Emission and Absorption

Chemical composition

Stellar atmosphere = mixture, composed of many chemical elements, present as atoms, ions, or molecules

Abundances, e.g., given as mass fractions β_k

- Solar abundances

$$\left.\begin{aligned}
\beta_H &= 0.71 \\
\beta_{He} &= 0.28 \\
\beta_C &= 0.004 \\
\beta_N &= 0.001 \\
\beta_O &= 0.009 \\
&\vdots \\
\beta_{Fe} &= 0.001 \\
&\vdots
\end{aligned}\right\}$$

Universal abundance for Population I stars

Chemical composition

- Population II stars

$$\beta_H = \beta_H^\odot$$
$$\beta_{He} = \beta_{He}^\odot$$
$$\beta_Z = 0.1 \cdots 0.00001\ \beta_Z^\odot$$

- Chemically peculiar stars, e.g., helium stars

$$\beta_H \le 0.002 << \beta_H^\odot$$
$$\beta_{He} = 0.964 >> \beta_{He}^\odot$$
$$\beta_C = 0.029 >> \beta_C^\odot$$
$$\beta_N = 0.003 \approx \beta_N^\odot$$
$$\beta_O = 0.002 < \beta_O^\odot$$

- Chemically peculiar stars, e.g., PG1159 stars

$$\beta_H \le 0.05 << \beta_H^\odot$$
$$\beta_{He} = 0.25 >> \beta_{He}^\odot$$
$$\beta_C = 0.55 >> \beta_C^\odot$$
$$\beta_N < 0.02$$
$$\beta_O = 0.15 >> \beta_O^\odot$$

Other definitions

- Particle number density N_k = number of atoms/ions of element k per unit volume
  relation to mass density:

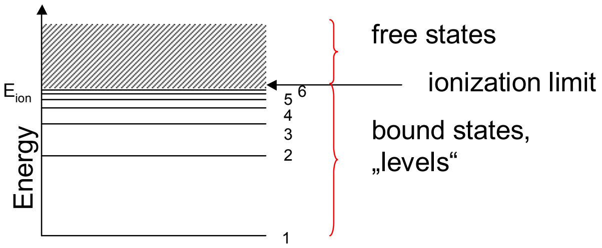
$$\beta_k \rho = A_k m_H N_k$$

  with A_k = mean mass of element k in atomic mass units (AMU)
  m_H = mass of hydrogen atom
- Particle number fraction $\dfrac{N_k}{\sum N_{k'}}$
- logarithmic $\varepsilon_k = \log(N_k / N_H) + 12.00$
- Number of atoms per 10^6 Si atoms (meteorites)

The model atom

The population numbers (=occupation numbers)

n_i = number density of atoms/ions of an element, which are in the level i



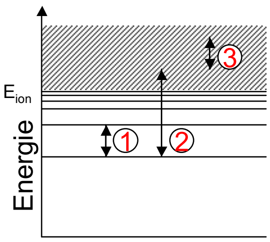
E_i = energy levels, quantized

E_1 = E(ground state) = 0

E_{ion} = ionization energy

Photon absorption cross-sections

Transitions in atoms/ions



1. bound-bound transitions = lines
2. bound-free transitions = ionization and recombination processes
3. free-free transitions = Bremsstrahlung

We look for a relation between macroscopic quantities $\kappa(\nu), \eta_\nu(\nu)$ and microscopic (quantum mechanical) quantities, which describe the state transitions within an atom

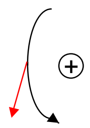
Photon absorption cross-sections

Line transitions: $\Delta E_{\mathrm{bb}} = \pm\left(E_{\mathrm{up}} - E_{\mathrm{low}}\right)$

Bound-free transitions: thermal average of electron velocities v (Maxwell distribution, i.e., electrons in thermodynamic equilibrium)

$$\text{unbound state} = \text{ion} + \text{free electron } \left(1/2\ \mathrm{m_e v^2}\right)$$

$$\left|\Delta \mathrm{E_{bf}}\right| > \mathrm{E_{th}} = \mathrm{E_{ion}} - \mathrm{E_{low}}$$



Free-free transition: free electron in Coulomb field of an ion, Bremsstrahlung, classically: jump into other hyperbolic orbit, ΔE_{ff} arbitrary

For all processes holds: ΔE can only be supplied or removed by:

- Inelastic collisions with other particles (mostly electrons), **collisional processes**
- By absorption/emission of a photon, **radiative processes**
- In addition: **scattering processes** = (in)elastic collisions of photons with electrons or atoms
  - scattering off free electrons: Thomson or Compton scattering
  - scattering off bound electrons: Rayleigh scattering

The line absorption cross-section

Classical description (H.A. Lorentz)

Harmonic oscillator in electromagnetic field

- Damped oscillations (1-dim), eigen-frequency ω_0
  Damping constant γ
- Periodic excitation with frequency ω by E-field

Equation of motion:

$$m\ddot{x} + \gamma m\dot{x} + m\omega_0^2 x = eE_0 e^{i\omega t}$$

inertia + damping + restoring force = excitation

Usual Ansatz for solution: $x(t) = x_0 e^{i\omega t}$

$$\left(-\omega^2 + i\omega\gamma + \omega_0^2\right)x = \frac{eE_0}{m} e^{i\omega t}$$

The line absorption cross-section

$$\left(-\omega^2+i\omega\gamma+\omega_0^2\right)x(t)=\frac{eE_0}{m}e^{i\omega t}$$

$$x(t)=\frac{eE_0}{m}e^{i\omega t}\cdot\frac{1}{\left(\omega_0^2-\omega^2+i\omega\gamma\right)}$$

expand $$x(t)=\frac{eE_0}{m}e^{i\omega t}\cdot\frac{\left(\omega_0^2-\omega^2-i\omega\gamma\right)}{(\omega_0^2-\omega^2)^2+\omega^2\gamma^2}$$

real part $$\mathrm{Re}(x(t))=\frac{eE_0}{m}\left[\frac{\omega_0^2-\omega^2}{(\omega_0^2-\omega^2)^2+\omega^2\gamma^2}\cos\omega t+\frac{\gamma\omega}{(\omega_0^2-\omega^2)^2+\omega^2\gamma^2}\sin\omega t\right]$$

Electrodynamics: radiated power

$$p(t)=\frac{2}{3}\frac{e^2}{c^3}(\ddot{x})^2$$

$$\ddot{x}(t)=\frac{eE_0}{m}\left[\frac{\omega_0^2-\omega^2}{(\omega_0^2-\omega^2)^2+\omega^2\gamma^2}(-\omega^2)\cos\omega t+\frac{\gamma\omega}{(\omega_0^2-\omega^2)^2+\omega^2\gamma^2}(-\omega^2)\sin\omega t\right]$$

$$(\ddot{x}(t))^2=\left(\frac{eE_0}{m}\right)^2\left[\frac{\left(\omega_0^2-\omega^2\right)^2\omega^4}{N^2}\cos^2\omega t+\frac{2\gamma\left(\omega_0^2-\omega^2\right)\omega^5}{N^2}\cos\omega t\sin\omega t+\frac{\gamma^2\omega^6}{N^2}\sin^2\omega t\right]$$

The line absorption coss-section

average over one period

$$\overline{\cos^2\omega t}=\overline{\sin^2\omega t}=1/2,\quad \overline{\cos\omega t\sin\omega t}=0$$

$$\overline{(\ddot{x})^2}=\frac{1}{2}\left(\frac{eE_0\omega^2}{m}\right)^2\left[\frac{\left(\omega_0^2-\omega^2\right)^2+\gamma^2\omega^2}{\left(\left(\omega_0^2-\omega^2\right)^2+\gamma^2\omega^2\right)^2}\right]$$

$$\overline{(\ddot{x})^2}=\frac{1}{2}\left(\frac{eE_0}{m}\right)^2\left[\frac{\omega^4}{\left(\omega_0^2-\omega^2\right)^2+\gamma^2\omega^2}\right]$$

power, averaged over one period

$$\bar{p}=\frac{2}{3}\frac{e^2}{c^3}\overline{(\ddot{x})^2}=\left(\frac{e^4E_0^2}{3m^2c^3}\right)\left[\frac{\omega^4}{\left(\omega_0^2-\omega^2\right)^2+\gamma^2\omega^2}\right]$$

$$\bar{p}=\frac{e^4E_0^2}{3m^2c^3}\varphi(\nu)/C$$ C=normalization constant $(\nu=\omega/2\pi)$

$$\varphi(\nu)=\frac{\nu^4C}{\left(\nu_0^2-\nu^2\right)^2+(\gamma/2\pi)^2\nu^2}$$ profile function

The line absorption cross-section

since $\Delta\nu = \nu\text{-}\nu_0 << \nu, \nu_0$: $\quad \nu \approx \nu_0$

$$(\nu_0^2 - \nu^2)^2 = ((\nu_0 + \nu)(\nu_0 - \nu))^2 \approx 4\nu_0^2(\nu_0 - \nu)^2$$

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

now: calculating the normalization constant

$$\int_{\nu_0 - \infty}^{\nu_0 + \infty} \varphi(\nu)d\nu = 1$$

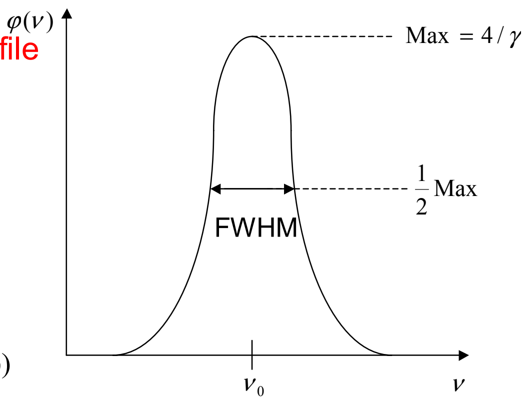
substitution: $\quad x := \frac{4\pi}{\gamma}(\nu_0 - \nu)$

$$\int_{\nu_0 - \infty}^{\nu_0 + \infty} \varphi(\nu)d\nu = \frac{C}{4}\nu_0^2 \frac{4\pi}{\gamma} \underbrace{\int_{-\infty}^{+\infty} \frac{dx}{1 + x^2}}_{=\pi} = C\frac{\nu_0^2 \pi^2}{\gamma} \Rightarrow C = \frac{\gamma}{\nu_0^2 \pi^2}$$

