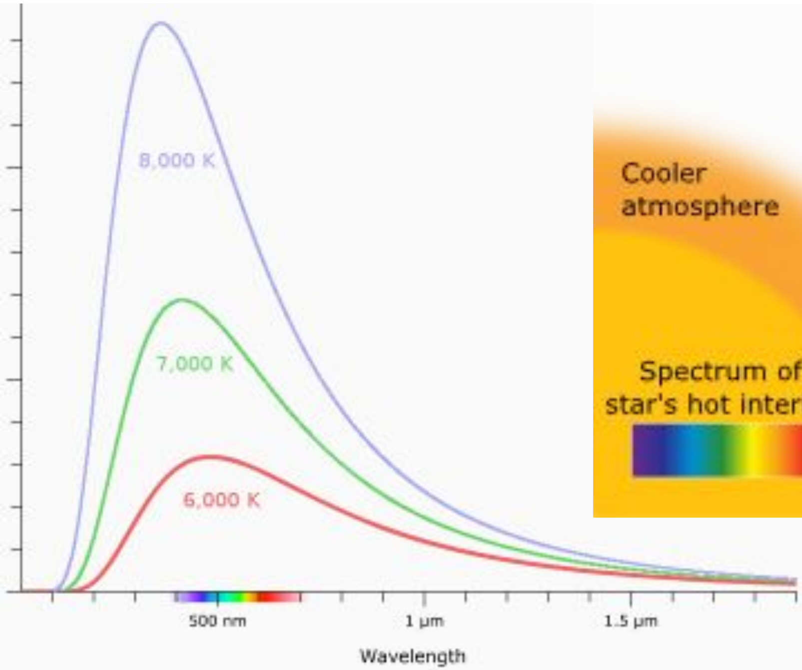
Stellar atmospheres - Why are we interested?

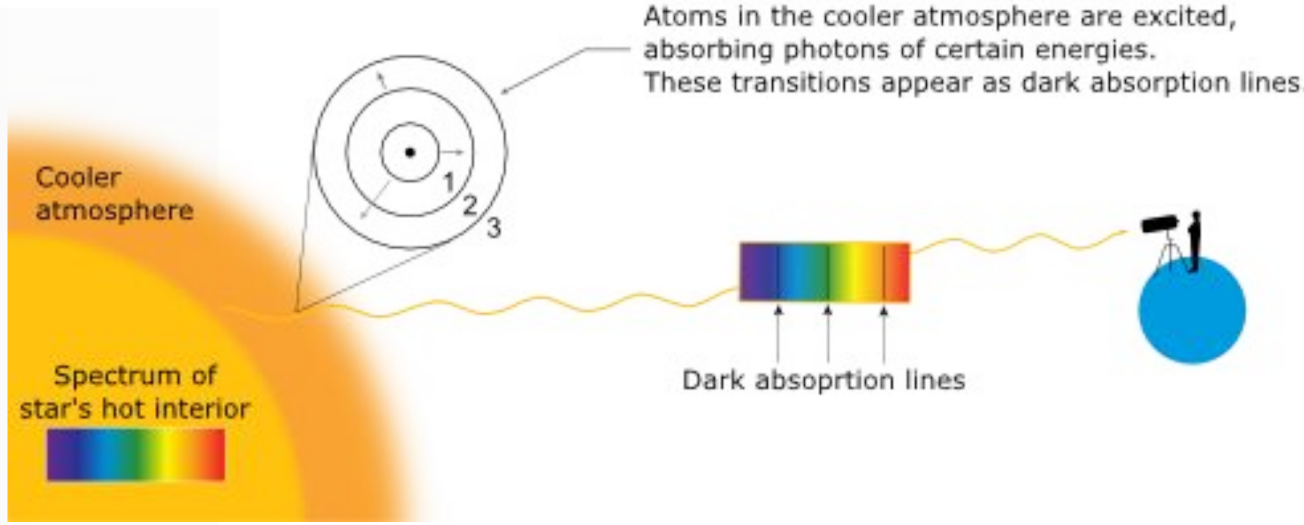
- Directly visible part of stars:
  - layers from which radiation can escape into space
- Outer boundary of stars, carrying information of the interior
- Most information (80%) we acquire by light comes from stars
- Stars are black bodies, but the black body radiation is insufficient to analyse observations →energy redistribution!
- Absolute parameters require us to understand the atmosphere based on fundamental microphysics (atomic, molecular data, processes)

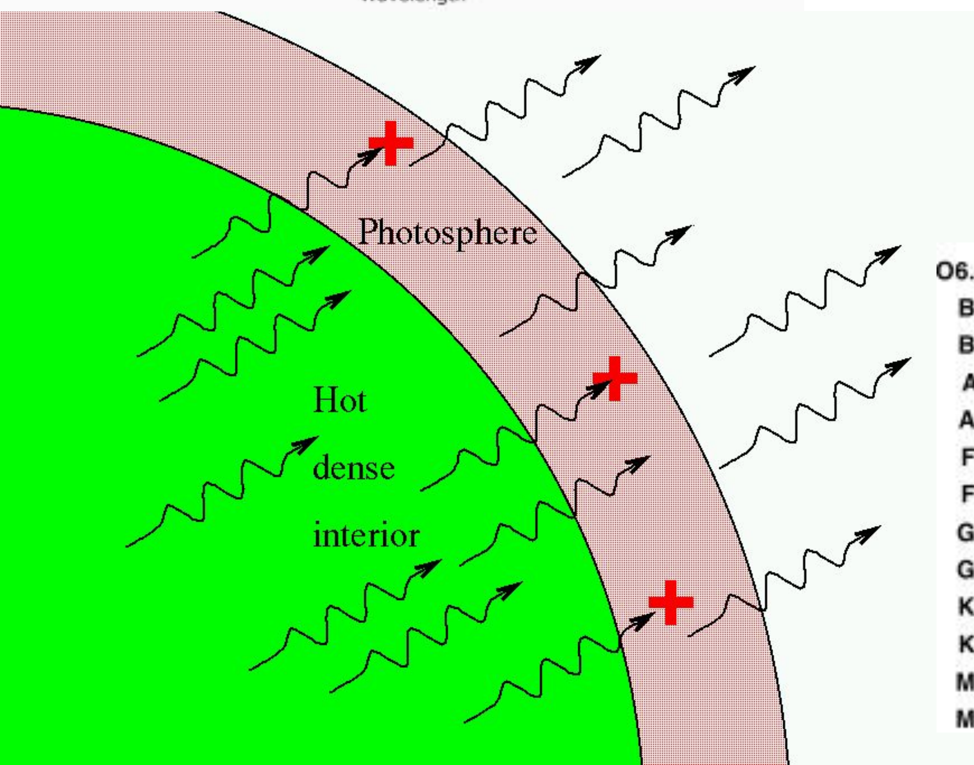




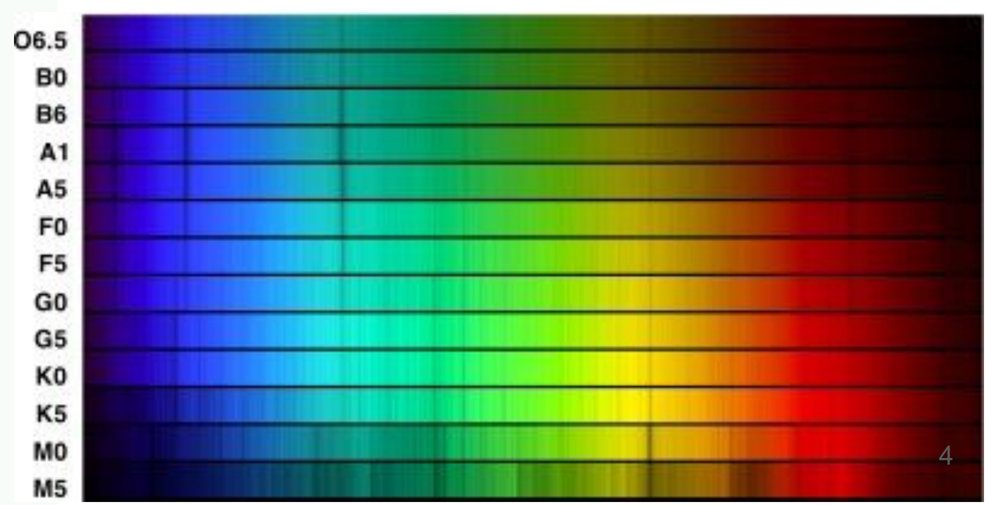

OBSERVATIONS
SPECTRA COLOURS
COMPARISON
SENSITIVITY FUNCTIONS
SYNTHETIC SPECTRUM
ABUNDANCES
LUMINOSITIES
....Teff, log g, ξt....
MODEL ATMOSPHERE
PHYSICS: DATA
IONIZATION AND DISSOCIATION ENERGIES
PARTITION FUNCTIONS
CONTINUOUS ABSORPTION
SPECTRAL LINE DATA
....−χ, gf, Γ....
COMPUTER PROGRAM
NUMERICAL ANALYSIS
EQUATIONS
PHYSICS: THEORY
BASIC MODEL ASSUMPTIONS





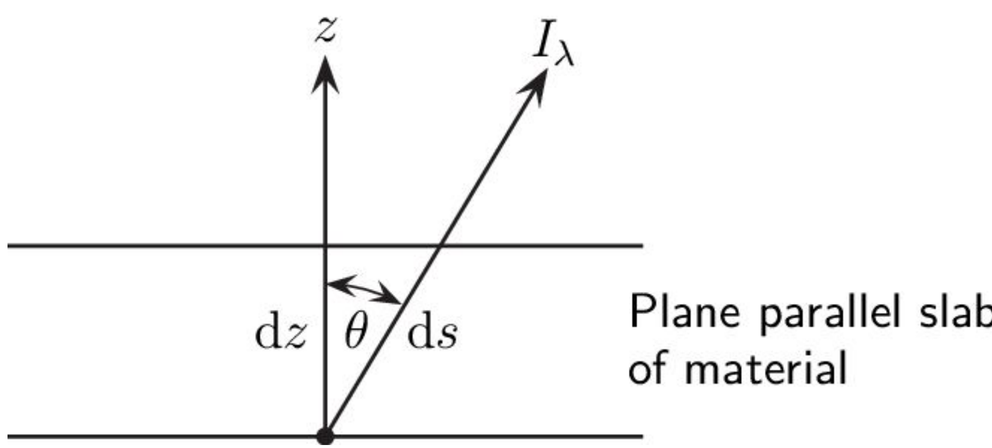


Opacity & temperature gradient!



Some disclaimers and assumptions

- Hydrostatic (v = 0), no wind, no velocity fields
- Stationary (d/dt = 0)
- Plane-parallel atmospheres (okay for most cases)
- Only radiation, no convection
- Few equations, only the basics
- Simple homogeneous atmospheres, no spots, caps, chemical gradients
- No fancy stuff, even though these are all possible to model:
  - diffusion, magnetic fields, molecules, 3D effects, pulsations, binary proximity effects, disks



$$\nu I_\nu = \lambda I_\lambda$$

The "hazy" circle of unknowns

- Work with distributions and mean values
- Unknown composition (abundances) and radiation field (energy distribution)

The state of the material determines the radiation field and the radiation field controls the state of the material.

Radiation determines the structure of the medium yet the medium is probed only by this radiation.

HARVARD OBSERVATORY MONOGRAPHS
HARLOW SHAPLEY, EDITOR

No. 1

STELLAR ATMOSPHERES

A CONTRIBUTION TO THE OBSERVATIONAL STUDY OF HIGH TEMPERATURE IN THE REVERSING LAYERS OF STARS

BY

CECILIA H. PAYNE

PUBLISHED BY THE OBSERVATORY
CAMBRIDGE, MASSACHUSETTS
1925

Stellar Atmospheres Theory: An Introduction

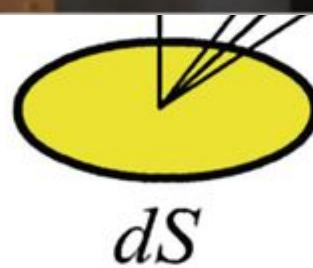
I. Hubeny

Universities Space Research Association, NASA Goddard Space Flight Center, Code 681, Greenbelt, MD 20771, USA

Specific intensity

Specific intensity: a measure of brightness, the amount of energy radiated per second from a small area in a particular direction.

Independent of distance! →



Flux

The rate at which energy at a certain frequency flows across an area or unit surface area.

Unit = erg / cm^2 / s / Hz

$$F_\nu = \oint I_\nu \cos\theta d\Omega \qquad F_\nu = 2\pi \oint_0^{\pi/2} I_\nu \sin\theta \cos\theta d\theta$$

Luminosity

Total energy radiated from the star, integrated for the entire surface

$$F = \sigma T^4$$

$$L = 4\pi R^2 \sigma T^4, \text{ or } L = 4\pi R^2 F, \text{ then } F = L/4\pi R^2$$

Radiation pressure, K integral

$$p = \frac{E}{c}$$

$$K_\nu = \oint I_\nu \cos^2 \theta d\Omega$$

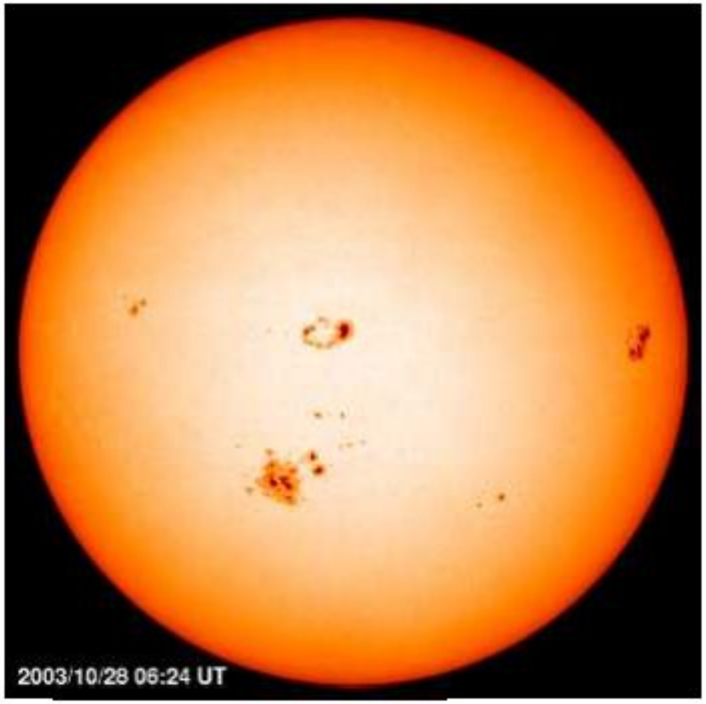
$$P_{rad} = \frac{4\sigma}{3c} T^4$$

Eddington approximation

I_ν is independent of direction (isotropic) within the outgoing hemisphere, then:

$$F_\nu = \pi I_\nu$$

$$T^4 = \frac{3}{4} T_{\mathrm{eff}}^4 \left(\tau_{\mathrm{v}} + \frac{2}{3} \right)$$