The line absorption cross-section

Profile function, Lorentz profile

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



properties:

- Symmetry:

$$\varphi(+(\nu_0 - \nu)) = \varphi(-(\nu_0 - \nu))$$

- Asymptotically:

$$\varphi(\nu) \to 1/(\nu_0 - \nu)^2 = 1/\Delta\nu^2$$

- FWHM:

$$\frac{2}{\gamma} = \frac{\gamma/4\pi^2}{(\Delta\nu_{\mathrm{FWHM}}/2)^2 + (\gamma/4\pi)^2} \Rightarrow \Delta\nu_{\mathrm{FWHM}} = \frac{2\gamma}{4\pi} = \frac{\gamma}{2\pi}$$

The damping constant

- Radiation damping, classically (other damping mechanisms later)
- Damping force ("friction") $F = \gamma m \dot{x}(t)$

  power=force ·velocity $p(t) = \gamma m(\dot{x}(t))^2$

  electrodynamics $p(t) = \frac{2}{3}\frac{e^2}{c^3}(\ddot{x}(t))^2$
- Hence, Ansatz for frictional force is not correct
- Help: define γ such, that the power is correct, when time-averaged over one period: $\gamma m\omega^2 = \frac{2}{3}\frac{e^2}{c^3}\omega^4$ (where we used $x(t) = x_0 e^{i\omega t}$)

$\omega \approx \omega_0 \Rightarrow \boxed{\gamma = \frac{2}{3}\frac{e^2\omega_0^2}{mc^3}}$ classical radiation damping constant

☛

Half-width

Insert into expression for FWHM:

$$\Delta\nu_{\text{FWHM}} = \frac{\gamma}{2\pi} = \frac{4\pi e^2\nu_0^2}{3mc^3}$$

$$\frac{\Delta\nu_{\text{FWHM}}}{\nu} = \frac{\Delta\lambda_{\text{FWHM}}}{\lambda} \Rightarrow \Delta\lambda_{\text{FWHM}} = \frac{c}{\nu^2}\Delta\nu_{\text{FWHM}} = \frac{4\pi e^2}{3mc^2} = \boxed{1.18\cdot 10^{-4}\,\text{Å}}$$

The absorption cross-section

Definition absorption coefficient κ $\quad dI_\nu = -\kappa(\nu) I_\nu ds$

with n_{low} = number density of absorbers: $\kappa(\nu) = \sigma(\nu) n_{\mathrm{low}}$

$\sigma(\nu)$ absorption cross-section (definition), dimension: area

Separating off frequency dependence: $\sigma(\nu) = \sigma_0 \varphi(\nu)$

Dimension σ_0: area · frequency

Now: calculate absorption cross-section of classical harmonic oscillator for plane electromagnetic wave:

$$E_x = E_0 e^{i\omega t}$$

$$I_\nu(\nu', \mu) = \frac{c}{8\pi} E_0^2 \delta(\nu - \nu') \delta(\mu - 1)$$

Power, averaged over one period, extracted from the radiation field:

$$\bar{p} = \frac{e^4 E_0^2}{3m^2 c^3} \frac{\pi^2 \nu_0^2}{\gamma} \varphi(\nu) \quad \text{with} \quad \gamma = \gamma_{\text{class.}} = \frac{2}{3} \frac{e^2 \omega_0^2}{mc^3}$$

$$\bar{p} = \frac{e^4 E_0^2}{3m^2 c^3} \frac{\pi^2 \nu_0^2 3mc^3}{2e^2 4\pi^2 \nu_0^2} \varphi(\nu) \quad = \frac{e^2 E_0^2}{8m} \varphi(\nu)$$

On the other hand: $\bar{p} = \sigma(\nu) \int_{\nu'} \int_{\mu} I(\nu', \mu) d\nu' d\mu = \sigma(\nu) \frac{c}{8\pi} E_0^2$

Equating: $$\sigma(\nu) \frac{c}{8\pi} E_0^2 = \frac{e^2 E_0^2}{8m} \varphi(\nu)$$

$$\sigma(\nu) = \frac{\pi e^2}{mc} \varphi(\nu) \Rightarrow \sigma_0 = 0.026537 \text{ cm}^2 \text{ Hz}$$

Classically: independent of particular transition

Quantum mechanically: correction factor, oscillator strength

$$\boxed{\sigma_{\mathrm{lu}} = \frac{\pi e^2}{mc} f_{\mathrm{lu}} \qquad \kappa(\nu) = n_{\mathrm{low}} \frac{\pi e^2}{mc} f_{\mathrm{lu}} \varphi(\nu)}$$

index "lu" stands for transition lower→upper level

Oscillator strengths

Oscillator strengths f_{lu} are obtained by:

- Laboratory measurements
- Solar spectrum
- Quantum mechanical computations (Opacity Project etc.)

λ/Å	Line	f_{lu}	g_{low}	g_{up}
1215.7	Ly α	0.41	2	8
1025.7	Ly β	0.07	2	18
972.5	Ly γ	0.03	2	32
6562.8	H α	0.64	8	18
4861.3	H β	0.12	8	32
4340.5	H γ	0.04	8	50

- Allowed lines: $f_{lu} \approx 1$,
- Forbidden: <<1 e.g. He I $1s^2\,{}^1S \rightarrow 1s2s\,{}^3S$ $f_{lu} = 2\ 10^{-14}$

Opacity status report

Connecting the (macroscopic) opacity with (microscopic) atomic physics

Classical crossection

$$\kappa(\nu) = n_{\mathrm{low}} \underbrace{\frac{\pi e^2}{mc} f_{\mathrm{low,up}} \varphi(\nu)}_{\sigma_{low,up}}$$

Profile function

QM correction factor

Population number of lower level

View atoms as harmonic oscillator

- Eigenfrequency: transition energy
- Profile function: reaction of an oscillator to extrenal driving (EM wave)
- Classical crossection: radiated power = damping

Extension to emission coefficient

Alternative formulation by defining Einstein coefficients:

$$\kappa(\nu) = n_{\text{low}} \frac{h\nu_0}{4\pi} B_{\text{lu}} \varphi(\nu)$$

$$\text{i.e.} \quad \frac{h\nu_0}{4\pi} B_{\text{lu}} = \frac{\pi e^2}{mc} f_{\text{lu}}$$

Similar definition for emission processes:

$$\eta_\nu^{\text{induced}} = n_{\text{up}} \frac{h\nu_0}{4\pi} B_{\text{ul}} I_\nu \psi(\nu)$$

$$\eta_\nu^{\text{spontaneous}} = n_{\text{up}} \frac{h\nu_0}{4\pi} A_{\text{ul}} \psi(\nu)$$

$\psi(\nu)$ profile function, complete redistribution: $\varphi(\nu) = \psi(\nu)$

Relations between Einstein coefficients

Derivation in TE; since they are atomic constants, these relations are valid independent of thermodynamic state

In TE, each process is in equilibrium with its inverse, i.e., within one line there is no netto destruction or creation of photons (detailed balance)

$$\text{emitted intensity} = \text{absorbed intensity}$$

$$B_{\text{ul}} \frac{h\nu_0}{4\pi} I_\nu n_{\text{up}} + A_{\text{ul}} \frac{h\nu_0}{4\pi} n_{\text{up}} = B_{\text{lu}} \frac{h\nu_0}{4\pi} I_\nu n_{\text{low}} \quad \text{TE: } I_\nu = B_\nu(T)$$

$$\left(B_{\text{ul}} B_\nu(T) + A_{\text{ul}}\right) n_{\text{up}} = B_{\text{lu}} B_\nu(T) n_{\text{low}}$$

$$B_\nu(T)\left(n_{\text{low}} B_{\text{lu}} - n_{\text{up}} B_{\text{ul}}\right) = n_{\text{up}} A_{\text{ul}}$$

$$B_\nu(T) = \frac{A_{\text{ul}}}{B_{\text{ul}}} \left(\frac{n_{\text{low}} B_{\text{lu}}}{n_{\text{up}} B_{\text{ul}}} - 1 \right)^{-1}$$

Relations between Einstein coefficients

$$B_\nu(T)=\frac{A_{\rm ul}}{B_{\rm ul}}\left(\frac{n_{\rm low}B_{\rm lu}}{n_{\rm up}B_{\rm ul}}-1\right)^{-1} \quad \text{with Boltzmann equation:} \quad \frac{n_{\rm up}}{n_{\rm low}}=\frac{g_{\rm up}}{g_{\rm low}}e^{-h\nu_0/kT}$$

$$B_\nu(T)=\frac{A_{\rm ul}}{B_{\rm ul}}\left(\frac{g_{\rm low}B_{\rm lu}}{g_{\rm up}B_{\rm ul}}e^{h\nu_0/kT}-1\right)^{-1} \quad \text{comparison with Planck blackbody radiation:}$$

$$B_\nu(T)=\frac{2h\nu_0^3}{c^2}\left(e^{h\nu_0/kT}-1\right)^{-1}$$

$$\boxed{\begin{aligned}&\Rightarrow \frac{A_{\rm ul}}{B_{\rm ul}}=\frac{2h\nu_0^3}{c^2}\\ &\Rightarrow \frac{g_{\rm low}B_{\rm lu}}{g_{\rm up}B_{\rm ul}}=1\Rightarrow g_{\rm low}B_{\rm lu}=g_{\rm up}B_{\rm ul}\end{aligned}}$$

Relation to oscillator strength

$$B_{\rm lu}=\frac{4e^2\pi^2}{mch\nu_0}f_{\rm lu}$$

$$B_{\rm ul}=\frac{g_{\rm up}}{g_{\rm low}}B_{\rm lu}=\frac{g_{\rm up}}{g_{\rm low}}\frac{4e^2\pi^2}{mch\nu_0}f_{\rm lu}$$

$$A_{\rm ul}=\frac{2h\nu_0^3}{c^2}B_{\rm ul}=\frac{g_{\rm up}}{g_{\rm low}}\frac{8e^2\nu_0^2\pi^2}{mc^3}f_{\rm lu}=3\gamma_{\rm ul}\frac{g_{\rm up}}{g_{\rm low}}f_{\rm lu}$$ dimension $\mathrm{A_{ul}}$ $1/\mathrm{time}$

Interpretation of $1/A_{\rm ul}$ as lifetime of the excited state

order of magnitude: $A_{\rm ul}\approx\gamma_{\rm ul}$
at 5000 Å: $10^8\,\mathrm{s}^{-1}$
lifetime: $10^{-8}\,\mathrm{s}$

Comparison induced/spontaneous emission

When is spontaneous or induced emission stronger?

with $I_\nu = B_\nu$

$$\frac{\eta_\nu^{\text{spontaneous}}}{\eta_\nu^{\text{induced}}} = \frac{A_{\text{ul}} h\nu_* n_{\text{up}}\, \psi(\nu)/4\pi}{B_\nu(T^*) B_{\text{ul}} h\nu_* n_{\text{up}}\, \psi(\nu)/4\pi} = \frac{A_{\text{ul}}}{B_{\text{ul}}} \frac{1}{B_\nu(T^*)} = \frac{2h\nu_*^3}{c^2} \frac{c^2}{2h\nu_*^3}\left(e^{h\nu_*/kT^*} - 1\right)$$

$$:= 1 \Rightarrow e^{h\nu_*/kT^*} = 2 \Rightarrow h\nu_*/kT^* = \ln 2$$

$$\text{e.g. } T^* = 10000\,\text{K} : \lambda_* = 20000\,\mathring{\text{A}}$$

$$T^* = 50000\,\text{K} : \lambda_* = 4160\,\mathring{\text{A}}$$

At wavelengths shorter than λ_* spontaneous emission is dominant

Induced emission as negative absorption

Radiation transfer equation:

$$\frac{dI_\nu}{ds} = \eta_\nu - \kappa I_\nu \quad \text{with } \eta_\nu = \eta_\nu^{\text{spontaneous}} + \eta_\nu^{\text{induced}}$$

$$\frac{dI_\nu}{ds} = \eta_\nu^{\text{spontaneous}} + \eta_\nu^{\text{induced}} - \kappa I_\nu$$

transition low→up $\quad \kappa_{\text{lu}} = B_{\text{lu}} \frac{h\nu_0}{4\pi} n_{\text{low}} \varphi(\nu), \quad \eta_{\text{lu}}^{\text{induced}} = B_{\text{ul}} \frac{h\nu_0}{4\pi} n_{\text{up}} I_\nu \varphi(\nu)$

Useful definition: κ corrected for induced emission:

$$\frac{dI_\nu}{ds} = \eta_\nu^{\text{spontaneous}} + \left(B_{\text{ul}} n_{\text{up}} - B_{\text{lu}} n_{\text{low}}\right) \frac{h\nu_0}{4\pi} \varphi(\nu) I_\nu$$

So we get (formulated with oscillator strength instead of Einstein coefficients):

$$\kappa_{\text{lu}} = \frac{\pi e^2}{mc} f_{\text{lu}} \left(n_{\text{low}} - \frac{g_{\text{low}}}{g_{\text{up}}} n_{\text{up}} \right) \varphi(\nu)$$

$$\eta_{\text{lu}}^{\text{spontaneous}} = \frac{2h\nu_0^3}{c^2} \frac{\pi e^2}{mc} f_{\text{lu}} \frac{g_{\text{low}}}{g_{\text{up}}} n_{\text{up}} \varphi(\nu)$$

The line source function

General source function: $S_\nu = \eta_\nu / \kappa$

Special case: emission and absorption by one line transition:

$$S_\nu^{\mathrm{lu}} = \frac{\eta_\nu^{\mathrm{lu}}}{\kappa^{\mathrm{lu}}} = \frac{A_{\mathrm{ul}} n_{\mathrm{up}} \frac{h\nu_0}{4\pi}\varphi(\nu)}{\left(B_{\mathrm{lu}} n_{\mathrm{low}} - B_{\mathrm{ul}} n_{\mathrm{up}}\right)\frac{h\nu_0}{4\pi}\varphi(\nu)} = \frac{2h\nu_0^3}{c^2} \frac{n_{\mathrm{up}}}{\frac{g_{\mathrm{up}}}{g_{\mathrm{low}}} n_{\mathrm{low}} - n_{\mathrm{up}}}$$

$$\boxed{S_\nu^{\mathrm{lu}} = \frac{2h\nu_0^3}{c^2}\left[\frac{g_{\mathrm{up}}}{g_{\mathrm{low}}}\frac{n_{\mathrm{low}}}{n_{\mathrm{up}}} - 1\right]^{-1}}$$

- Not dependent on frequency
- Only a function of population numbers
- In LTE:

$$S_\nu^{\mathrm{lu}} = \frac{2h\nu_0^3}{c^2}\left[e^{h\nu_0/kT} - 1\right]^{-1} = B_\nu(\nu_0, T)$$

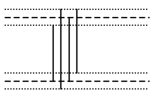
Line broadening: Radiation damping

Every energy level has a finite lifetime τ against radiative decay (except ground level) $\tau = 1 \big/ \sum_{\mathrm{l<u}} A_{\mathrm{ul}}$

Heisenberg uncertainty principle: $\Delta E \cdot \tau = \hbar$

Energy level not infinitely sharp

q.m. $\Rightarrow$ profile function = Lorentz profile



$$\gamma = \frac{1}{\tau_{\mathrm{u}}} + \frac{1}{\tau_l} = \sum_{\mathrm{k<u}} A_{\mathrm{uk}} + \sum_{\mathrm{j}<l} A_{l\mathrm{j}}$$

Simple case: resonance lines (transitions to ground state)

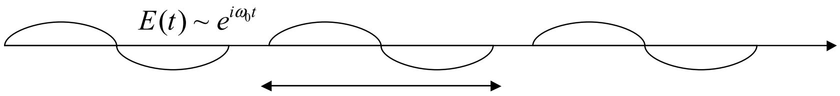
example Lyα (transition 2$\rightarrow$1): $\gamma = \mathrm{A}_{21} = 3\gamma_{\mathrm{cl}}\, \mathrm{g}_1/\mathrm{g}_2\, \mathrm{f}_{12} = 3\gamma_{\mathrm{cl}}\, 2/8 \cdot 0.41 = 0.31\gamma_{\mathrm{cl}}$

example Hα (3$\rightarrow$2):

$$\gamma = 3\gamma_{\mathrm{cl}}\left(\frac{\mathrm{g}_1}{\mathrm{g}_2}\mathrm{f}_{12} + \frac{\mathrm{g}_2}{\mathrm{g}_3}\mathrm{f}_{23} + \frac{\mathrm{g}_1}{\mathrm{g}_3}\mathrm{f}_{13}\right) = 3\gamma_{\mathrm{cl}}\left(\frac{2}{8}0.41 + \frac{8}{18}0.64 + \frac{2}{18}0.07\right) = 1.18\gamma_{\mathrm{cl}}$$

Line broadening: Pressure broadening

Reason: collision of radiating atom with other particles
⇒Phase changes, disturbed oscillation



t_0 = time between two collisions

Line broadening: Pressure broadening

Reason: collision of radiating atom with other particles
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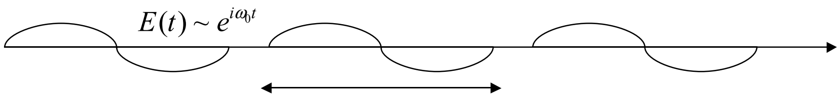


t_0 = time between two collisions

Intensity spectrum (=power spectrum) of the cut wave train:

$$I_1 \sim \left|\text{Fourier transform}\right|^2$$

$$I_1(\omega) \sim \left| \int_{-t_0/2}^{t_0/2} e^{i\omega_0 t} e^{i\omega t} dt \right|^2 = \left[\frac{\sin\left(\frac{\omega-\omega_0}{2} t\right)}{\frac{\omega-\omega_0}{2}} \right]^2$$

Line broadening: Pressure broadening

Probability distribution for t_0

$$W(t_0)dt_0 = e^{-t_0/\tau}\left(dt_0/\tau\right) \qquad \tau = \text{average time between two collisions}$$

Averaging over all t_0 gives

$$I_\nu(\omega) = \text{const}\cdot\int_0^\infty \left[\sin\left(\frac{\omega-\omega_0}{2}t\right)\Big/\frac{\omega-\omega_0}{2}\right]^2 e^{-t_0/\tau}dt_0/\tau$$

Performing integration and normalization gives profile function of intensity spectrum: $\varphi(\omega) = \dfrac{1/\pi\tau}{(\omega-\omega_0)^2+(1/\tau)^2}$

i.e. profile function for collisional broadening is a Lorentz profile with

$$\gamma = 2/\tau,\quad \tau \sim N^{-1} \qquad N = \text{particle density of colliders}$$

$$\gamma = N\cdot\gamma' \qquad \gamma' \text{ approximately constant}$$

(to calculate γ': calculation of τ necessary; for that: assumption about phase shift needed, e.g., given by semi-classical theory)

Line broadening: Pressure broadening

- Semi-classical theory (Weisskopf, Lindholm), „Impact Theory“

  Phase shifts $\Delta\omega$:

  $$\text{Ansatz: } \Delta\omega = C_p/r^p,\ \ p = 2,3,4,6\ ,\ r(t) = \text{distance to colliding particle}$$

  find constants C_p by laboratory measurements, or calculate

p=	name	dominant at
2	linear Stark effect	hydrogen-like ions
3	resonance broadening	neutral atoms with each other, H+H
4	quadratic Stark effect	ions
6	van der Waals broadening	metals + H

- Good results for p=2 (H, He II): „Unified Theory“
  - H Vidal, Cooper, Smith 1973
  - He II Schöning, Butler 1989
- For p=4 (He I)
  - Barnard, Cooper, Shamey; Barnard, Cooper, Smith; Beauchamp et al.