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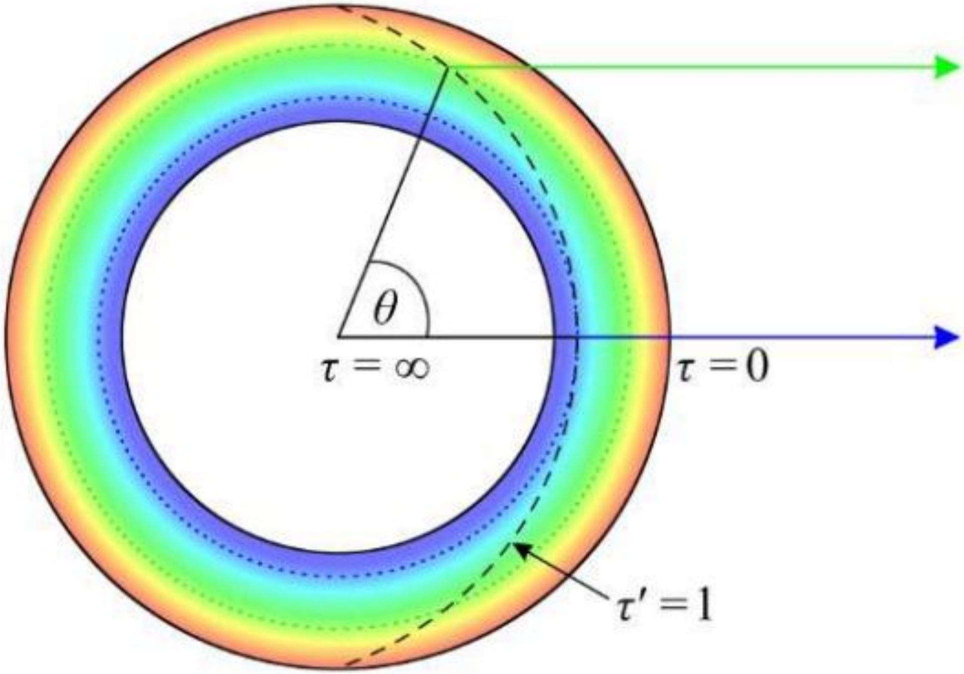


Distributions in LTE

- Maxwellian velocity distribution of particles:

$$f(\mathbf{v})\mathrm{d}\mathbf{v} = (m/2\pi kT)^{3/2}\ \exp(-mv^2/2kT)\,\mathrm{d}\mathbf{v}$$

- Boltzmann excitation equation:

$$(n_j/n_i) = (g_j/g_i)\ \exp\left[-(E_j - E_i)/kT\right]$$

- Saha ionization equation:

$$\frac{N_I}{N_{I+1}} = n_\mathrm{e}\,\frac{U_I}{U_{I+1}}\,C\,T^{-3/2}\ \exp(\chi_I/kT)$$

$$U = \sum_1^\infty g_i \exp(-E_i/kT)$$

$$C = (h^2/2\pi mk)^{3/2}$$

Basics

The specific intensity:

$$\mathrm{d}E = I(\mathbf{r}, \mathbf{n}, \nu, t)\, \mathrm{d}S\ \cos\theta\, \mathrm{d}\omega\ \mathrm{d}\nu\, \mathrm{d}t$$

$$I = (ch\nu)\, f$$

Then the energy density:

$$E = \oint (h\nu) f\, \mathrm{d}\omega = (1/c) \oint I\, \mathrm{d}\omega$$

The flux:

$$\mathbf{F} = \oint (h\nu) \cdot (c\, \mathbf{n})\, f\, \mathrm{d}\omega = \oint \mathbf{n}\, I\, \mathrm{d}\omega$$

Radiation pressure:

$$\mathrm{P} = \oint (h\nu)\, \mathbf{n}\mathbf{n}\, f\, \mathrm{d}\omega = (1/c) \oint \mathbf{n}\mathbf{n}\, I\, \mathrm{d}\omega$$

Basics

Absorption coefficient (related to the mean free path):

$$\mathrm{d}E = \chi(\mathbf{r}, \mathbf{n}, \nu, t)\, I(\mathbf{r}, \mathbf{n}, \nu, t)\, \mathrm{d}S\, \mathrm{d}\omega\, \mathrm{d}\nu\, \mathrm{d}t$$

$$\chi(\mathbf{r}, \mathbf{n}, \nu, t) = \kappa(\mathbf{r}, \mathbf{n}, \nu, t) + \sigma(\mathbf{r}, \mathbf{n}, \nu, t)$$

Emission coefficient:

$$\mathrm{d}E = \eta(\mathbf{r}, \mathbf{n}, \nu, t)\, \mathrm{d}S\, \mathrm{d}\omega\, \mathrm{d}\nu\, \mathrm{d}t$$

Planck function:

$$B(\nu, T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1}$$

$$\eta/\chi = B$$

Source function in LTE

Basics

The transfer equation:

$$[I(\mathbf{r}+\Delta\mathbf{r},\mathbf{n},\nu,t+\Delta t)-I(\mathbf{r},\mathbf{n},\nu,t)]\,\mathrm{d}S\,\mathrm{d}\omega\,\mathrm{d}\nu\,\mathrm{d}t\;=$$
$$[\eta(\mathbf{r},\mathbf{n},\nu,t)-\chi(\mathbf{r},\mathbf{n},\nu,t)I(\mathbf{r},\mathbf{n},\nu,t)]\,\mathrm{d}s\,\mathrm{d}S\,\mathrm{d}\omega\,\mathrm{d}\nu\,\mathrm{d}t$$

$$\left(\frac{1}{c}\frac{\partial}{\partial t}+\mathbf{n}\cdot\nabla\right)I(\mathbf{r},\mathbf{n},\nu,t)=\eta(\mathbf{r},\mathbf{n},\nu,t)-\chi(\mathbf{r},\mathbf{n},\nu,t)\,I(\mathbf{r},\mathbf{n},\nu,t)$$

For a one dimensional planar and static case:

$$\mu\frac{\mathrm{d}I(\nu,\mu,z)}{\mathrm{d}z}=\eta(\nu,\mu,z)-I(\nu,\mu,z)\,\chi(\nu,\mu,z)$$

$$\mu\frac{\mathrm{d}I_\nu}{\mathrm{d}z}=\eta_\nu-\chi_\nu I_\nu$$

$$S_\nu\equiv\frac{\eta_\nu}{\chi_\nu}$$

$$\mathrm{d}\tau_\nu\equiv-\chi_\nu\,\mathrm{d}z$$

Transfer equation:

$$\mu\,\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu}=I_\nu-S_\nu$$

Basics

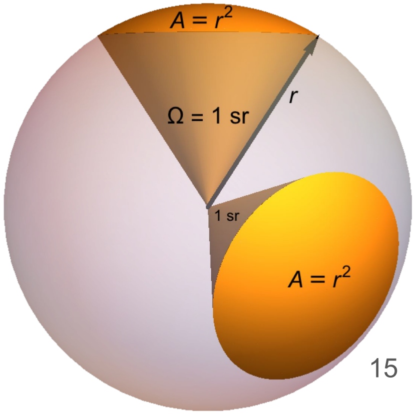
Moments of the specific intensity:

$$\begin{pmatrix} cE_\nu \\ \mathbf{F}_\nu \\ c\mathrm{P}_\nu \end{pmatrix} = \oint \begin{pmatrix} 1 \\ \mathbf{n} \\ \mathbf{nn} \end{pmatrix} I_\nu \, \mathrm{d}\omega$$

Analogously, the angle averaged, time independent moments:

$$\begin{pmatrix} J_\nu \\ \mathbf{H}_\nu \\ \mathrm{K}_\nu \end{pmatrix} = \frac{1}{4\pi} \begin{pmatrix} cE_\nu \\ \mathbf{F}_\nu \\ c\mathrm{P}_\nu \end{pmatrix} = \frac{1}{4\pi} \oint \begin{pmatrix} 1 \\ \mathbf{n} \\ \mathbf{nn} \end{pmatrix} I_\nu \, \mathrm{d}\omega$$

4π = surface of unit sphere (12.566 steradian)



Basics

Moments of the RTE in a plane-parallel approximation are all scalar quantities:

$$J_\nu = \frac{1}{2}\int_{-1}^{1} I_\nu(\mu)\mathrm{d}\mu$$

$$H_\nu = \frac{1}{2}\int_{-1}^{1} \mu\, I_\nu(\mu)\mathrm{d}\mu$$

$$K_\nu = \frac{1}{2}\int_{-1}^{1} \mu^2 I_\nu(\mu)\mathrm{d}\mu$$

The moment equations are not closed!

$$\frac{\mathrm{d}H_\nu}{\mathrm{d}\tau_\nu} = J_\nu - S_\nu \ ,$$

$$\frac{\mathrm{d}K_\nu}{\mathrm{d}\tau_\nu} = H_\nu \ .$$

$$f_\nu^{\mathrm{K}} \equiv K_\nu / J_\nu$$

Variable Eddington factor

$$\frac{\mathrm{d}^2(f_\nu^{\mathrm{K}} J_\nu)}{\mathrm{d}\tau_\nu^2} = J_\nu - S_\nu$$

Angle independent form of the RTE
But not solvable even if S is known, must be iterated with the Eddington factor.

Diffusion approximation

Deep in the atmosphere the source function approaches the Planck function (S → B) because virtually no photons escape and thus the medium approaches the thermal equilibrium. LTE always prevails!

$$S_\nu(t_\nu) = \sum_{n=0}^{\infty} \frac{\mathrm{d}^n B_\nu}{\mathrm{d}\tau_\nu^n} \frac{(t_\nu - \tau_\nu)^n}{n!}$$

$$I_\nu(t_\nu, \mu) = \sum_{n=0}^{\infty} \mu^n \frac{\mathrm{d}^n B_\nu}{\mathrm{d}\tau_\nu^n} = B_\nu(\tau_\nu) + \mu \frac{\mathrm{d}B_\nu}{\mathrm{d}\tau_\nu} + \mu^2 \frac{\mathrm{d}^2 B_\nu}{\mathrm{d}\tau_\nu^2} + \ldots \quad .$$

Applying these in the moments:

$$J_\nu(\tau_\nu) = B_\nu(\tau_\nu) + \frac{1}{3} \frac{\mathrm{d}^2 B_\nu}{\mathrm{d}\tau_\nu^2} + \cdots \quad ,$$

$$H_\nu(\tau_\nu) = \frac{1}{3} \frac{\mathrm{d}B_\nu}{\mathrm{d}\tau_\nu} + \cdots \quad ,$$

$$K_\nu(\tau_\nu) = \frac{1}{3} B_\nu(\tau_\nu) + \frac{1}{5} \frac{\mathrm{d}^2 B_\nu}{\mathrm{d}\tau_\nu^2} + \cdots \quad .$$

Diffusion approximation

At large depths:

- The mean intensity approaches the Planck function.
- The radiation field is isotropic and the variable Eddington factor approach 1/3.

$$f_\nu^{\mathrm{K}} \equiv K_\nu / J_\nu$$

$$J_\nu(\tau_\nu) = B_\nu(\tau_\nu) + \frac{1}{3}\frac{\mathrm{d}^2 B_\nu}{\mathrm{d}\tau_\nu^2} + \cdots \quad ,$$

$$H_\nu(\tau_\nu) = \frac{1}{3}\frac{\mathrm{d}B_\nu}{\mathrm{d}\tau_\nu} + \cdots \quad ,$$

$$K_\nu(\tau_\nu) = \frac{1}{3}B_\nu(\tau_\nu) + \frac{1}{5}\frac{\mathrm{d}^2 B_\nu}{\mathrm{d}\tau_\nu^2} + \cdots \quad .$$

Diffusion approximation

At large depths:

- The mean intensity approaches the Planck function.
- The radiation field is isotropic and the variable Eddington factor approach 1/3.

$$f_\nu^{\mathrm{K}} \equiv K_\nu / J_\nu$$

- The monochromatic flux is the derivative of the Planck function with respect to the optical depth:

$$H_\nu = \frac{1}{3}\frac{\mathrm{d}B_\nu}{\mathrm{d}\tau_\nu} = -\frac{1}{3}\frac{1}{\chi_\nu}\frac{\mathrm{d}B_\nu}{\mathrm{d}z} = -\frac{1}{3}\frac{1}{\chi_\nu}\frac{\mathrm{d}B_\nu}{\mathrm{d}T}\frac{\mathrm{d}T}{\mathrm{d}z}$$

  At depth the transfer problem is a single equation!

  Radiative diffusion coefficient: $-\frac{1}{3}\frac{1}{\chi_\nu}\frac{\mathrm{d}B_\nu}{\mathrm{d}T}$

- Integrating over frequencies we get the total radiation flux in the diffusion approximation:

$$H = -\left(\frac{1}{3}\frac{1}{\chi_{\mathrm{R}}}\frac{\mathrm{d}B}{\mathrm{d}T}\right)\frac{\mathrm{d}T}{\mathrm{d}z} \qquad \frac{1}{\chi_{\mathrm{R}}}\frac{\mathrm{d}B}{\mathrm{d}T} = \int_0^\infty \frac{1}{\chi_\nu}\frac{\mathrm{d}B_\nu}{\mathrm{d}T}\,\mathrm{d}\nu$$

Rosseland mean opacity

$$H = -\left(\frac{1}{3}\frac{1}{\chi_{\mathrm{R}}}\frac{\mathrm{d}B}{\mathrm{d}T}\right)\frac{\mathrm{d}T}{\mathrm{d}z} \qquad \frac{1}{\chi_{\mathrm{R}}}\frac{\mathrm{d}B}{\mathrm{d}T} = \int_0^\infty \frac{1}{\chi_\nu}\frac{\mathrm{d}B_\nu}{\mathrm{d}T}\,\mathrm{d}\nu$$

Opacity weighted mean. The integrand makes the largest contributions at lowest opacities.

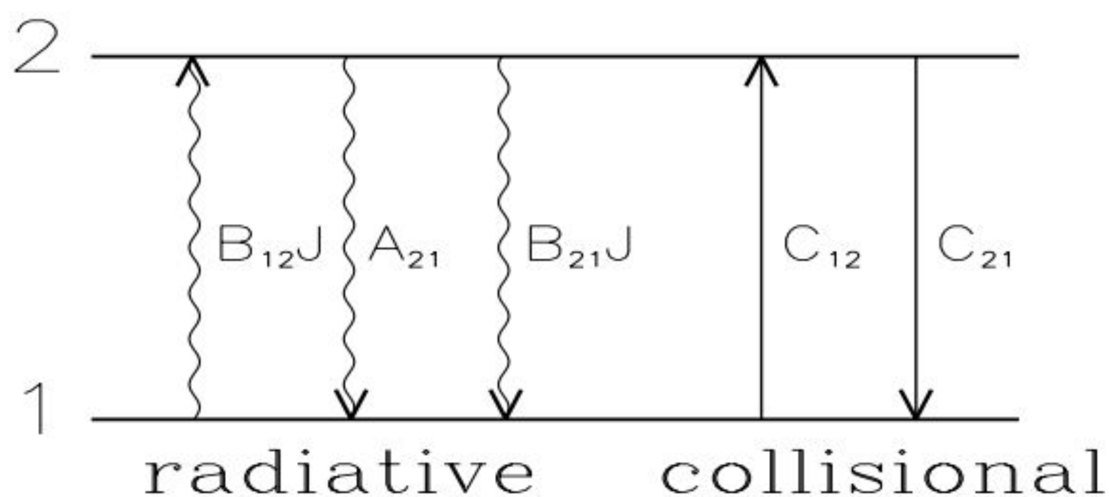
It yields the correct temperature structure at depth.

Looking at it another way: at different frequencies and monochromatic opacities we see different depths (radii) of the star, with the Rosseland mean opacity we have a radius by definition.