Film logg

Thermal broadening

Thermal motion of atoms (Doppler effect)

Velocities distributed according to Maxwell, i.e.

$$w_x(\mathrm{v}_x) \sim e^{-1/2 m_\mathrm{A} \mathrm{v}_x^2 / kT}$$

for one spatial direction x (line-of-sight)

Thermal (most probable) velocity v_th:

$$\mathrm{v}_\mathrm{th} = \sqrt{2kT/m_\mathrm{A}} = 12.85\left(T/10^4\,\mathrm{A}\right)^{1/2}\ \ \mathrm{km/s}$$

example: $\mathrm{T} = 6000\mathrm{K},\ \mathrm{A} = 56$ (iron): $\mathrm{v}_\mathrm{th} = 1.33$ km/s

i.e. $w_\mathrm{x}(\mathrm{v}_x) = C \cdot e^{-\mathrm{v}_x^2/\mathrm{v}_\mathrm{th}^2}$, with $\int_0^\infty w_\mathrm{x}(\mathrm{v}_x) d\mathrm{v}_x = 1$ we obtain:

$$\mathrm{C} \cdot \int_0^\infty e^{-\mathrm{v}_x^2/\mathrm{v}_\mathrm{th}^2} d\mathrm{v}_x = \mathrm{C} \cdot \mathrm{v}_\mathrm{th} \int_0^\infty e^{-x^2} d\mathrm{x} = 1 \Rightarrow C\sqrt{\pi}\mathrm{v}_\mathrm{th} = 1 \Rightarrow C = \frac{1}{\sqrt{\pi}\mathrm{v}_\mathrm{th}}$$

$$\boxed{w_\mathrm{x}(\mathrm{v}_x) = \frac{1}{\sqrt{\pi}\mathrm{v}_\mathrm{th}} e^{-\mathrm{v}_x^2/\mathrm{v}_\mathrm{th}^2}}$$

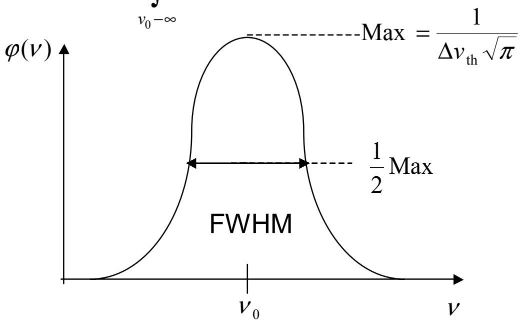
Line profile

Doppler effect: $\frac{\Delta\nu}{\nu_0} = \frac{\mathrm{v}}{c}$, $\frac{\Delta\nu_\mathrm{th}}{\nu_0} = \frac{\mathrm{v}_\mathrm{th}}{c}$

profile function:

$$w_x(\mathrm{v}_x) \Rightarrow \varphi(\nu) = \frac{C_1}{\sqrt{\pi}\Delta\nu_\mathrm{th}} \frac{\nu_0}{c} e^{-\Delta\nu^2/\Delta\nu_\mathrm{th}^2}, \quad \text{with} \int_{\nu_0-\infty}^{\nu_0+\infty} \varphi(\nu) d\nu = 1 \quad \text{we obtain:}$$

$$\boxed{\varphi(\nu) = \frac{1}{\sqrt{\pi}\Delta\nu_\mathrm{th}} e^{-(\nu-\nu_0)^2/\Delta\nu_\mathrm{th}^2}}$$



Line profile = Gauss curve

- Symmetric about ν_0
- Maximum: $1/\Delta\nu_\mathrm{th}\sqrt{\pi}$
- Half width: $\Delta\nu_\mathrm{FWHM} = 2\sqrt{\ln 2}\Delta\nu_\mathrm{th} = 1.67\Delta\nu_\mathrm{th}$
- Temperature dependency: $\Delta\nu_\mathrm{th} \sim \sqrt{T}$

Examples

At λ_0=5000Å:

T=6000K, A=56 (Fe): $\Delta \lambda_{th}$=0.02Å

T=50000K, A=1 (H): $\Delta \lambda_{th}$=0.5Å

Compare with radiation damping: $\Delta \lambda_{FWHM}$=1.18 10^{-4}Å

But: decline of Gauss profile in wings is much steeper than for Lorentz profile:

$$\text{Gauss } (10\Delta\lambda_{th}) \quad : \quad e^{-10^2} \approx 10^{-43}$$

$$\approx$$

$$\text{Lorentz } (1000\Delta\lambda_{rad}) : \; 1/1000^2 \approx 10^{-6}$$

In the line wings the Lorentz profile is dominant

Line broadening: Microturbulence

Reason: chaotic motion (turbulent flows) with length scales smaller than photon mean free path

Phenomenological description:

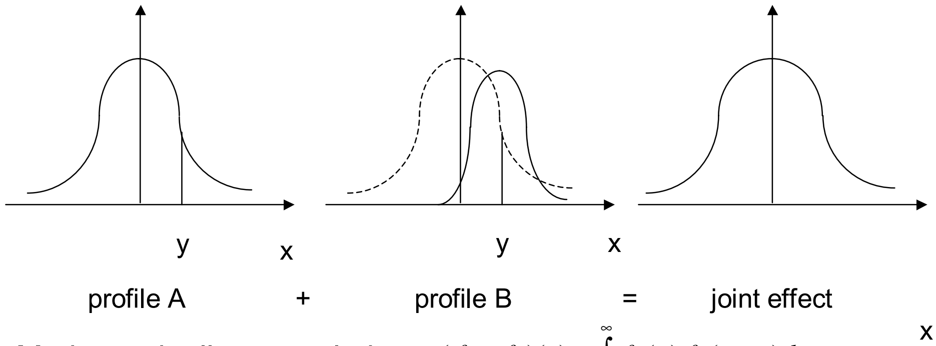
Velocity distribution: $w_x(v_x) = \frac{1}{\sqrt{\pi} v_{micro}} e^{-v_x^2/v_{micro}^2}$

i.e., in analogy to thermal broadening

v_{micro} is a free parameter, to be determined empirically

Solar photosphere: v_{micro} =1.3 km/s

Joint effect of different broadening mechanisms



Mathematically: convolution $(f_A * f_B)(x) = \int_{-\infty}^{\infty} f_A(y) f_B(x-y)\,dy$

commutative: $f_A * f_B = f_B * f_A$

multiplication of areas: $\int_{-\infty}^{\infty} (f_A * f_B)(x)\,dx = \int_{-\infty}^{\infty} f_A(x)\,dx \cdot \int_{-\infty}^{\infty} f_B(x)\,dx$

Fourier transformation: $\widetilde{f_A * f_B} = \sqrt{2\pi}\, \tilde{f}_A \cdot \tilde{f}_B$

i.e.: in Fourier space the convolution is a multiplication

Application to profile functions

Convolution of two Gauss profiles (thermal broadening + microturbulence)

$$G_A(x) = 1\big/ A\sqrt{\pi} \quad e^{-x^2/A^2} \qquad G_B(x) = 1\big/ B\sqrt{\pi} \quad e^{-x^2/B^2}$$

$$\mathrm{G_C}(x) = G_A(x) * G_B(x) = 1\big/ C\sqrt{\pi} \quad e^{-x^2/C^2} \quad \text{with} \quad \mathrm{C}^2 = A^2 + B^2$$

Result: Gauss profile with quadratic summation of half-widths; proof by Fourier transformation, multiplication, and back-transformation

Convolution of two Lorentz profiles (radiation + collisional damping)

$$L_A(x) = \frac{A/\pi}{x^2 + A^2} \qquad L_B(x) = \frac{B/\pi}{x^2 + B^2}$$

$$L_C(x) = L_A(x) * L_B(x) = \frac{C/\pi}{x^2 + C^2} \quad \text{with} \quad C = A + B$$

Result: Lorentz profile with sum of half-widths; proof as above

Application to profile functions

Convolving Gauss and Lorentz profile (thermal broadening + damping)

$$G(\nu)=\frac{1}{\Delta\nu_D\sqrt{\pi}}\,e^{-(\nu-\nu_0)^2/\Delta\nu_D^2}\qquad L(\nu)=\frac{\gamma/4\pi^2}{(\nu-\nu_0)^2+(\gamma/4\pi)^2}$$

$$V=G*L \quad \text{depends on} \quad \nu,\Delta\nu,\gamma,\Delta\nu_D:\quad V(\nu)=\int_{-\infty}^{\infty}G(\nu')L(\nu-\nu')d\nu'$$

$$\text{Transformation:}\ \mathrm{v}:=(\nu-\nu_0)/\Delta\nu_D\quad a:=\gamma/(4\pi\Delta\nu_D)\quad y:=(\nu'-\nu_0)/\Delta\nu_D$$

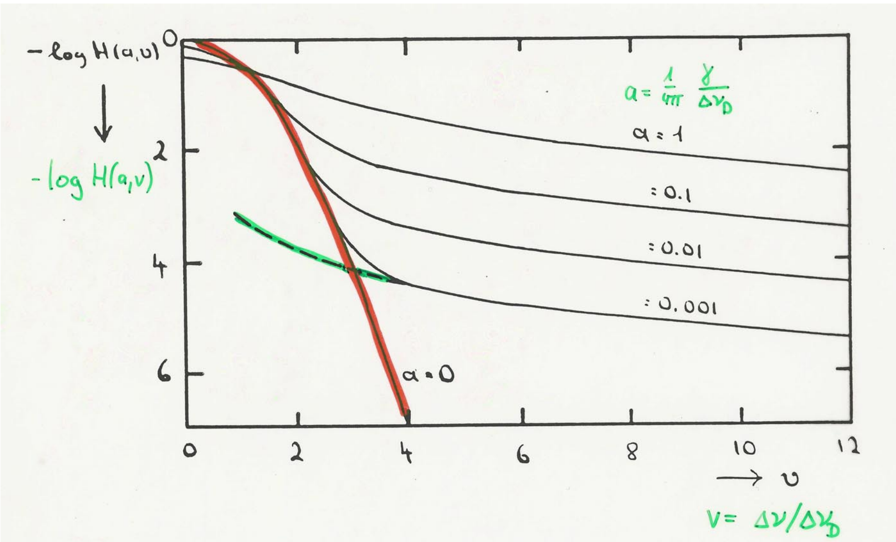
$$G(y)=\frac{1}{\Delta\nu_D\sqrt{\pi}}\,e^{-y^2}\quad L(y)=\frac{a/\Delta\nu_D\pi}{y^2+a^2}\quad V=\frac{1}{\Delta\nu_D\sqrt{\pi}}\frac{a}{\pi}\int_{-\infty}^{\infty}\frac{e^{-y^2}}{(\mathrm{v}-y)^2+a^2}dy$$

$$\text{Def:}\ V=\frac{1}{\Delta\nu_D\sqrt{\pi}}H(a,\mathrm{v})\quad \text{with}\quad \boxed{H(a,\mathrm{v})=\frac{a}{\pi}\int_{-\infty}^{\infty}\frac{e^{-y^2}}{(\mathrm{v}-y)^2+a^2}dy}$$

Voigt function, no analytical representation possible.
(approximate formulae or numerical evaluation)

$$\text{Normalization:}\quad \int_{-\infty}^{\infty}H(a,\mathrm{v})d\mathrm{v}=\sqrt{\pi}$$

Voigt profile, line wings



Treatment of very large number of lines

Example: bound-bound opacity for 50Å interval in the UV:

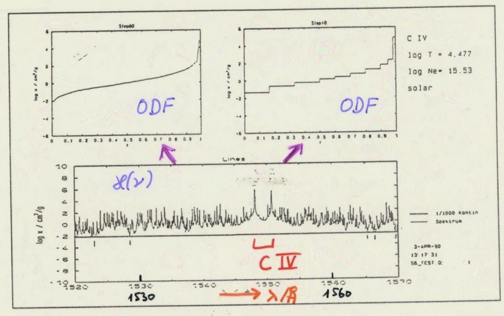


Abbildung 31: ODF des Intervalles von 1520 Å bis 1570 Å bei solaren Häufigkeiten. Hervorstechend sind die Kohlenstofflinien 1548 Å und 1550 Å .

Möller
Diploma thesis
Kiel University 1990

Direct computation would require very much frequency points

- Opacity Sampling
- Opacity Distribution Functions ODF (Kurucz 1979)

Bound-free absorption and emission

Einstein-Milne relations, Milne 1924: Generalization of Einstein relations to continuum processes: photoionization and recombination

Recombination spontaneous + induced

Transition probabilities:

P_ν : probability for photoionization in $[\nu, \nu + d\nu]$

$F(\mathrm{v})$: spontaneous recapture probability of electron in $[\mathrm{v}, \mathrm{v} + d\mathrm{v}]$

$G(\mathrm{v})$: corresponding induced probability v=electron velocity

I) number of photoionizations $n_{\text{low}} P_\nu I_\nu d\nu dt$

II) number of recombinations $n_{\text{up}} n_{\text{e}}(\mathrm{v})[F(\mathrm{v}) + G(\mathrm{v}) I_\nu] \mathrm{v} d\mathrm{v} dt$

Photon energy $h\nu = E_{\text{ion}} + 1/2\, m\mathrm{v}^2 \rightarrow d\nu = m/h\, \mathrm{v} d\mathrm{v}$

In TE, detailed balancing: I) = II)

Einstein-Milne relations

$$n_{\text{low}} P_\nu I_\nu d\nu dt = n_{\text{up}} n_{\text{e}}(\text{v}) \left[F(\text{v}) + G(\text{v}) I_\nu \right] h/m \;\, d\nu dt \quad \text{with} \quad I_\nu = B_\nu$$

$$n_{\text{low}} P_\nu B_\nu = n_{\text{up}} n_{\text{e}}(\text{v}) \left[F(\text{v}) + G(\text{v}) B_\nu \right] h/m$$

$$B_\nu = \frac{F(\text{v})}{G(\text{v})} \left[\frac{n_{\text{low}} P_\nu m}{n_{\text{up}} n_{\text{e}}(\text{v}) h G(\text{v})} - 1 \right]^{-1} = \frac{2h\nu^3}{c^2} \left[e^{h\nu/kT} - 1 \right]^{-1}$$

$$\boxed{\Rightarrow \frac{F(\text{v})}{G(\text{v})} = \frac{2h\nu^3}{c^2}}$$

$$\Rightarrow \frac{n_{\text{low}} P_\nu m}{n_{\text{up}} n_{\text{e}}(\text{v}) h G(\text{v})} = e^{h\nu/kT}$$

- $n_{\text{low}}/n_{\text{up}}$ from Saha equation: $\dfrac{n_{\text{low}}}{n_{\text{up}}} = \dfrac{2}{n_{\text{e}}} \left(\dfrac{2\pi m k T}{h^2} \right)^{3/2} \dfrac{g_{\text{up}}}{g_{\text{low}}} e^{-E_{\text{ion}}/kT}$
- $n_{\text{e}}(\text{v})$: Maxwell distribution: $n_{\text{e}}(\text{v}) d\text{v} = n_{\text{e}} \left(\dfrac{m}{2\pi k T} \right)^{3/2} e^{-m\text{v}^2/2kT} 4\pi \text{v}^2 d\text{v}$

Einstein-Milne relations

$$\frac{P_\nu}{G(\text{v})} = \frac{h}{m} e^{h\nu/kT} \frac{n_{\text{up}}}{n_{\text{low}}} n_{\text{e}}(\text{v})$$

$$= \frac{h}{m} e^{h\nu/kT} \frac{2}{n_{\text{e}}} \left(\frac{2\pi m k T}{h^2} \right)^{3/2} \frac{g_{\text{up}}}{g_{\text{low}}} e^{-E_{\text{ion}}/kT} n_{\text{e}} \left(\frac{m}{2\pi k T} \right)^{3/2} e^{-m\text{v}^2/2kT} 4\pi \text{v}^2$$

$$= \frac{h}{m} 2 \left(\frac{m}{h^2} \right)^{3/2} \frac{g_{\text{up}}}{g_{\text{low}}} m^{3/2} 4\pi \text{v}^2$$

$$\boxed{\frac{P_\nu}{G(\text{v})} = \frac{8\pi m^2}{h^3} \frac{g_{\text{up}}}{g_{\text{low}}} \text{v}^2}$$

Einstein-Milne relations, continuum analogs to A_{ji}, B_{ji}, B_{ij}

Absorption and emission coefficients

absorption coefficient (opacity) $\kappa(\nu) = n_{\text{low}} P_\nu h\nu = n_{\text{low}}\sigma_\nu$ definition. of cross-section σ

emission coefficient (emissivity) $\eta_\nu(\nu) = n_{\text{up}} n_{\text{e}}(\text{v})[F(\text{v}) + G(\text{v})I_\nu]h^2\nu/m$

And again: induced emission as negative absorption

$$\kappa(\nu) = n_{\text{low}} P_\nu h\nu - n_{\text{up}} n_{\text{e}}(\text{v}) G(\text{v}) h\nu^2/m$$

$$= n_{\text{low}} P_\nu h\nu \left[1 - \frac{n_{\text{up}}}{n_{\text{low}}} n_{\text{e}}(\text{v}) \frac{G(\text{v})}{P_\nu} \frac{h}{m}\right] = \ldots = \sigma_\nu \left[n_{\text{low}} - n_{\text{up}} \left(\frac{n_{\text{up}}}{n_{\text{low}}}\right)^* e^{-h\nu/kT}\right]$$

and $\eta_\nu(\nu) = \ldots = \frac{2h\nu}{\text{c}^3} \sigma_\nu n_{\text{up}} \left(\frac{n_{\text{up}}}{n_{\text{low}}}\right)^* e^{-h\nu/kT}$ (using Einstein-Milne relations)

LTE: $\kappa(\nu) = n_{\text{low}} P_\nu h\nu \left[1 - e^{-h\nu/kT}\right]$

$$\eta_\nu(\nu) = n_{\text{up}} n_{\text{e}}(\text{v}) F(\text{v}) h\text{v}^2/m$$

$$\vdots$$

$$\eta_\nu(\nu) = \kappa(\nu) B_\nu$$

Continuum absorption cross-sections

H-like ions: semi-classical Kramers formula

$$\sigma(\nu) = \begin{cases} \sigma_{\text{th}} \left(\nu_{\text{th}}/\nu\right)^3 & \text{for } \nu > \nu_{\text{th}} \\ 0 & \text{else} \end{cases}$$

$$\nu_{\text{th}} = \text{ threshold frequency}, \quad \sigma_{\text{th}} = \frac{8h^3}{3\sqrt{3}\pi^2 m^2 c e^2} \frac{n}{Z^2} = 7.906 \cdot 10^{-18}\,\text{cm}^2 \frac{n}{Z^2}$$