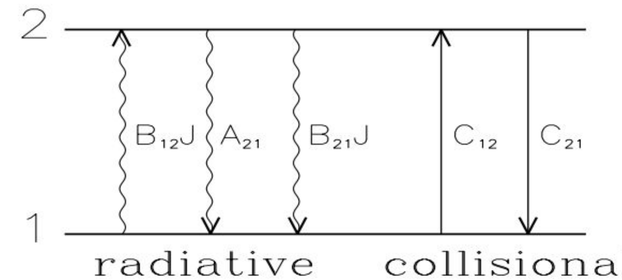
$$\chi_R = \frac{\int_0^\infty \frac{\mathrm{d}B_\nu}{\mathrm{d}T}\mathrm{d}\nu}{\int_0^\infty \frac{1}{\chi_\nu}\frac{\mathrm{d}B_\nu}{\mathrm{d}T}\mathrm{d}\nu} \qquad \mathrm{d}\tau_\nu \equiv -\chi_\nu\,\mathrm{d}z$$

Let us “calculate” a model atmosphere

- T_{eff} : measures the total energy output of the plasma
- R : radius, with T_{eff} defines L
- log g: constant in p-p (thin) atmospheres
- Composition
- Maxwell velocity distribution: particle speed (collisions)
- Eddington and diffusion approximations
- We need transitions! Connection between material and radiation field. Not a simple function of energy, but fundamental properties of material.



Transition types



- Bound - Bound:
  - Einstein coefficients (independent of T):

    • Spontaneous Emission: $N_{i \to j} = N_i A_{ij} dt$

    • Absorption: $N_{j \to i} = N_j B_{ji} I_{\nu_{ij}} dt$

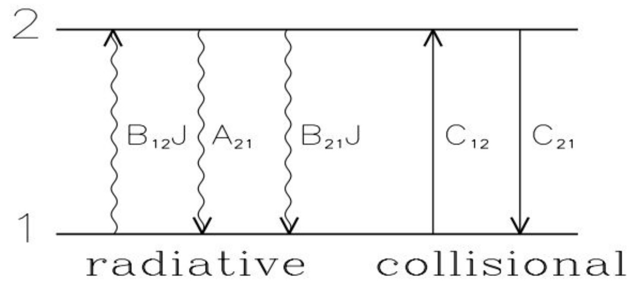
    • Stimulated Emission (enhanced in the presence of a photon of the same energy as the spontaneous transition) $N_{i \to j} = N_i B_{ij} I_{\nu_{ij}} dt$

  - In *detailed balance* (strict TE):

$$N_j B_{ji} B_{\nu_{ij}}(T) = N_i \left[A_{ij} + B_{ij} B_{\nu_{ij}}(T) \right]$$

- A and B are based on lab measurements!

Transition types



- Bound - Free: photoionization

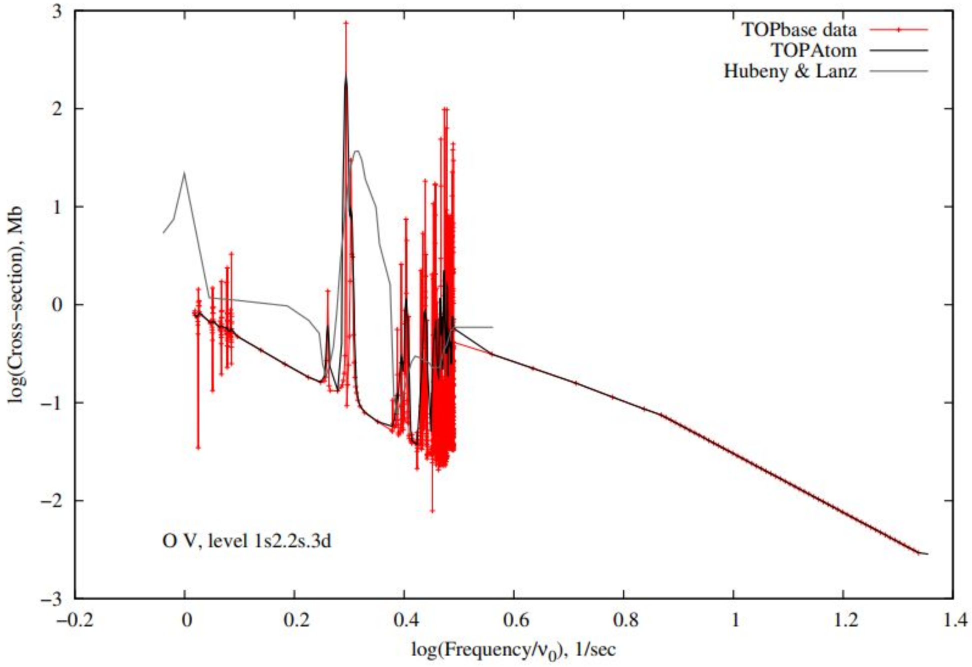
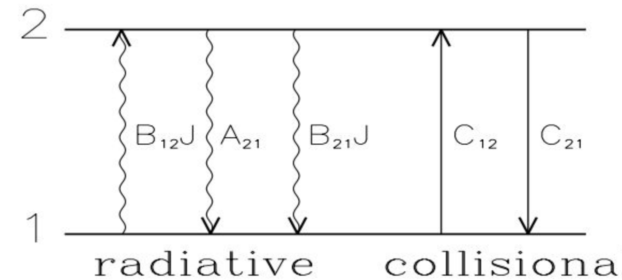


Figure 3.2: Photoionization cross-section of the O V, `1s2.2s.3d` level. ν_0 is the ionization edge frequency. The original data consists of 967 data points and are shown here in red. The TOPAtom RAP smoothed data is black, it has 192 data points. For comparison the cross-section from TLUSTY's web site is plotted with grey.

Transition types



- Free - Free:

  A free electron cannot absorb a photon. Scattering!

- Collisional excitation, de-excitation. Local interaction!

Absorption and emission coefficients

$$\kappa_\nu = \frac{h\nu_0}{4\pi}\left(n_1 B_{12} - n_2 B_{21}\right)\phi(\nu)$$

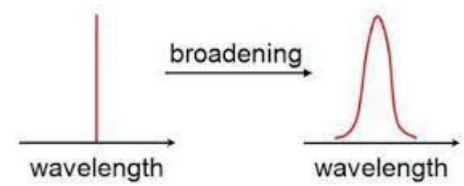
$$\eta_\nu = \frac{h\nu_o}{4\pi} n_2 A_{21}\phi(\nu)$$

$$S_\nu \equiv \frac{\eta_\nu}{\kappa_\nu} = \frac{n_2 A_{21}}{n_1 B_{12} - n_2 B_{21}} \equiv S^{\mathrm{L}}$$

Normalized Doppler line profile:

$$x \equiv \frac{\nu - \nu_0}{\Delta\nu_D} \qquad \Delta\nu_D = (\nu_0/c)v_{\mathrm{th}} \qquad v_{\mathrm{th}} = (2kT/m)^{1/2}$$

$$\phi(x) = \exp(-x^2)/\sqrt{\pi} \qquad \int_0^\infty \phi(\nu)\mathrm{d}\nu = 1$$



Voigt profile:

$$\phi(x) = H(a,x)/\sqrt{\pi}, \qquad H(a,x) = \frac{a}{\pi}\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-y^2}}{(x-y)^2 + a^2}\mathrm{d}y$$

$$a = \Gamma/(4\pi\Delta\nu_D)$$

We assume the absorption, emission, and stimulated emission profiles are all identical! CRD

- Data files were converted to same data format
- Level identification … based configuration and term
- Cross-correlation, T… …vels and transitions were replaced with NIST:
  - …ilding config…ra… …(string…
  - …00… …(in…
- Cross-…orr…tion provid… …ynspec

Log(gf)

Wavelength, nm

Element ID

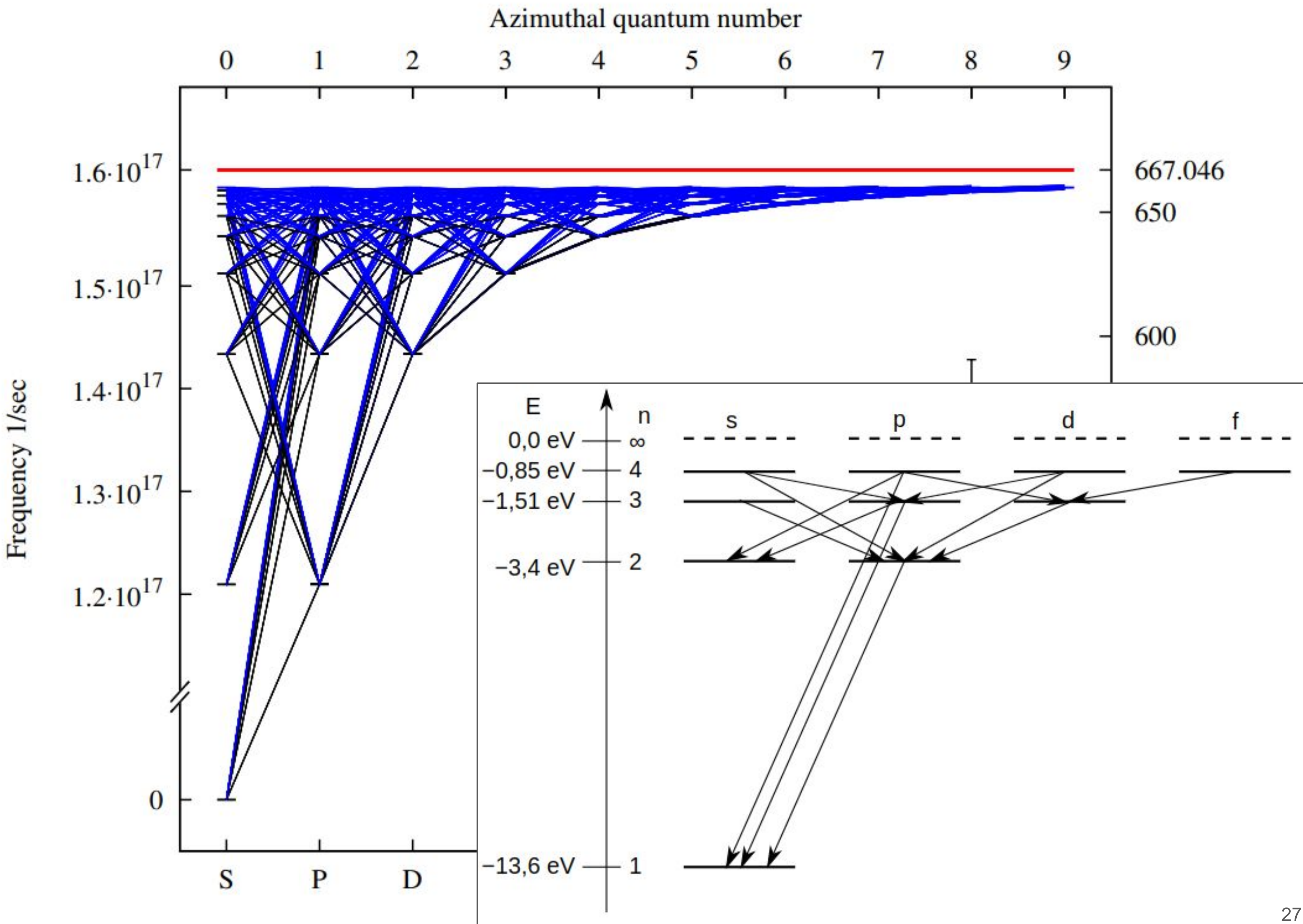
Upper level energy and stat. weight

Natural broadening parameter $\log(A_{ij})$

Lower level energy and stat. weight

2.2688	07.05	-2.983	0.000	0.0	4407643.300	1.0	10.13	0.00	0.00	0	!TBtr
2.2736	07.05	-2.844	0.000	0.0	4398403.418	1.0	10.27	0.00	0.00	0	!TBtr
2.2765	07.05	-2.688	0.000	0.0	4392710.000	1.0	10.42	0.00	0.00	0	!TBtr
2.2870	07.05	-2.510	0.000	0.0	4372540.000	1.0	10.59	0.00	0.00	0	!TBtr
2.3024	07.05	-1.824	0.000	0.0	4343290.000	1.0	10.80	0.00	0.00	0	!NISTtr
2.3277	07.05	-1.575	0.000	0.0	4296090.000	1.0	11.04	0.00	0.00	0	!NISTtr
2.3771	07.05	-1.264	0.000	0.0	4206810.000	1.0	11.33	0.00	0.00	0	!NISTtr
2.3828	07.05	-10.932	0.000	0.0	4196800.000	1.0	1.66	0.00	0.00	0	!NISTtr
2.4898	07.05	-0.842	0.000	0.0	4016390.000	1.0	11.71	0.00	0.00	0	!NISTtr
2.4914	07.05	-4.747	0.000	0.0	4013770.000	2.0	7.59	0.00	0.00	0	!NISTtr
2.5051	07.05	-10.627	0.000	0.0	3991860.000	1.0	1.92	0.00	0.00	0	!NISTtr
[illegible]	07.05	-0.171	0.000	0.0	3473790.000	1.0	12.26	0.00	0.00	0	!NISTtr
[illegible]	[illegible]	[illegible]	0.000	0.0	3438610.000	2.0	5.01	0.00	0.00	0	!NISTtr
[illegible]	[illegible]	[illegible]	0.000	0.0	3385890.000	1.0	2.41	0.00	0.00	0	!NISTtr
[illegible]	07.05	-2.444	3385890.000	1.0	4412500.000	2.0	8.93	0.00	0.00	0	!TBtr
[illegible]	07.05	-2.301	3385890.000	1.0	4403100.000	2.0	9.06	0.00	0.00	0	!TBtr
[illegible]	07.05	-2.135	3385890.000	1.0	4390900.000	2.0	9.22	0.00	0.00	0	!TBtr

...


Azimuthal quantum number
0
1
2
3
4
5
6
7
8
9
Frequency 1/sec
1.6·10^17
1.5·10^17
1.4·10^17
1.3·10^17
1.2·10^17
0
667.046
650
600
S
P
D
E
n
0,0 eV
∞
−0,85 eV
4
−1,51 eV
3
−3,4 eV
2
−13,6 eV
1
s
p
d
f

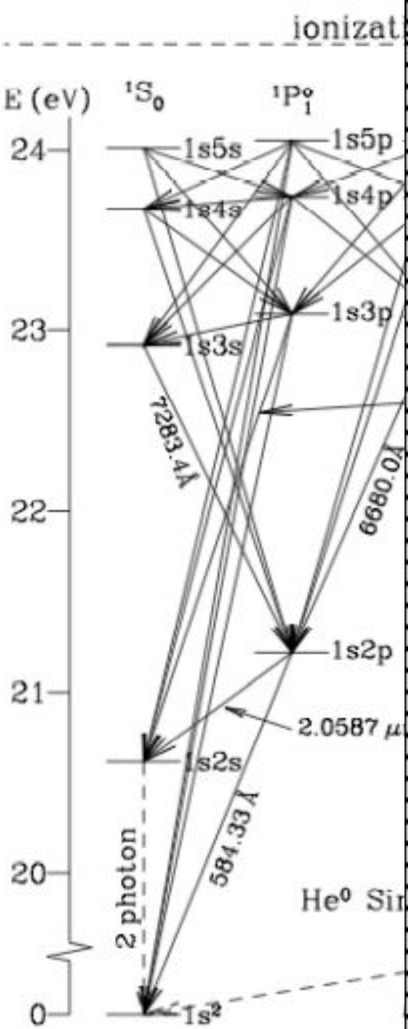
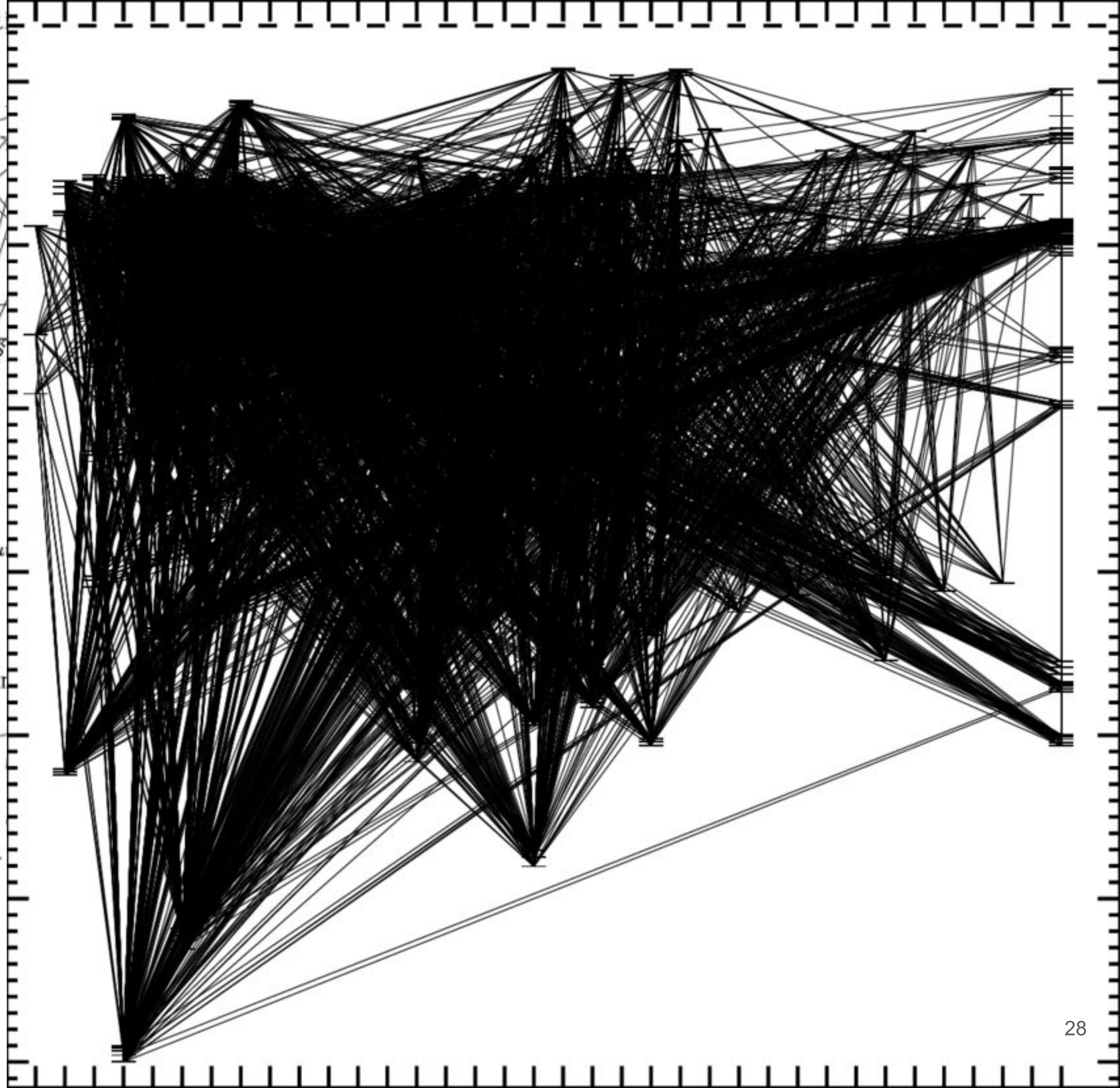


Figure 14.3 Radiative
by vacuum wavelength.



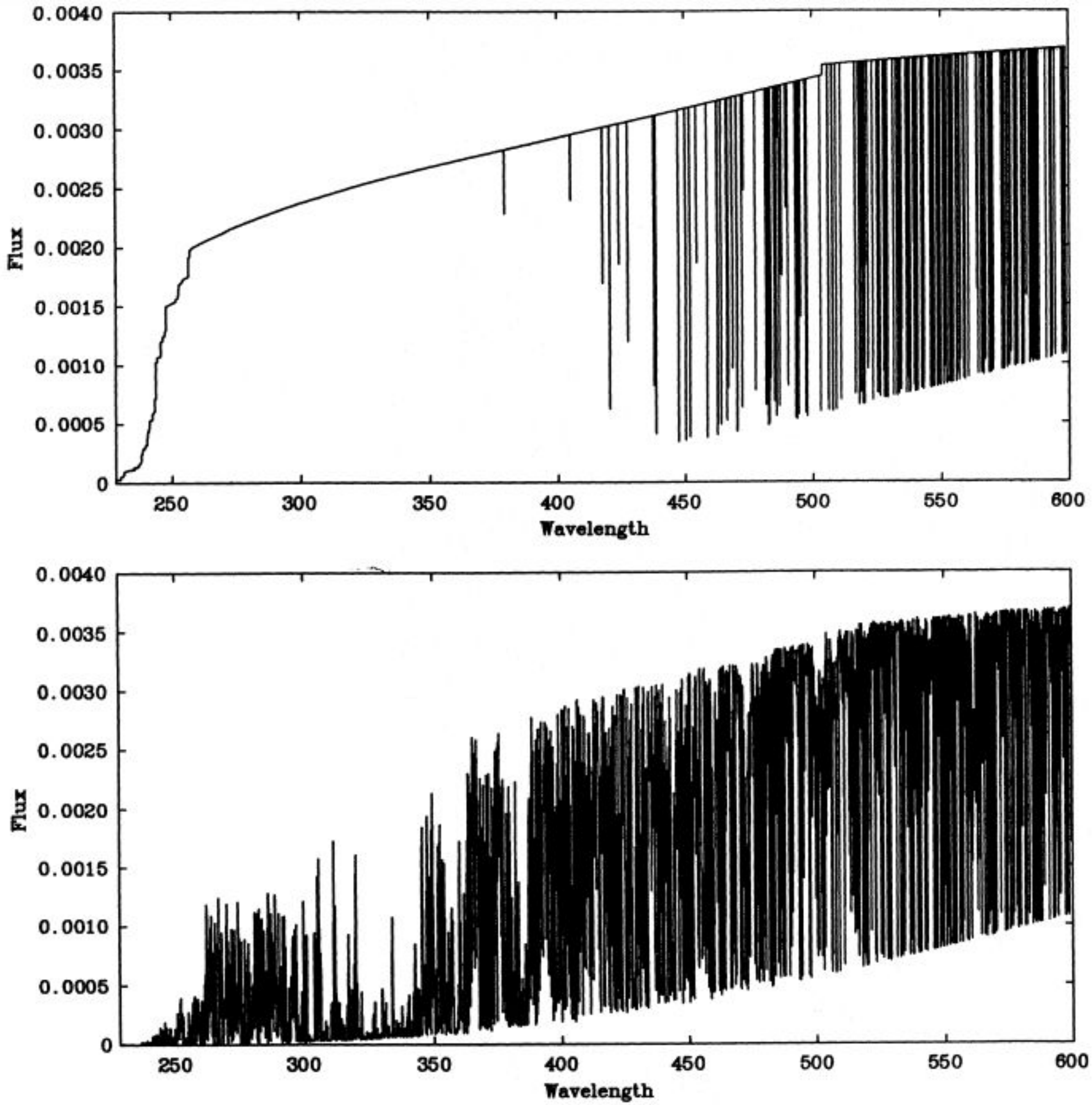


Fig. 7. Comparison of the emergent fluxes without (upper) and with (lower) line blocking in the important 228 – 600 Å spectral region

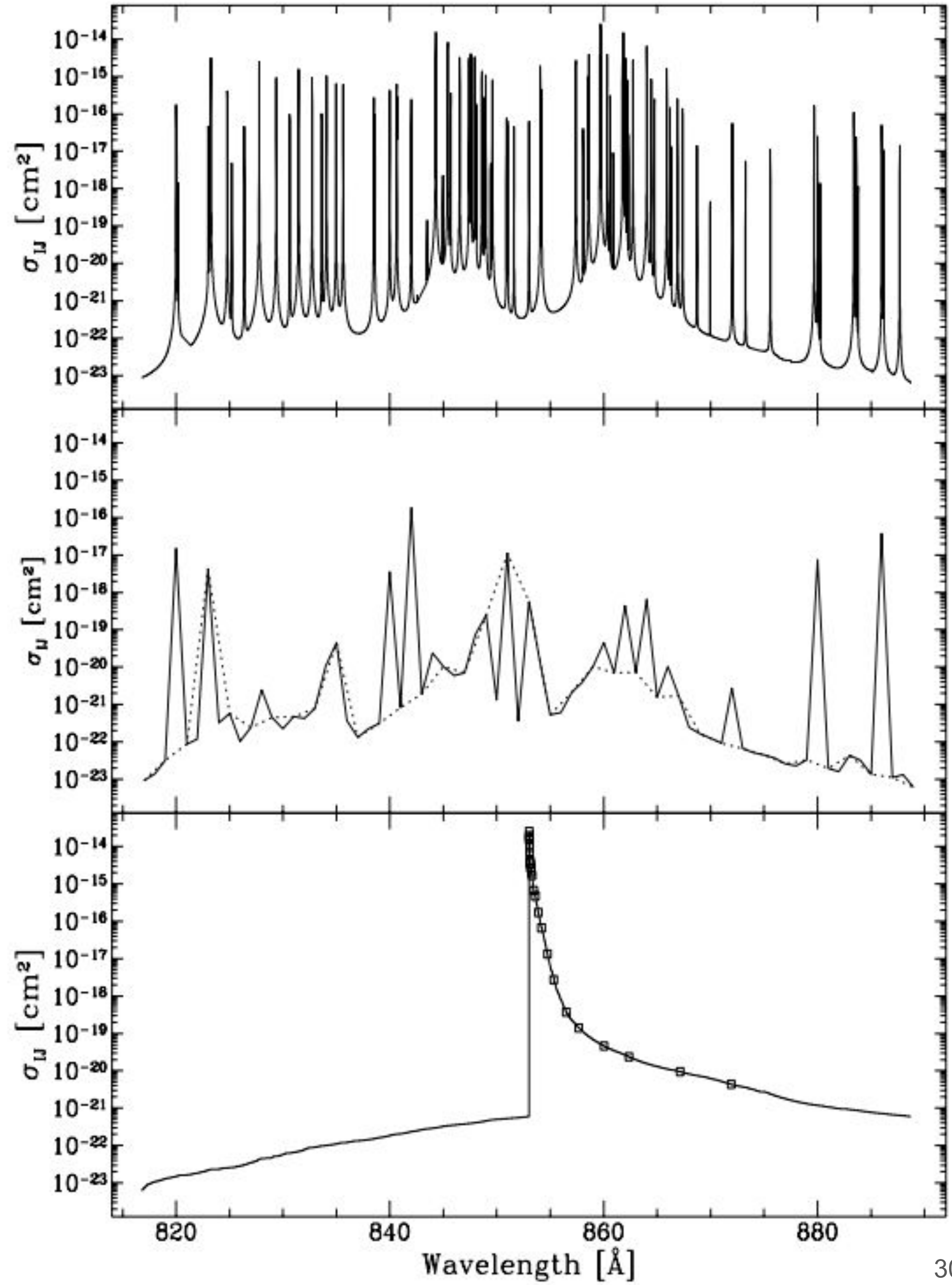
ODF function

Actual opacity:

Opacity Sampling:

$$x \equiv \frac{\nu - \nu_0}{\Delta \nu_D}$$

Opacity Distribution Function:



Scattering

- … how is it different from absorption?
- Must be treated along with absorption and emission.

$$\chi_\nu = \kappa_\nu + \kappa_\nu^{\rm sc}$$

Extinction (true absorption) and scattering coefficients

$$\kappa_\nu = \sum_i \sum_{j>i} [n_i - n_j G_{ij}(\nu)]\, \sigma_{ij}(\nu) + \sum_i \left[n_i - n_k G_{ik}(\nu) e^{-h\nu/kT}\right] \sigma_{ij}(\nu) + \sum_\kappa n_{\rm e} n_\kappa \sigma_{\kappa\kappa}(\nu, T) \left(1 - e^{-h\nu/kT}\right) + \kappa_\nu^{\rm add}$$

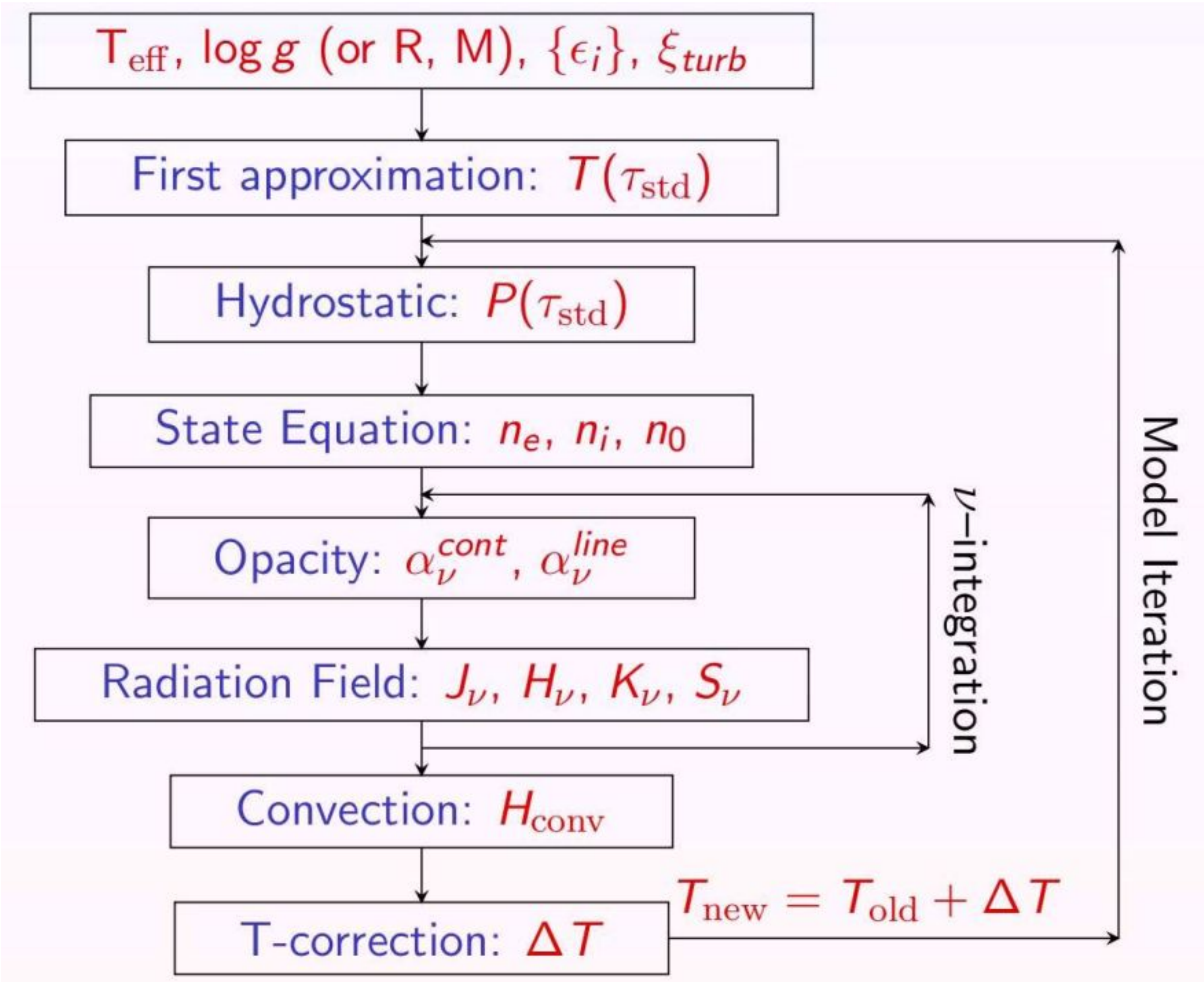
$$\sigma_{ij}(\nu) = \frac{\pi e^2}{m_{\rm e} c} f_{ij} \phi_{ij}(\nu)$$

$$\kappa_\nu^{\rm sc} = n_{\rm e}\sigma_{\rm e} + \sum_i n_i \sigma_{{\rm Ray},i}$$