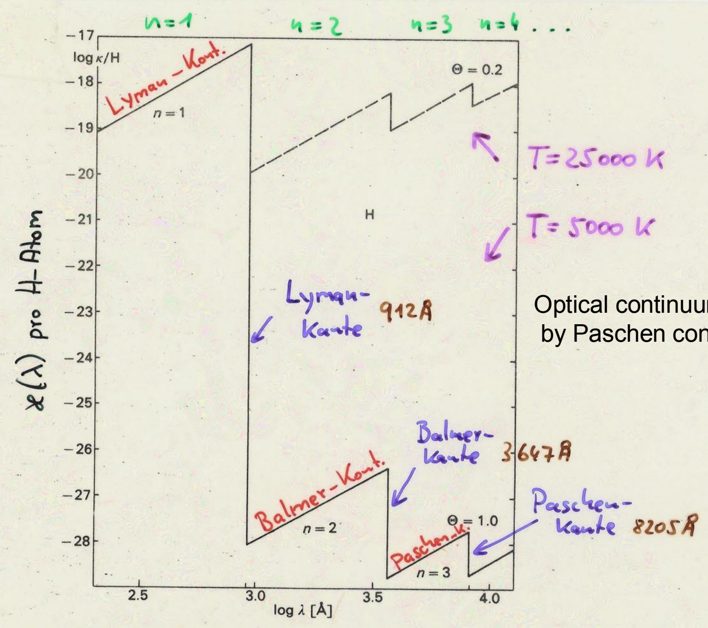
n principal quantum number, Z nuclear charge

Quantum mechanical calculations yield correction factors

$$\sigma(\nu) = \sigma_{\text{th}} \left(\nu_{\text{th}}/\nu\right)^3 g_{\text{bf}}(n,\nu) \quad , \quad g_{\text{bf}}(n,\nu) \;\; \text{Gaunt factor}$$

Adding up of bound-free absorptions from all atomic levels:
example hydrogen

$$\kappa_{\text{bf}}^{\text{tot}}(\nu) = \sum_{n=1}^{n_{\max}} \sigma_{\text{bf}}^n(\nu) n_n$$



Optical continuum dominated by Paschen continuum

Fig. 7.3. The hydrogen absorption coefficient κ_λ per hydrogen atom is shown as a function of wavelength for two temperatures $\Theta = 5040/T = 0.2$ and for $\Theta = 5040/T = 1.0$. Higher temperatures lead to higher values of κ_λ in the visual spectral region.

(Böhm-Vitense)

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The solar continuum spectrum and the H⁻ ion

H^- ion has one bound state, ionization energy 0.75 eV
Absorption edge near 17000Å,
hence, can potentially contribute to opacity in optical band

$$\text{Sun: } T = 6000\text{K},\ \log n_e = 13.6 \quad \text{Saha equation: } \frac{n_{H^+}}{n_{H^0}} = 10^{-4}, \frac{n_{H^-}}{n_{H^0}} = 10^{-7.5}$$

H almost exclusively neutral, but in the optical Paschen-continuum, i.e. population of H(n=3) decisive:

$$\frac{n_{H^0}(n=3)}{n_{H^0}(n=1)} = \frac{g_3}{g_1} e^{-12.1\text{eV}/kT} = \frac{18}{2} e^{-23.4} = 6 \cdot 10^{-10}$$

$$\frac{n_{H^-}}{n_{H^0}(n=3)} = \frac{n_{H^-}}{n_{H^0}(n=1)} \frac{n_{H^0}(n=1)}{n_{H^0}(n=3)} = \frac{3 \cdot 10^{-8}}{6 \cdot 10^{-10}} = 500$$

Bound-free cross-sections for H^- and H^0 are of similar order

H^- bound-free opacity therefore dominates the visual continuum spectrum of the Sun

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Stel

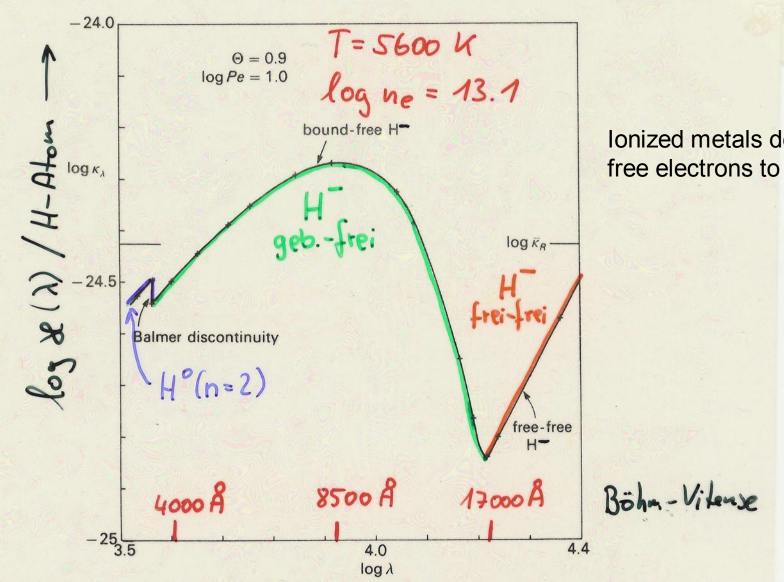

Fig. 7.5. The continuous absorption coefficient per particle is shown for $\Theta = 0.9$, which means $T = 5600$, and log $P_e = 1.0$. The contributions from the bound-free and free-free continua of H^- are dominant. The small contribution from the Balmer continuum of hydrogen is visible at log $\lambda = 3.562$. $\bar{\kappa}_R$ is the Rosseland mean absorption coefficient; see section 8.4.

Ionized metals deliver free electrons to build H^-

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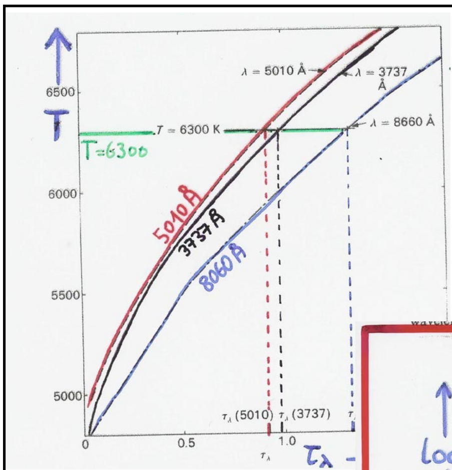
spectrum and the H^- ion



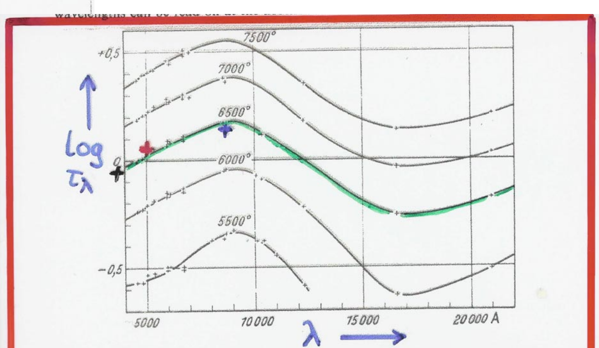
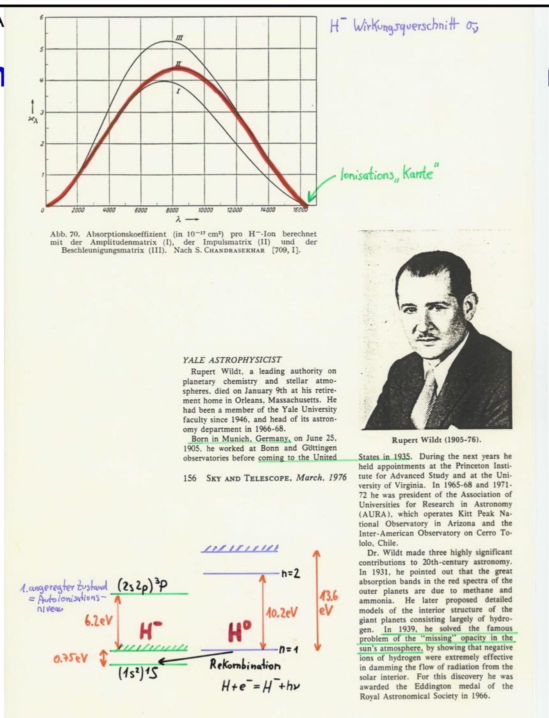


Fig. 6.4. The wavelength dependence of the continuous absorption coefficient κ_λ in the solar photosphere as determined by Chalonge and Kourganoff in 1946. (From Unsöld, 1955, p. 116.)