Thomson and Rayleigh scattering cross sections

$$S_\nu^{\rm tot} = \frac{\eta_\nu}{\chi_\nu} + \frac{\kappa_\nu^{\rm sc}}{\chi_\nu} J_\nu$$

Now we can calculate a model



thermal structure

$T = T(z)$

$p = p(z)$

Based on Eddington's first approximation, in LTE:

$$S = B = \sigma T^4/\pi$$

And the temperature structure is:

$$T^4 = \frac{3}{4} T_{\rm eff}^4 \left(\tau_{\rm v} + \frac{2}{3} \right)$$

Next, the hydrostatic equilibrium provides the pressure:

$$\frac{\mathrm{d}P}{\mathrm{d}z} = -\rho\, g \qquad \mathrm{d}m = -\rho\, \mathrm{d}z \qquad \frac{\mathrm{d}P}{\mathrm{d}m} = g \ ,$$

$$P = P_{\rm gas} + P_{\rm rad} + P_{\rm turb} = NkT + \frac{4\pi}{c}\int_0^\infty K_\nu \mathrm{d}\nu + \frac{1}{2}\rho\, v_{\rm turb}^2$$

$$\frac{\mathrm{d}P_{\rm gas}}{\mathrm{d}m} = g - \frac{4\pi}{c}\int_0^\infty \frac{\mathrm{d}K_\nu}{\mathrm{d}m} = g - \frac{4\pi}{c}\int_0^\infty \frac{\chi_\nu}{\rho} H_\nu \mathrm{d}\nu$$

thermal structure

$T = T(z)$

$p = p(z)$

ionisation
level population

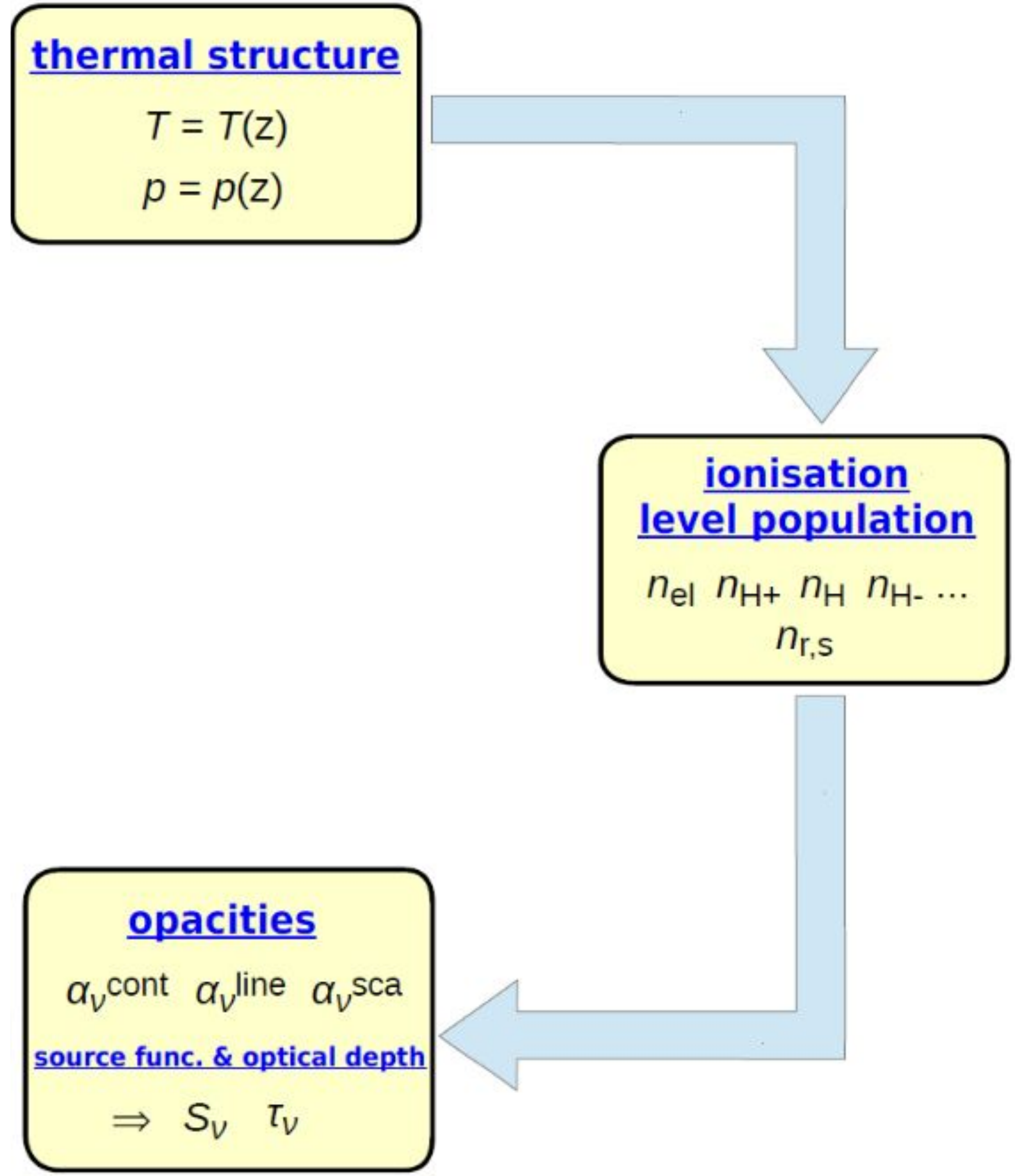
n_{el} n_{H+} n_H n_{H-} ...

$n_{r,s}$

$$\frac{n_{i+1} n_e}{n_i} = \frac{2}{\lambda^3} \frac{g_{i+1}}{g_i} \exp\left[-\frac{(\epsilon_{i+1} - \epsilon_i)}{k_B T} \right]$$

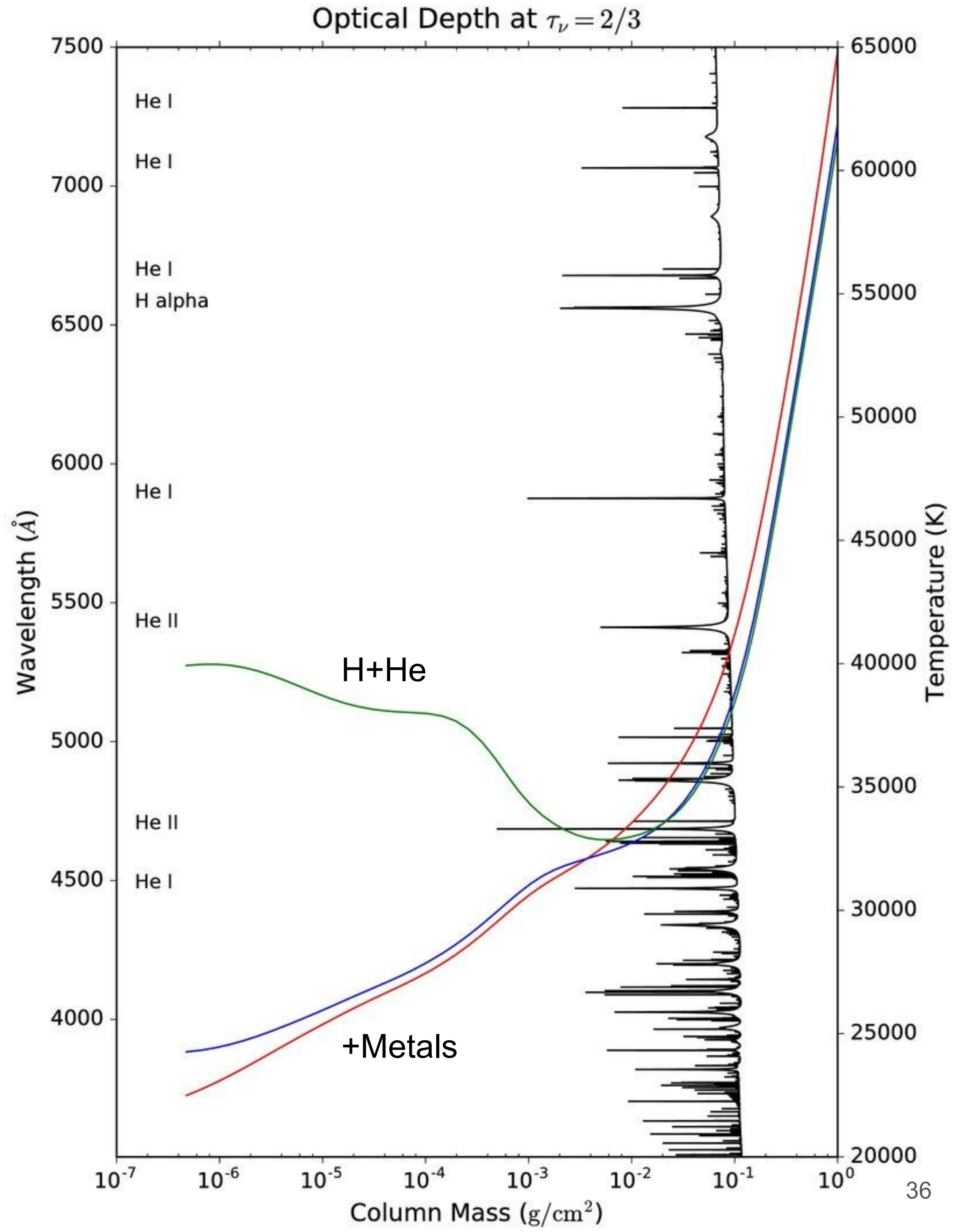
$$\lambda \stackrel{\text{def}}{=} \sqrt{\frac{h^2}{2\pi m_e k_B T}}$$

$$\sum_i n_i Z_i - n_{\mathrm{e}} = 0$$

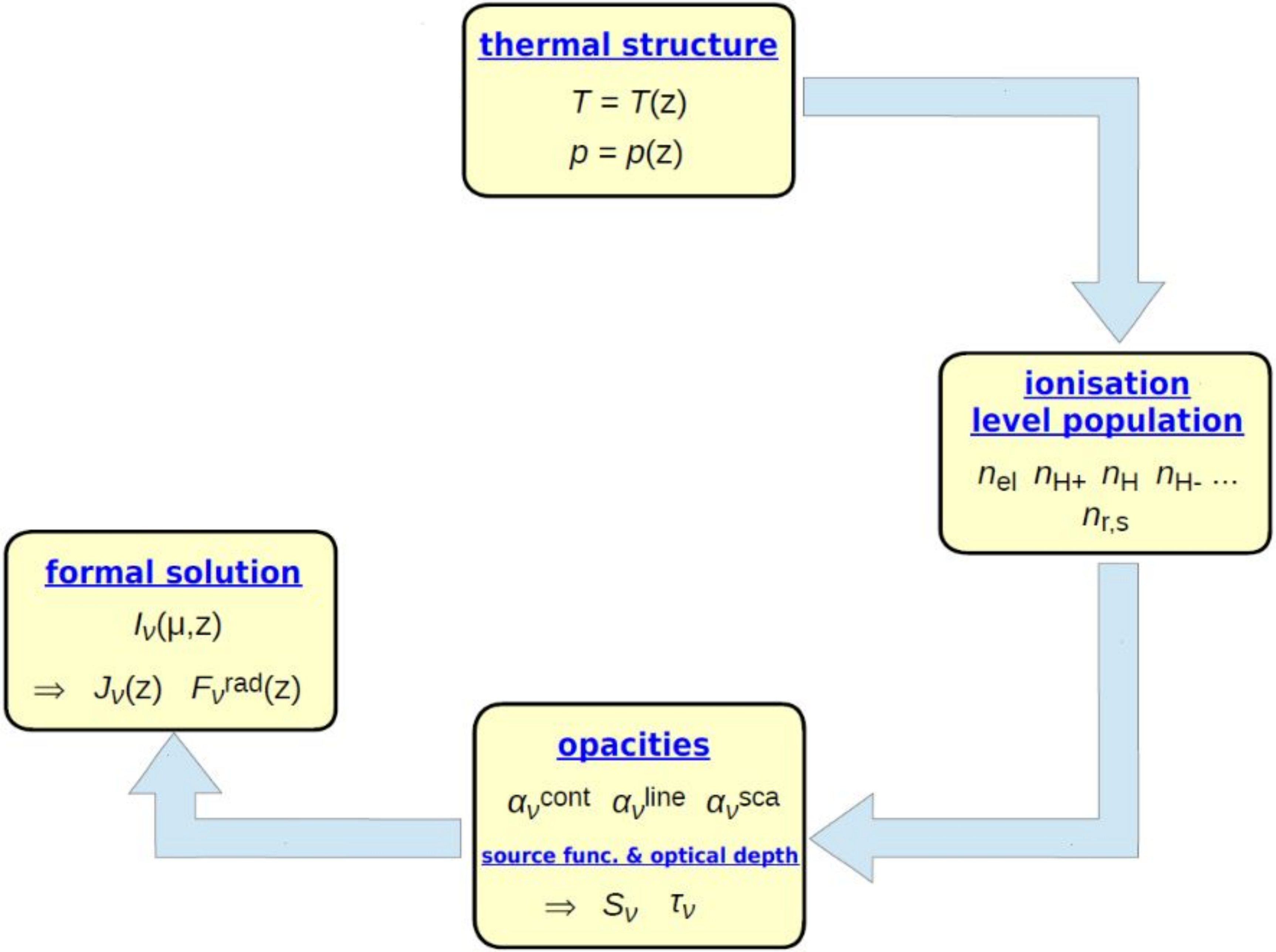

thermal structure
$T = T(z)$
$p = p(z)$
ionisation
level population
n_{el} n_{H+} n_{H} n_{H-} ...
$n_{r,s}$
opacities
α_ν^{cont} α_ν^{line} α_ν^{sca}
source func. & optical depth
$\Rightarrow$ S_ν τ_ν

Optical depth

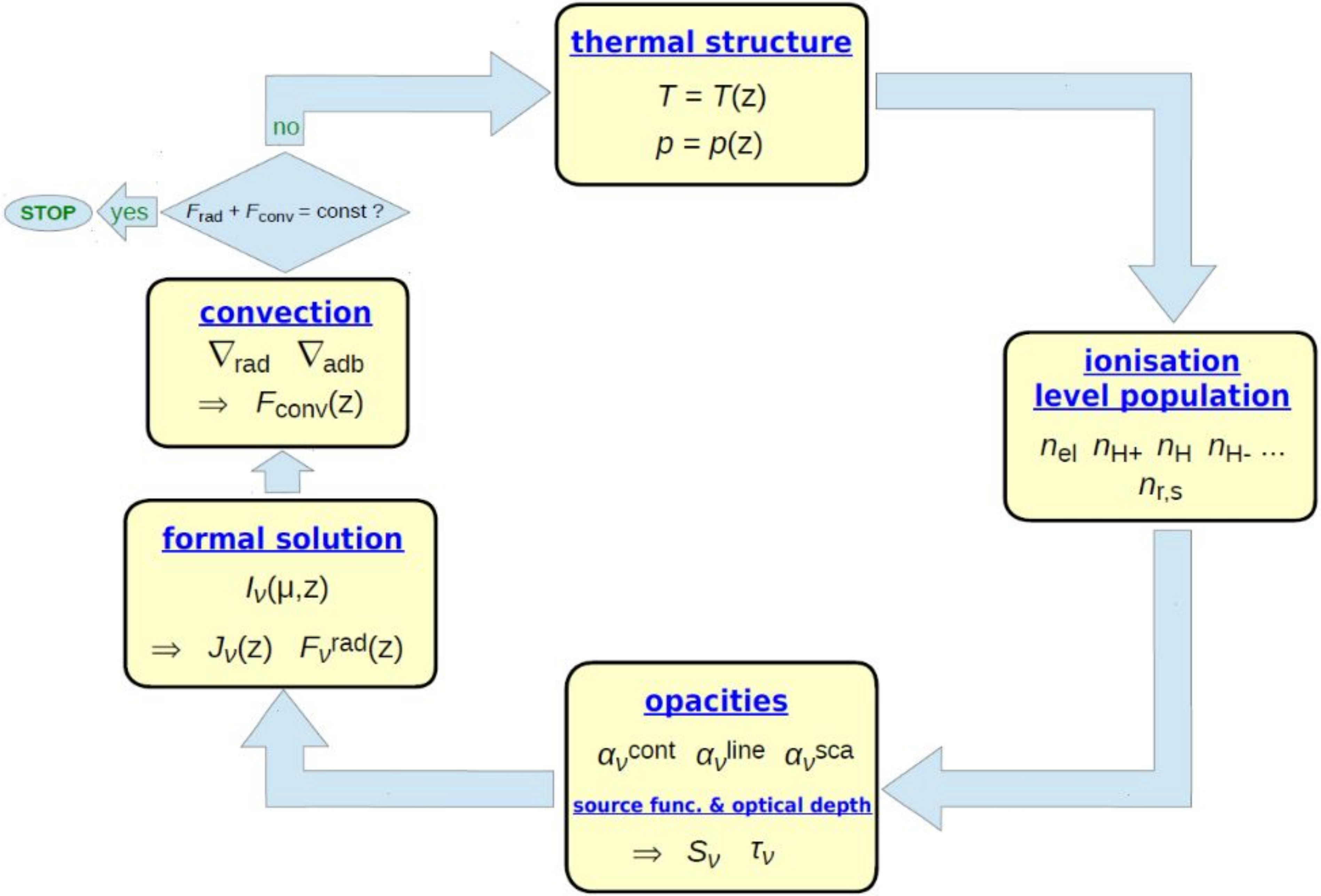
- Opacity varies
- So does R



Dorsch et al. 2018



thermal structure
$T = T(z)$
$p = p(z)$
ionisation
level population
n_{el} n_{H+} n_H n_{H-} ...
$n_{r,s}$
opacities
α_ν^{cont} α_ν^{line} α_ν^{sca}
source func. & optical depth
$\Rightarrow$ S_ν τ_ν
formal solution
$I_\nu(\mu,z)$
$\Rightarrow$ $J_\nu(z)$ $F_\nu^{rad}(z)$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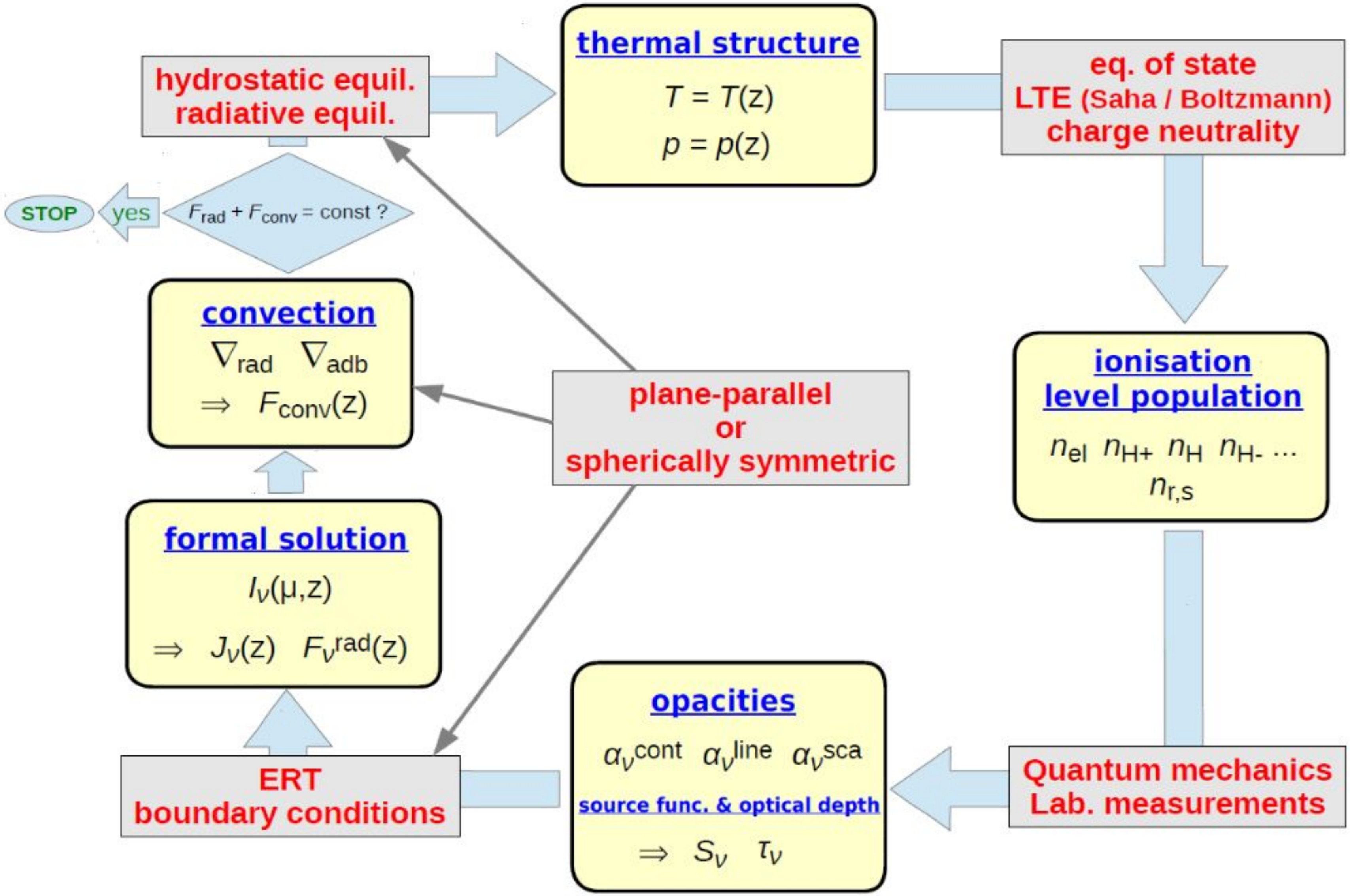
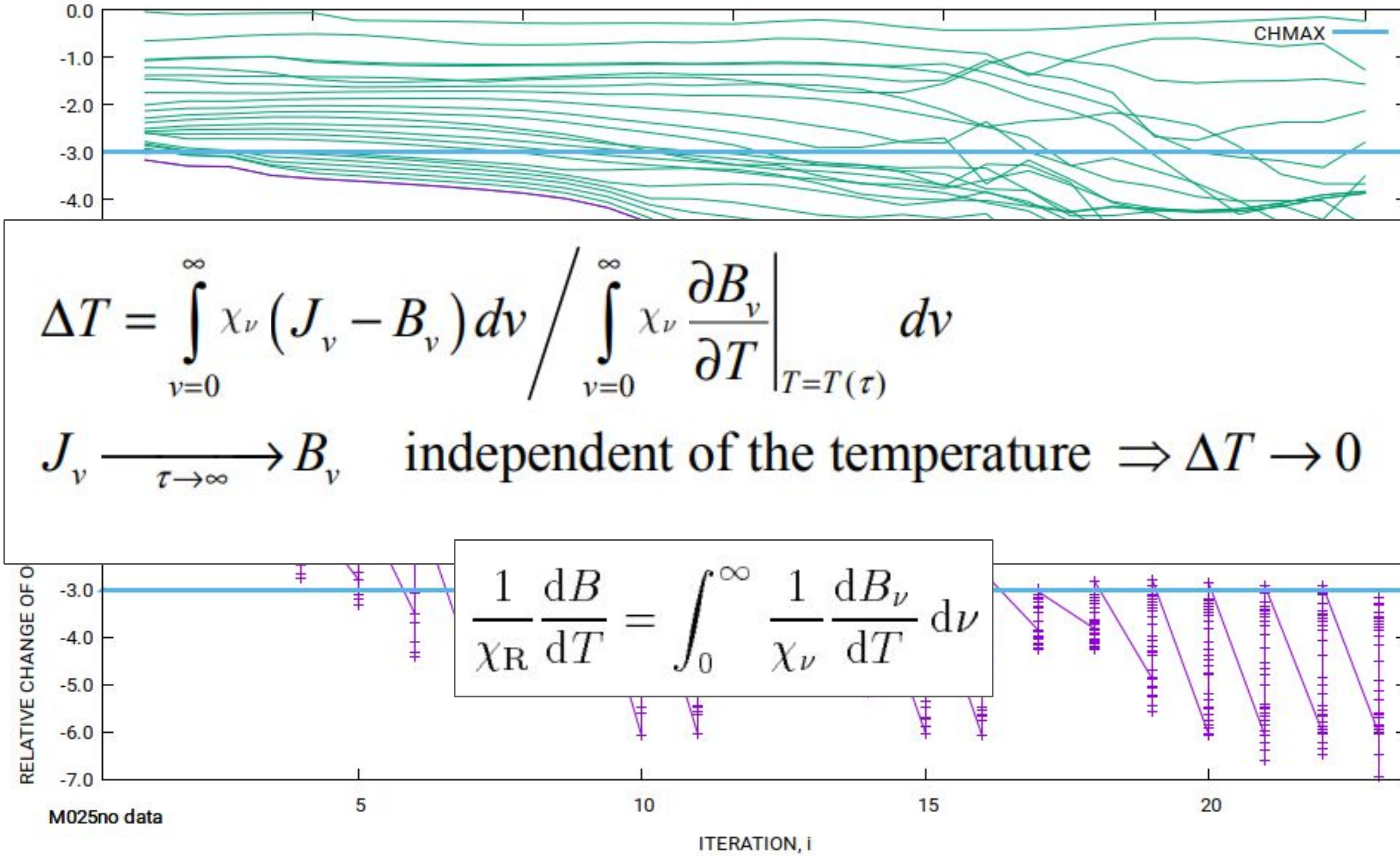
α_ν^{cont} α_ν^{line} α_ν^{sca}
source func. & optical depth
$\Rightarrow S_\nu \quad \tau_\nu$
formal solution
$I_\nu(\mu,z)$
$\Rightarrow J_\nu(z) \quad F_\nu^{rad}(z)$
convection
$\nabla_{rad} \quad \nabla_{adb}$
$\Rightarrow F_{conv}(z)$
$F_{rad} + F_{conv} = const$?
yes
STOP
no

basic stellar atmosphere model



Temperature correction

If the convergence criteria are not met, any of the model parameters differ more than the target threshold (0.1%) between consecutive global iterations:



$$\Delta T = \int_{\nu=0}^{\infty} \chi_\nu (J_\nu - B_\nu)\, d\nu \Bigg/ \int_{\nu=0}^{\infty} \chi_\nu \left.\frac{\partial B_\nu}{\partial T}\right|_{T=T(\tau)} d\nu$$

$$J_\nu \xrightarrow[\tau\to\infty]{} B_\nu \quad \text{independent of the temperature} \Rightarrow \Delta T \to 0$$

$$\frac{1}{\chi_\mathrm{R}} \frac{\mathrm{d}B}{\mathrm{d}T} = \int_0^\infty \frac{1}{\chi_\nu} \frac{\mathrm{d}B_\nu}{\mathrm{d}T}\, \mathrm{d}\nu$$

Recap: structural equations

$$\frac{d^2(f_\nu J_\nu)}{d\tau_\nu^2} = J_\nu - S_\nu$$

Radiative transfer

$$\frac{dP_{\text{gas}}}{dm} = g - \frac{4\pi}{c}\int_0^\infty \frac{dK_\nu}{dm} = g - \frac{4\pi}{c}\int_0^\infty \frac{\chi_\nu}{\rho} H_\nu d\nu$$

Hydrostatic equilibrium

$$\int_0^\infty H_\nu d\nu = \int_0^\infty \frac{d(f_\nu J_\nu)}{dm} d\nu = \frac{\sigma}{4\pi} T_{\text{eff}}^4$$