Stellar A

Th… nd the H$^-$ ion



Scattering processes

Thomson scattering at free electrons

Absorption coefficient $\kappa = n_e \sigma_e$ follows from power of harmonic oscillator (σ_e Thomson cross-section)

$$\overline{p} = \left(\frac{e^4 E_0^2}{3m^2 c^3} \right) \left[\frac{\nu^4}{\left(\nu_0^2 - \nu^2\right)^2 + \left(\gamma/2\pi\right)^2 \nu^2} \right]$$

free electrons: no resonance frequency, no friction: $\nu_0 = 0; \gamma = 0$

$$\rightarrow \overline{p} = \frac{e^4 E_0^2}{3m^2 c^3} \ , \quad \text{on the other hand we had} \quad \overline{p} = \sigma_e \frac{c}{8\pi} E_0^2$$

$$\boxed{\sigma_e = \frac{8\pi}{3} \frac{e^4}{m^2 c^4} = 6.65 \cdot 10^{-25} \ \text{cm}^2}$$

Thomson cross-section is wavelength-independent

Scattering processes

Rayleigh scattering of photons on electrons bound in atoms or molecules

$$\overline{p} = \left(\frac{e^4 E_0^2}{3m^2c^3}\right)\left[\frac{\nu^4}{\left(\nu_0^2-\nu^2\right)^2+\left(\gamma/2\pi\right)^2\nu^2}\right]$$

semi-classical: $\nu \ll \nu_0 = \nu_{lu}$

$$\rightarrow \overline{p} = \frac{e^4 E_0^2}{3m^2c^3}\frac{\nu^4}{\nu_{lu}{}^4} \quad \text{on the other hand we had} \quad \overline{p} = \sigma_{\mathrm{R}}\frac{c}{8\pi}E_0^2$$

$$\boxed{\sigma_{\mathrm{R}} = \frac{8\pi}{3}\frac{e^4}{m^2c^4}\frac{\nu^4}{\nu_{lu}{}^4}f_{\mathrm{lu}} = \sigma_{\mathrm{e}} f_{\mathrm{lu}}\frac{\nu^4}{\nu_{lu}{}^4}}$$

(here we have included the oscillator strength as the quantum mechanical correction)

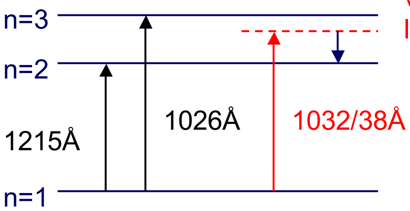
$$\rightarrow \kappa_{\mathrm{R}}(\nu) = \sum_l n_l \sigma_{\mathrm{e}} f_{\mathrm{lu}}\frac{\nu^4}{\nu_{lu}{}^4}$$

Rayleigh scattering on Lyα important for stellar spectral types G and K

Raman scattering

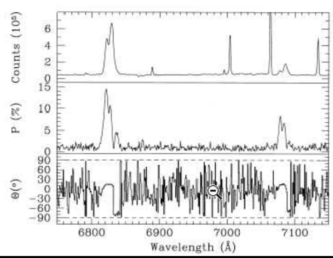
Discovered in symbiotic nova RR Tel

Raman scattering of O VI resonance line (Schmid 1987)



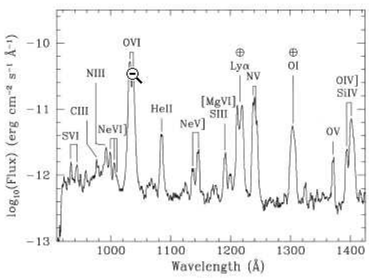
Raman-scattered line 6825/7082Å

$$\frac{1}{\lambda} = \frac{1}{\lambda_{\mathrm{OVI}}} - \frac{1}{\lambda_{\mathrm{Ly}\,\alpha}}$$



Schmid 1989,

Espey et al. 1995



Two-photon processes

Reader Comments

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Contributions

Publications

Honors

Additional Information

Maria Goeppert Mayer

1906-1972

Some Important Contributions:

NUCLEAR SHELL MODEL:

Discovery of the magic numbers and their explanation in terms of a nuclear shell model with strong spin-orbit coupling. For this she won the 1963 Nobel Prize in Physics, with J.H.D. Jensen who had independently proposed the strong spin-orbit coupling.

She was the first person to investigate the theoretical basis of nuclear pairing, which plays an important role in the shell model of the atomic nucleus.

OTHER IMPORTANT CONTRIBUTIONS:

Maria Goeppert Mayer was an accomplished physicist from the beginning of her career until the end and she made numerous contributions to the field of physics. She was the first person to investigate the phenomenon of double quantum emission and, a few years later, double beta decay. Mayer and Herzefeld were the first to study the effect of magnetic susceptibility on the refractive index of a gas. Mayer and Sachs pioneered the application of the new idea of a Yukawa potential between neutron and proton to the nuclear two-body system. Mayer was the first person to work out the atomic properties of transuranic elements as well. Mayer's last contribution, with Lawson, was the use of the center of mass and relative coordinates for the calculation of shell model interaction energies.

Some Important Publications:

Free-free absorption and emission

Assumption (also valid in non-LTE case):

Electron velocity distribution in TE, i.e. Maxwell distribution

$$S_\nu^{ff}(\nu) = \eta_\nu^{ff}(\nu) / \kappa^{ff}(\nu) = B_\nu(\nu, T)$$

Free-free processes always in TE

Similar to bound-free process we get:

$$\kappa^{ff}(\nu) = \sigma_{ff}(\nu) n_e n_k \left(1 - e^{-h\nu/kT}\right)$$

$$\sigma_{ff}(\nu) = \frac{16\pi^2}{3\sqrt{3}} \cdot \frac{Z^2 e^6}{hc(2\pi m)^{3/2}} \cdot \frac{1}{\nu^3} \frac{1}{\sqrt{T}} g_{ff}(n, \nu, T)$$

generalized Kramers formula, with Gauntfaktor from q.m.

- Free-free opacity important at higher energies, because less and less bound-free processes present
- Free-free opacity important at high temperatures

$$\sigma_{ff} \sim T^{-1/2}, \text{ but } \sigma_{bf} \sim T^{-3/2} \text{ (Saha), therefore: } \kappa_{ff}/\kappa_{bf} \propto T$$

Computation of population numbers

General case, non-LTE: $n_i = n_i(\rho, T, I_\nu)$
In LTE, just $n_i = n_i(\rho, T)$

In LTE completely given by:
- Boltzmann equation (excitation within an ion)
- Saha equation (ionization)

Boltzmann equation

Derivation in textbooks

$$\boxed{\frac{n_i}{n_j} = \frac{g_i}{g_j} e^{-(E_i - E_j)/kT}}$$

g_i statistical weight
E_i excitation energy

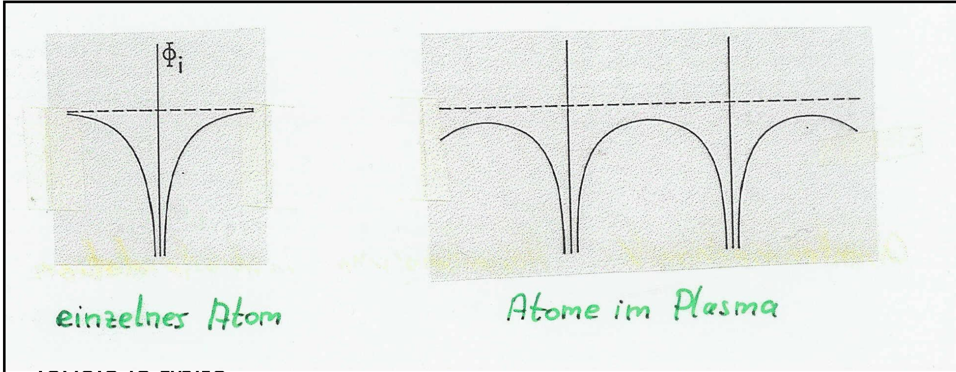
Other formulations:
- Related to ground state (E_1=0)

$$\frac{n_i}{n_1} = \frac{g_i}{g_1} e^{-E_i/kT}$$

- Related to total number density N of respective ion

$$\frac{n_i}{\sum n_j} = \frac{n_i}{n_1} \frac{n_1}{\sum n_j} = \frac{n_i}{n_1} \frac{1}{\sum \frac{n_j}{n_1}} = \frac{n_i}{n_1} \frac{g_1}{\sum g_j e^{-E_j/kT}}$$

$$\rightarrow \frac{n_i}{N} = \frac{n_i}{n_1} \frac{g_1}{U(T)}, \quad \text{with partition function } U(T) := \sum g_j e^{-E_j/kT}$$



levels is finite.

Very highly excited levels cannot exist because of interaction with neighbouring particles, radius H atom: $r(n) = a_0 n^2$

At density 10^{15} atoms/cm^3 $\rightarrow$ mean distance about 10^{-5} cm

$r(n_{max}) = 10^{-5}$ cm $\rightarrow$ $n_{\max}$ ~43

Levels are "dissolved"; description by concept of occupation probabilities p_i (Mihalas, Hummer, Däppen 1991)

$$g_i \rightarrow g_i p_i \quad \text{with} \quad p_i \rightarrow 0 \quad \text{when} \quad i \rightarrow \infty$$

Hummer-Mihalas occupation probabilities

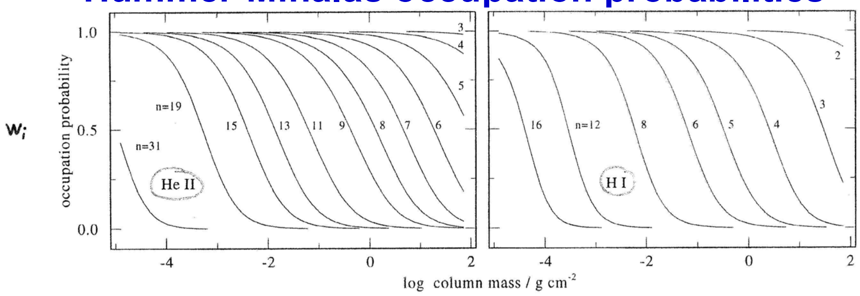
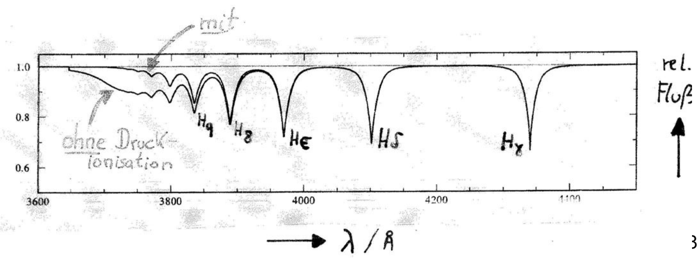


Fig. 2. Occupation probabilities of atomic He II levels (left) and H I levels (right) as a function of depth in the DO model atmosphere with $T_{\rm eff}$=100 000 K, log g =7.5, and H/He=0.1%.