Radiative equilibrium

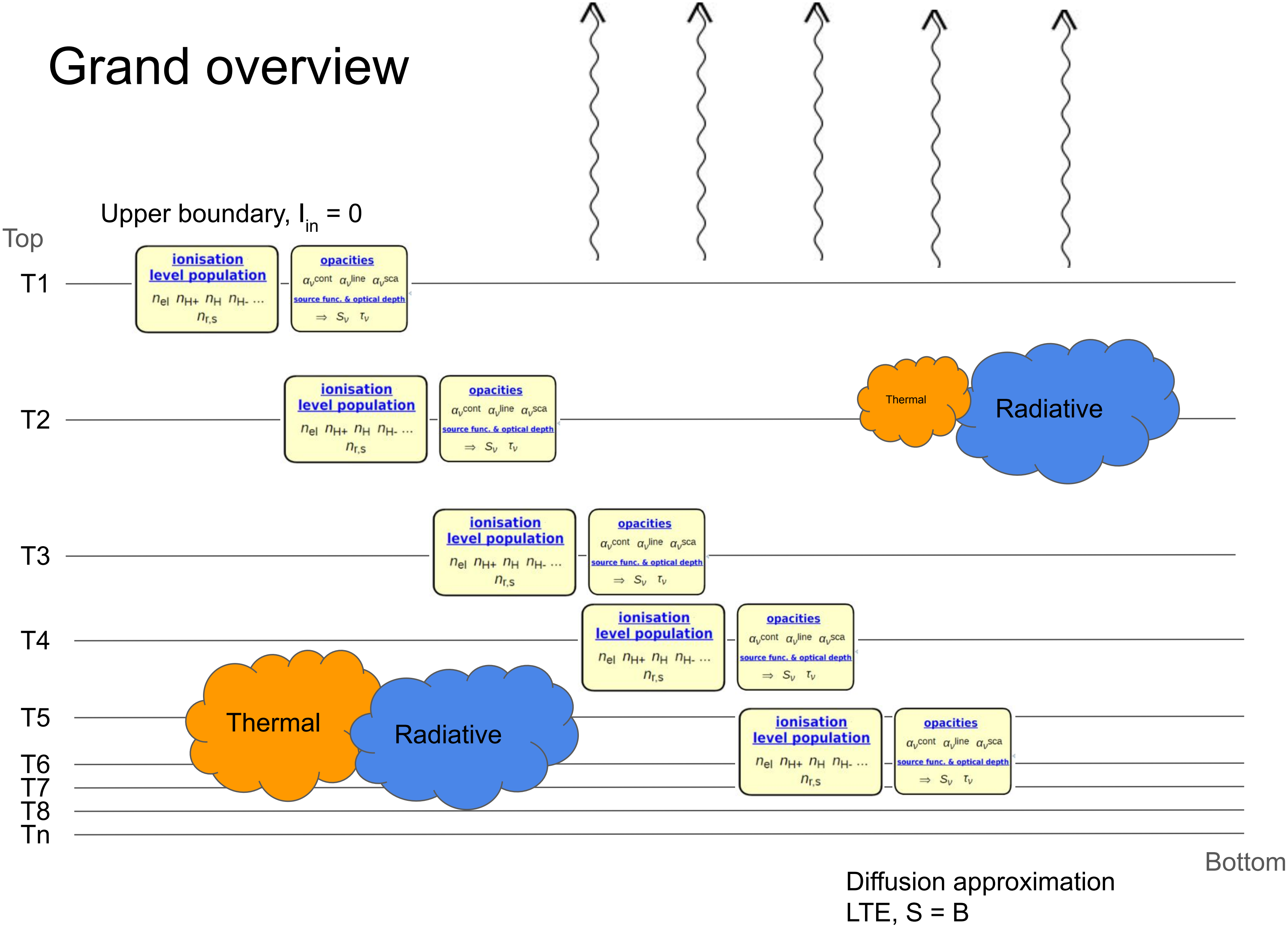
$$\frac{n_{i+1} n_e}{n_i} = \frac{2}{\lambda^3}\frac{g_{i+1}}{g_i}\exp\left[-\frac{(\epsilon_{i+1}-\epsilon_i)}{k_B T}\right]$$

Saha equation, Local!

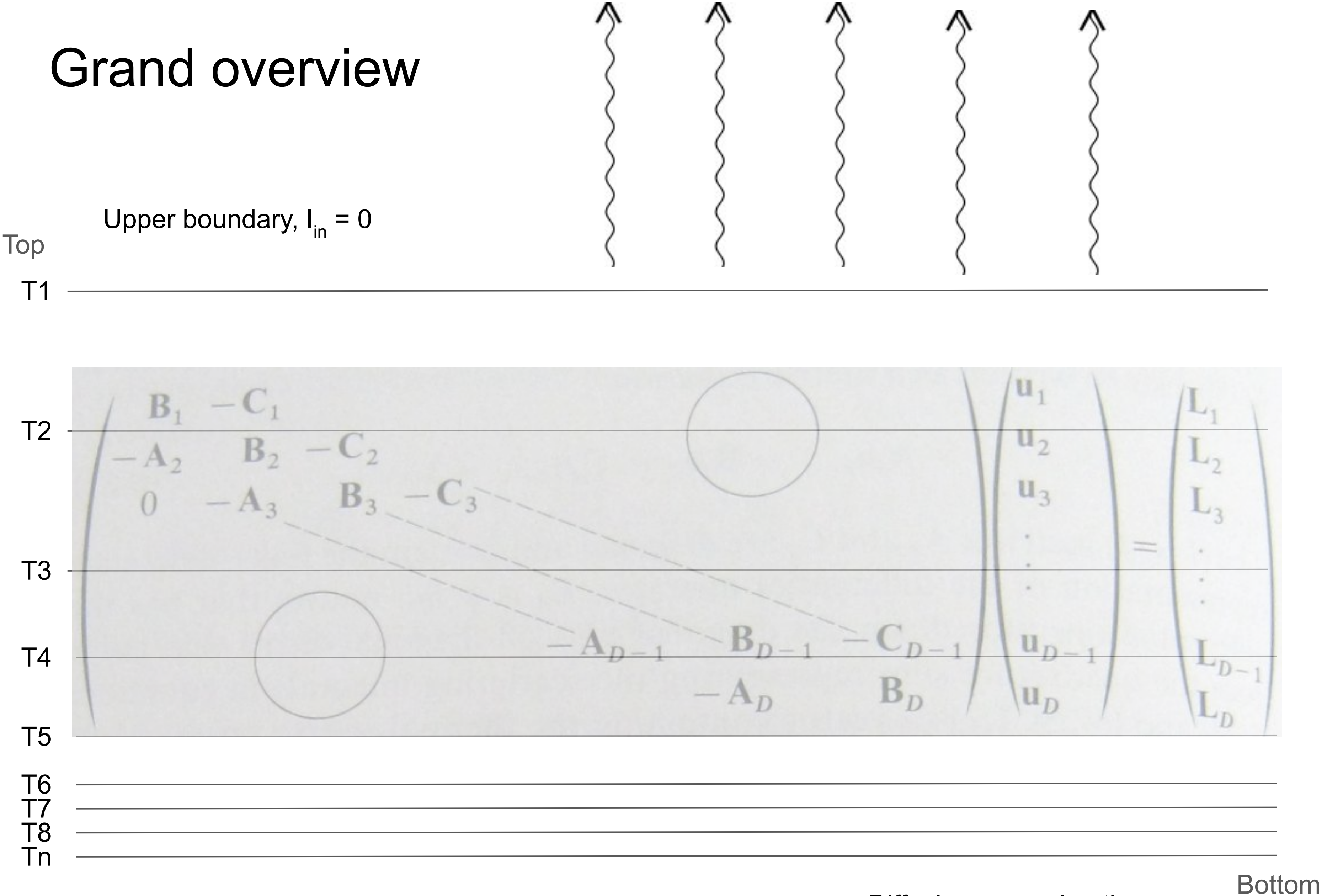
$$\sum_i n_i Z_i - n_{\text{e}} = 0$$

Charge neutrality

Grand overview



Grand overview



$$\begin{pmatrix} B_1 & -C_1 & & & \\ -A_2 & B_2 & -C_2 & & \\ 0 & -A_3 & B_3 & -C_3 & \\ & & \ddots & \ddots & \ddots \\ & & -A_{D-1} & B_{D-1} & -C_{D-1} \\ & & & -A_D & B_D \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{D-1} \\ u_D \end{pmatrix} = \begin{pmatrix} L_1 \\ L_2 \\ L_3 \\ \vdots \\ L_{D-1} \\ L_D \end{pmatrix}$$

Diffusion approximation
LTE, S = B

$$-\mathrm{A}_d\,\mathbf{u_{d-1}} + \mathrm{B}_d\,\mathbf{u_d} - \mathrm{C}_d\,\mathbf{u_{d+1}} = \mathrm{L}_d$$

Diagonal: differential op.
Off-diagonal:scattering terms

Finite difference representation of the differential op.

Depth vector, angle-frequency components

...pecialize the latter to the di...

THE FE... SOLUTION

The set ... equations (6-31), (6-34), and (6-36) have the overall structure

$$\begin{pmatrix} \mathbf{B}_1 & -\mathbf{C}_1 & & & & \\ -\mathbf{A}_2 & \mathbf{B}_2 & -\mathbf{C}_2 & & & \\ 0 & -\mathbf{A}_3 & \mathbf{B}_3 & -\mathbf{C}_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\mathbf{A}_{D-1} & \mathbf{B}_{D-1} & -\mathbf{C}_{D-1} \\ & & & & -\mathbf{A}_D & \mathbf{B}_D \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \mathbf{u}_3 \\ \vdots \\ \mathbf{u}_{D-1} \\ \mathbf{u}_D \end{pmatrix} = \begin{pmatrix} \mathbf{L}_1 \\ \mathbf{L}_2 \\ \mathbf{L}_3 \\ \vdots \\ \mathbf{L}_{D-1} \\ \mathbf{L}_D \end{pmatrix} \quad (6\text{-}3$$

Finite difference representation of the differential op.

Thermal source terms

Each element indicated is either an $(I \times I)$ matrix or a vector of length I; the grand matrix has a *block tridiagonal* structure, and the solution proceeds by an efficient forward-elimination and back-substitution procedure (209). In this scheme we in effect express each $\mathbf{u}_d$ in terms of $\mathbf{u}_{d+1}$ and substitute into the following equation. Thus from equation (6-34) we can write

$$\mathbf{u}_1 = \mathbf{B}_1^{-1}\mathbf{C}_1\mathbf{u}_2 + \mathbf{B}_1^{-1}\mathbf{L}_1 \equiv \mathbf{D}_1\mathbf{u}_2 + \mathbf{v}_1 \quad (6\text{-}38)$$

Substituting equation (6-38) into equation (6-31) for $d = 2$ yields $\mathbf{u}_2 = \mathbf{D}_2\mathbf{u}_3 + \mathbf{v}_2$ where $\mathbf{D}_2 = (\mathbf{B}_2 - \mathbf{A}_2\mathbf{D}_1)^{-1}\mathbf{C}_2$

and
$$\mathbf{v}_2 = (\mathbf{B}_2 - \mathbf{A}_2\mathbf{D}_1)^{-1}(\mathbf{L}_2 + \mathbf{A}_2\mathbf{v}_1)$$

We therefore have in general

$$\mathbf{u}_d = \mathbf{D}_d\mathbf{u}_{d+1} + \mathbf{v}_d \quad (6\text{-}39)$$

Forward elimination

where
$$\mathbf{D}_d \equiv (\mathbf{B}_d - \mathbf{A}_d\mathbf{D}_{d-1})^{-1}\mathbf{C}_d \quad (6\text{-}40)$$

and
$$\mathbf{v}_d \equiv (\mathbf{B}_d - \mathbf{A}_d\mathbf{D}_{d-1})^{-1}(\mathbf{L}_d + \mathbf{A}_d\mathbf{v}_{d-1}) \quad (6\text{-}41)$$

At d=D: $\mathbf{u_d}=\mathbf{v_d}$

for $d = 1, \ldots, D$. Starting at $d = 1$, we compute successive values for $\mathbf{D}_d$ and $\mathbf{v}_d$ through $d = D - 1$. At the last point, $d = D$, $\mathbf{C}_D \equiv 0$, hence $\mathbf{D}_D \equiv 0$, and $\mathbf{u}_D \equiv \mathbf{v}_D$ [which still follows from equation (6-41)]. Having found $\mathbf{u}_D$ we then perform successive back-substitutions into equation (6-39 to find $\mathbf{u}_d$, $(d = D - 1, \ldots, 2, 1)$. Having found u_{dmn}, we may then evaluate $J_{dn} = \sum_{m=1}^{M} b_m u_{dmn}$, and the source function, which involves frequency integrals of J_ν; e.g., $S_{dn} = \alpha_{dn} \sum_{n'} w_{n'} \phi_{dn'} J_{dn'} + \beta_{dn}$.

The forward-backward sweep described above accounts explicitly for scattering terms and the two-point boundary conditions. Feautrier's method

Diffusion approximation and back-solution

Little details we overlook

- Microturbulence
- Line broadening
- …

Hybrid CL/ALI method for evaluation of the transfer equation

Tlusty stores the physical state of the atmosphere for each depth point in vectors like:

$$\psi_d = \{J_1, ..., J_{NF}, N, T, n_e, n_1, ..., n_{NL}\}$$

The structural equations formally:

$$\mathbf{P}(\mathbf{x}) = 0$$

where $\mathbf{x} = \{\psi_1, ..., \psi_{ND}\}$ and using Newton-Raphson method for solving:

$$\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} - \frac{\mathbf{P}[\mathbf{x}^{(n)}]}{J[\mathbf{x}^{(n)}]}$$

$$J_{ij} = \partial P_i / \partial x_j$$

the ij-element of the Jacobian is the derivative of the ith equation with respect to the jth unknown. By block-Gaussian elimination this tridiagonal matrix can be reduced to an NN$\times$NN dimension matrix, where NN = NF + NL + 3. The total computation time scales as $\mathrm{N}_i \times$ ND $\times$ NN^3.

The ALI method reduces the number of unknowns more, as eliminates the frequency points. The mean intensity is expressed as:

$$J_\nu^{(i)} = \Lambda_\nu^* S_\nu^{(i)} + (\Lambda_\nu - \Lambda_\nu^*) S_\nu^{(i-1)}$$

or (ν subscript omitted):

$$J_d = \Lambda_d^* \frac{\eta_d}{\kappa_d} + \Delta J_d^{old}$$

From LTE to NLTE

- Velocity distribution remains Maxwellian (local)
- Saha-Boltzmann → Statistical equilibrium (rate eq.)
- Coupling between distant parts of the atmosphere (non-local)
- Source function deviates from the Planck function
- Computationally much more demanding
- Requires an initial guess (input model, LTE or NLTE)
- Not all models can be converged, or they just need a different approach
- LTE is strict, NLTE is anything beyond LTE
- Sophisticated processes vs. massive atomic data
- Costly transition from LTE to NLTE, but needed for a ~1% precision

- TLUSTY:
  - Full NLTE with line blanketing
  - Atomic data and physical processes are well separated (for metals)

Structural equations in NLTE

$$\frac{d^2(f_\nu J_\nu)}{d\tau_\nu^2} = J_\nu - S_\nu \qquad f_\nu = K_\nu / J_\nu$$

Radiative transfer

$$\frac{dP_{\text{gas}}}{dm} = g - \frac{4\pi}{c}\int_0^\infty \frac{dK_\nu}{dm} = g - \frac{4\pi}{c}\int_0^\infty \frac{\chi_\nu}{\rho} H_\nu d\nu$$

Hydrostatic equilibrium

$$\alpha\left[\int_0^\infty (\kappa_\nu J_\nu - \eta_\nu)\mathrm{d}\nu\right] + \beta\left[\int_0^\infty \frac{\mathrm{d}(f_\nu J_\nu)}{\mathrm{d}\tau_\nu}\mathrm{d}\nu - \frac{\sigma}{4\pi}T_{\text{eff}}^4\right] = 0$$

Radiative equilibrium

$$n_i \sum_{j\neq i}(R_{ij} + C_{ij}) = \sum_{j\neq i} n_j (R_{ij} + C_{ij})$$

Rate equation, non-local

$$\sum_i n_i Z_i - n_{\mathrm{e}} = 0$$

Charge neutrality

LTE vs. NLTE

When do departures from LTE become important?

LTE is a bad approximation, if:

1) Collisional rates are small $C_{ij} \sim n_e / \sqrt{T}$ $n_e \downarrow, T \uparrow \;\Rightarrow\; C_{ij} \downarrow$
2) Radiative rates are large $R_{ij} \sim T^{\alpha},\ \alpha > 1$ $T \uparrow \;\Rightarrow\; R_{ij} \uparrow$
3) Mean free path of photons is larger than that of electrons

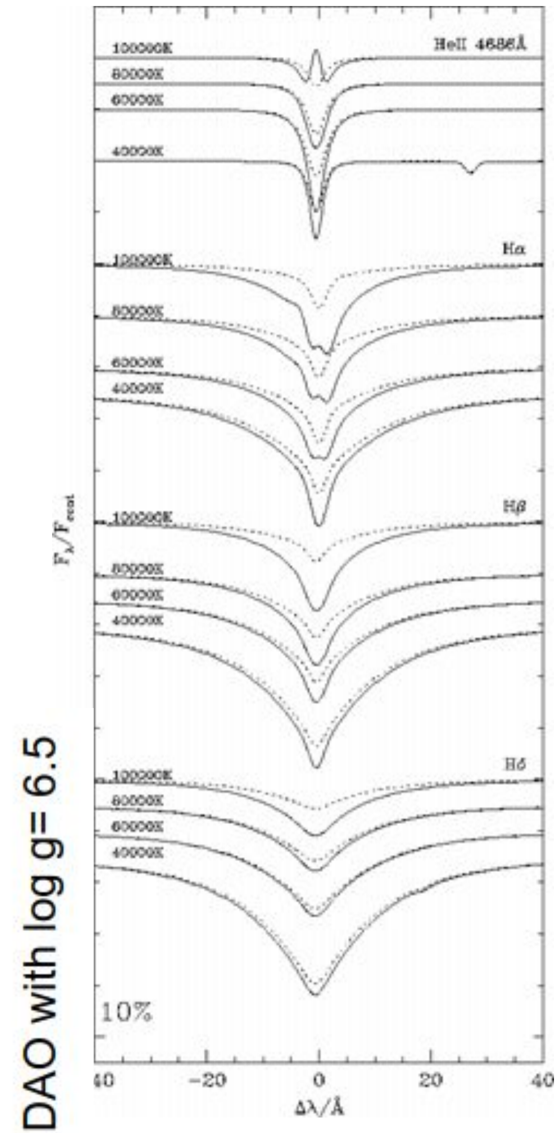
   Example: pure hydrogen plasma

$\Delta z \sim 1/n_H$ (density of neutral H)

Saha: $n_H \sim n_e n_p T^{-3/2} e^{\Delta E/kT} \;\rightarrow\; \Delta z \sim \dfrac{T^{3/2}}{n_e n_p} e^{-\Delta E/kT}$

$n_e \downarrow, T \uparrow \;\Rightarrow\; \Delta z \uparrow$

Departures from LTE occur, if temperatures are high and densities are low



Winds of hot stars!

https://slideplayer.com/slide/6269010/

NLTE effects

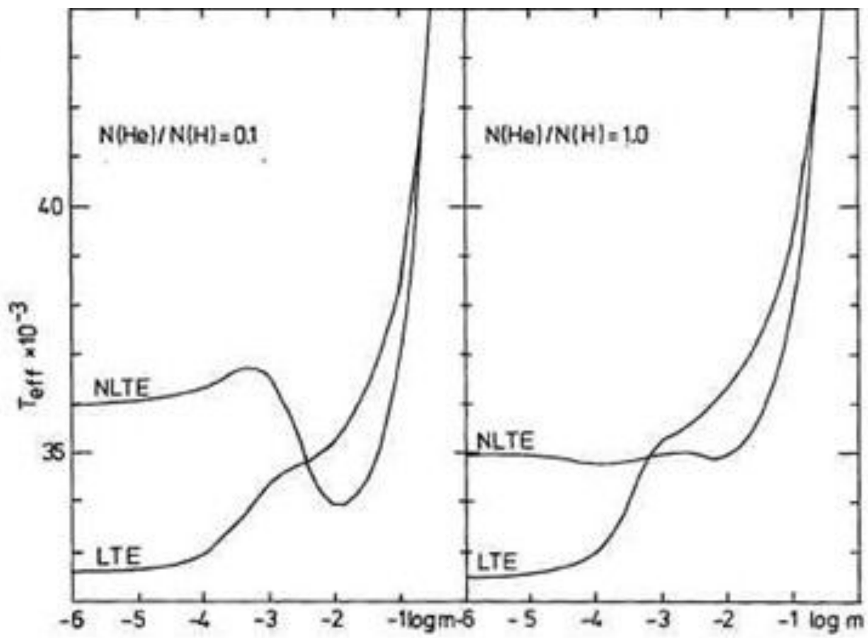


Fig. 4. Temperature stratification in NLTE and LTE for T_{eff} = 45000 K, $\log g = 5$ and two different helium abundances (N(He)/N(H) = 0.1 and 1.0)

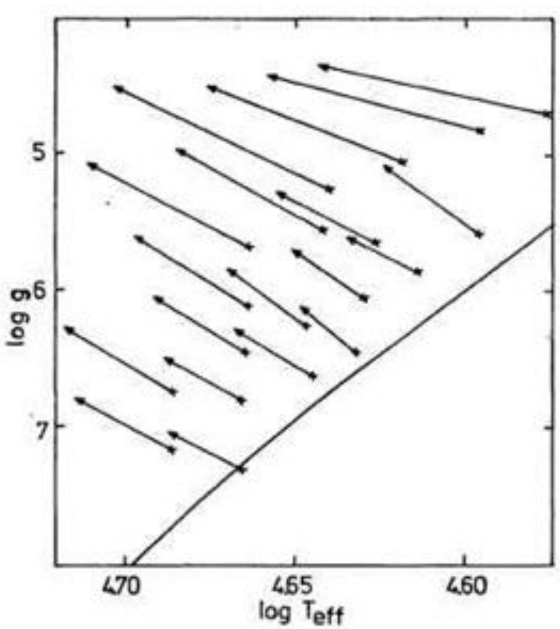


Fig. 8. "Non-LTE vectors" [Displacement due to non-LTE effects in the ($\log g$, $\log T_{eff}$)-diagram] for N(He)/N(H) = 0.1

https://slideplayer.com/slide/6269010/

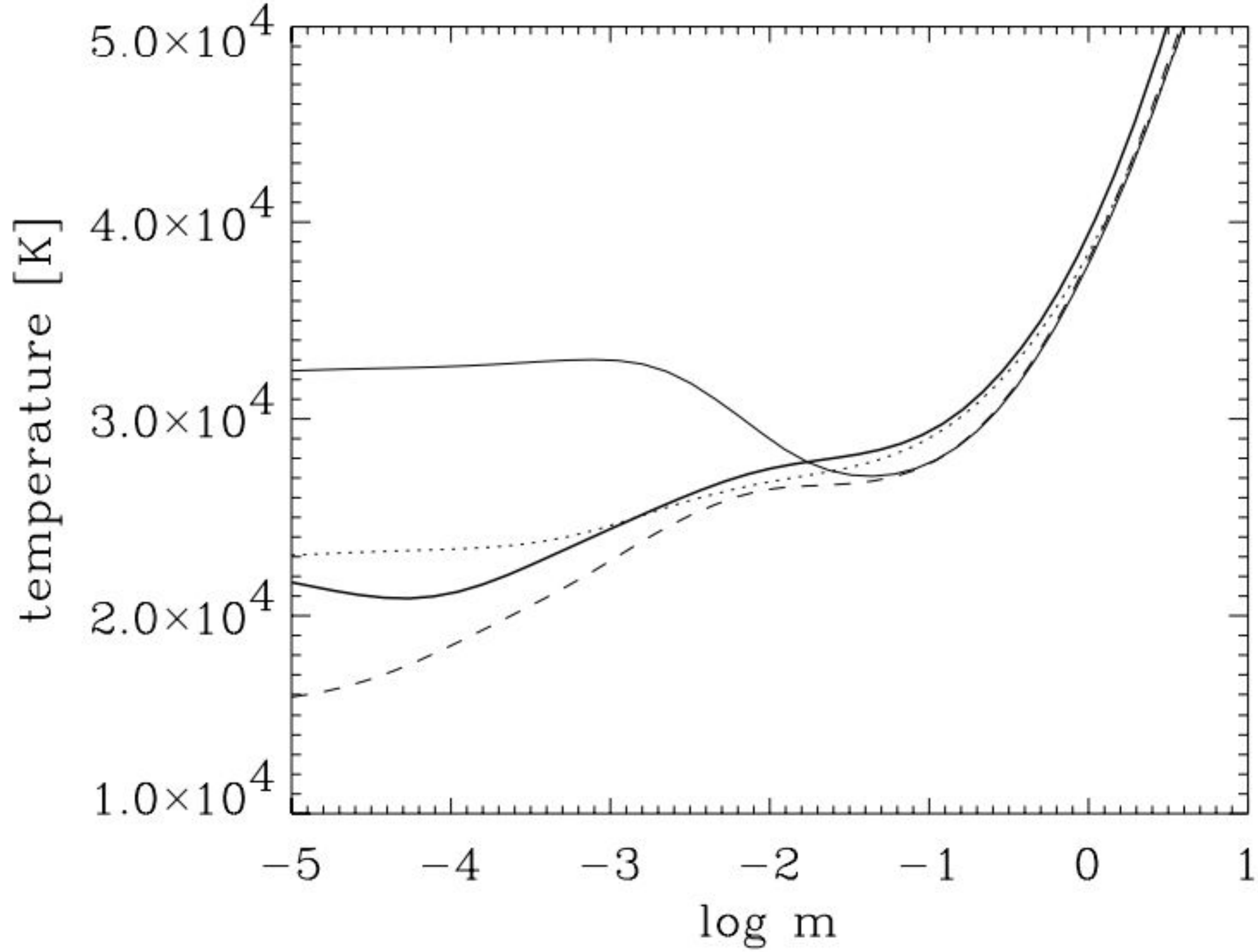
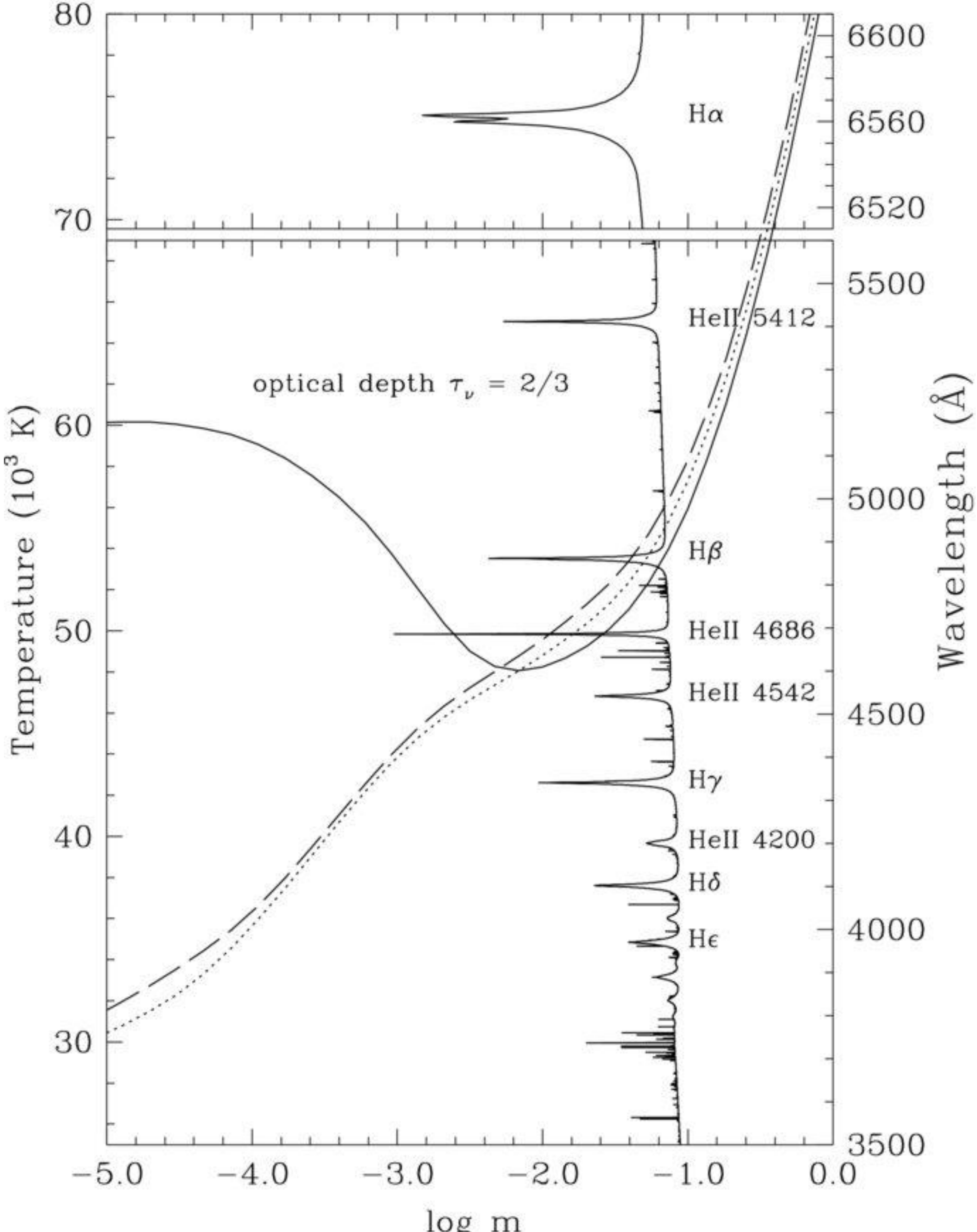


Fig. 6. Temperature structure for four model atmospheres with the same parameters: $T_{\rm eff} = 35\,000$ K, $\log g = 4$. Thick line: fully blanketed NLTE H-He-C-N-O-Si-Fe-Ni model; dashed line: NLTE model with light elements (H-He-C-N-O-Si); thin line: NLTE H-He model; dotted line: LTE H-He model.



Latour et al.
ApJ 733:100

Temperature stratification and monochromatic optical depth τv = 2/3 as functions of depth, where m is the column density, for NLTE models defined by Teff = 70,000 K, log g = 6.0, and log N(He)/N(H) = −0.5. The temperature structure is shown for models including H and He only (solid curve), H, He, and CNO in solar abundances (dotted curve), and H, He, and CNOFe in solar abundances (dashed curve). The τ_v = 2/3 curve is shown for the model with the most metals. The effective resolution is 0.1 Å.

Statistical equilibrium (rate equations)

Change of population number of a level with time: $\frac{d}{dt}n_i$

= Sum of all population processes into this level $= \sum_{j \neq i} n_j P_{ji}$

- Sum of all de-population processes out from this level $- n_i \sum_{j \neq i} P_{ij}$

$$\frac{d}{dt} n_i = \sum_{j \neq i} n_j P_{ji} - n_i \sum_{j \neq i} P_{ij}$$

One such equation for each level

The transition rate P_{ij} comprises radiative rates R_{ij}

and collision rates C_{ij}

In stellar atmospheres we often have the stationary case:

$$\frac{d}{dt} n_i = 0 \quad \text{hence} \quad \boxed{\sum_{j \neq i} n_j P_{ji} = n_i \sum_{j \neq i} P_{ij}} \quad \text{for all levels } i$$

These equations determine the population numbers.

https://slideplayer.com/slide/6269010/

TLUSTY – modeling the structure of stellar atmospheres

- … and accretion disks, even around BHs!
- Plane-parallel geometry
- Hydrostatic eq.
- Radiative eq.
- Detailed atoms for 14 elements
- LTE and NLTE line blanketed atmospheres
- "TLUSTY does NLTE, and does it in a more delicate way than many other codes."

We continue from here tomorrow!

How many of us are interested in TLUSTY?