Saha equation

Derivation with Boltzmann formula, but upper state is now a 2-particle state (ion plus free electron)

Energy: $\mathrm{E} = \mathrm{E}_{\mathrm{ion}} + \mathrm{p}^2 / 2\mathrm{m}_\mathrm{e}$ p=electron momentum)

Statistical weight: $g = g_{\mathrm{up}} \cdot G(p)$ weight of ion * weight of free electron

Insert into Boltzmann formula

$$\frac{n_{\mathrm{up}}(p)}{n_{\mathrm{low}}} = \frac{g_{\mathrm{up}} G(p)}{g_{\mathrm{low}}} e^{-(E_{\mathrm{ion}} + p^2/2m_\mathrm{e} - E_{\mathrm{low}})/kT}$$

Summarize over all final states
By integration over p

$$\rightarrow \frac{n_{\mathrm{up}}}{n_{\mathrm{low}}} = \frac{g_{\mathrm{up}}}{g_{\mathrm{low}}} e^{-(E_{\mathrm{up}} - E_{\mathrm{low}})/kT} \int_0^\infty G(p) e^{-p^2/2m_\mathrm{e}kT} dp$$

Statistical weight of free electron =number of available states in interval [p,p+dp] (Pauli principle):

$$G(p)dp = 2\frac{d\Omega(p)}{h^3} \quad 2 \text{ spins} \frac{\text{phase space volume}}{\text{phase space cell}}$$

$$d\Omega(p) = dxdydz \cdot dp_x dp_y dp_z = dV \cdot 4\pi p^2 dp = 1/n_\mathrm{e} \cdot 4\pi p^2 dp \rightarrow G(p) = 8\pi p^2 / h^3 n_\mathrm{e}$$

Saha equation

Insertion into Boltzmann formula gives:

$$\frac{n_{\mathrm{up}}}{n_{\mathrm{low}}} = \frac{g_{\mathrm{up}}}{g_{\mathrm{low}}} e^{-(E_{\mathrm{up}} - E_{\mathrm{low}})/kT} \int_0^\infty \frac{8\pi}{h^3 n_\mathrm{e}} p^2 e^{-p^2/2mkT_\mathrm{e}} dp \quad \text{with} \quad x = p/\sqrt{2m_\mathrm{e}kT}$$

$$= \frac{g_{\mathrm{up}}}{g_{\mathrm{low}}} e^{-(E_{\mathrm{up}} - E_{\mathrm{low}})/kT} \frac{8\pi}{h^3 n_\mathrm{e}} (2m_\mathrm{e}kT)^{3/2} \int_0^\infty x^2 e^{-x^2} dx$$

$$= \frac{g_{\mathrm{up}}}{g_{\mathrm{low}}} e^{-(E_{\mathrm{up}} - E_{\mathrm{low}})/kT} \frac{8\pi}{h^3 n_\mathrm{e}} (2m_\mathrm{e}kT)^{3/2} \frac{\sqrt{\pi}}{4}$$

$$\boxed{\frac{n_{\mathrm{up}}}{n_{\mathrm{low}}} = \frac{2}{n_\mathrm{e}} \left(\frac{2\pi m_\mathrm{e} kT}{h^3}\right)^{3/2} \frac{g_{\mathrm{up}}}{g_{\mathrm{low}}} e^{-(E_{\mathrm{up}} - E_{\mathrm{low}})/kT}}$$

Saha equation for two levels in adjacent ionization stages

Alternative: $\dfrac{n_{\mathrm{up}} n_\mathrm{e}}{n_{\mathrm{low}}} = f(T) = \dfrac{T^{3/2}}{C} \dfrac{g_{\mathrm{up}}}{g_{\mathrm{low}}} e^{-(E_{\mathrm{up}} - E_{\mathrm{low}})/kT} \quad C = 2.07 \cdot 10^{-16}\ \mathrm{K}^{3/2}\ \mathrm{cm}^3$

Example: hydrogen

Model atom with only one bound state:

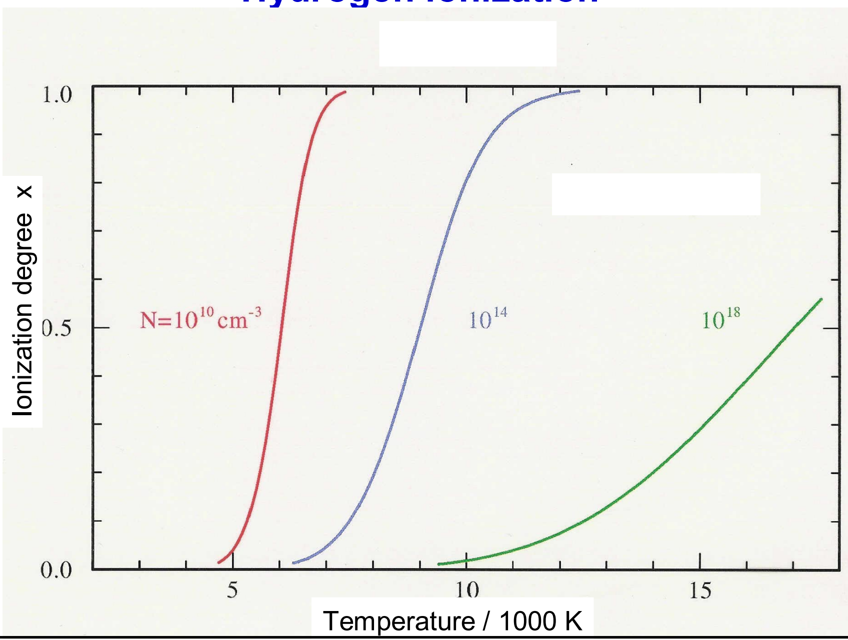
$$n_{\rm low} = n_{\rm I} = n(\text{H I ground state}) \qquad g_{\rm I} = 2$$
$$n_{\rm up} = n_{\rm II} = n(\text{H II}) \qquad g_{\rm II} = 1$$
$$\frac{n_e n_{\rm II}}{n_{\rm I}} = \frac{T^{3/2}}{C}\frac{1}{2}e^{-1.58\cdot 10^5\,\text{K}/T} = f(T)$$
pure hydrogen: $n_e = n_{\rm II}$, $N = n_{\rm I} + n_{II}$

ionization degree: $x = \frac{n_e}{N} = \frac{n_{\rm II}}{N}$

$$\Rightarrow \frac{x^2 N}{1-x} = f(T) \Rightarrow x^2 + \frac{f(T)}{N}x - \frac{f(T)}{N} = 0$$
$$\boxed{\Rightarrow x = -\frac{f(T)}{2N} + \sqrt{\left(\frac{f(T)}{2N}\right)^2 + \frac{f(T)}{N}}}$$
$$\Rightarrow x = x(T, N)$$

☛

Hydrogen ionization



More complex model atoms

$j=1,\ldots,J$ ionization stages

$i=1,\ldots,I(j)$ levels per ionization stage j

Saha equation for ground states of ionization stages j and $j+1$:

$$n_{1j} = n_{1j+1} n_e \frac{1}{2}\left(\frac{h^3}{2\pi m_e kT}\right)^{3/2} \frac{g_{1j}}{g_{1j+1}} e^{E_{\mathrm{Ion}}^{j}/kT}$$

With Boltzmann formula we get occupation number of i-th level:

$$n_{ij} = \frac{n_{ij}}{n_{1j}} n_{1j} = \frac{g_{ij}}{g_{1j}} e^{-E_i^j/kT} n_{1j+1} n_e C_1 T^{-3/2} \frac{g_{1j}}{g_{1j+1}} e^{E_{\mathrm{Ion}}^{j}/kT}$$

$$\boxed{\Rightarrow n_{ij} = \frac{g_{ij}}{g_{1j+1}} n_{1j+1} n_e C_1 T^{-3/2} e^{(E_{\mathrm{Ion}}^{j} - E_i^j)/kT}}$$

More complex model atoms

Related to total number of particles in ionization stage j+1

$$\frac{n_{ij+1}}{N_{j+1}} = \frac{n_{ij+1}}{n_{1j+1}} \frac{g_{1j+1}}{U_{j+1}} \underset{=}{\mathrm{i=1}} \frac{n_{1j+1}}{N_{j+1}} = 1 \cdot \frac{g_{1j+1}}{U_{j+1}} \rightarrow n_{1j+1} = \frac{g_{1j+1}}{U_{j+1}} N_{j+1}$$

$$\Rightarrow n_{ij} = \frac{g_{ij}}{g_{1j+1}} \frac{g_{1j+1}}{U_{j+1}} N_{j+1} n_e C_1 T^{-3/2} e^{(E_{\mathrm{Ion}}^{j} - E_i^j)/kT} \Rightarrow \boxed{n_{ij} = \frac{g_{ij}}{U_{j+1}} N_{j+1} n_e C_1 T^{-3/2} e^{(E_{\mathrm{Ion}}^{j} - E_i^j)/kT}}$$

N_j/N_{j+1}

$$N_j = \sum_i n_{ij} = \sum_i \frac{g_{ij}}{U_{j+1}} N_{j+1} n_e C_1 T^{-3/2} e^{(E_{\mathrm{Ion}}^{j} - E_i^j)/kT}$$

$$= \frac{N_{j+1}}{U_{j+1}} n_e C_1 T^{-3/2} e^{E_{\mathrm{Ion}}^{j}/kT} \sum_i g_{ij} e^{-E_i^j/kT} = \frac{N_{j+1}}{U_{j+1}} n_e C_1 T^{-3/2} e^{E_{\mathrm{Ion}}^{j}/kT} U_j$$

$$\boxed{\frac{N_j}{N_{j+1}} = \frac{U_j}{U_{j+1}} n_e C_1 T^{-3/2} e^{E_{\mathrm{Ion}}^{j}/kT} = n_e \Phi_j(T)}$$

Ionization fraction

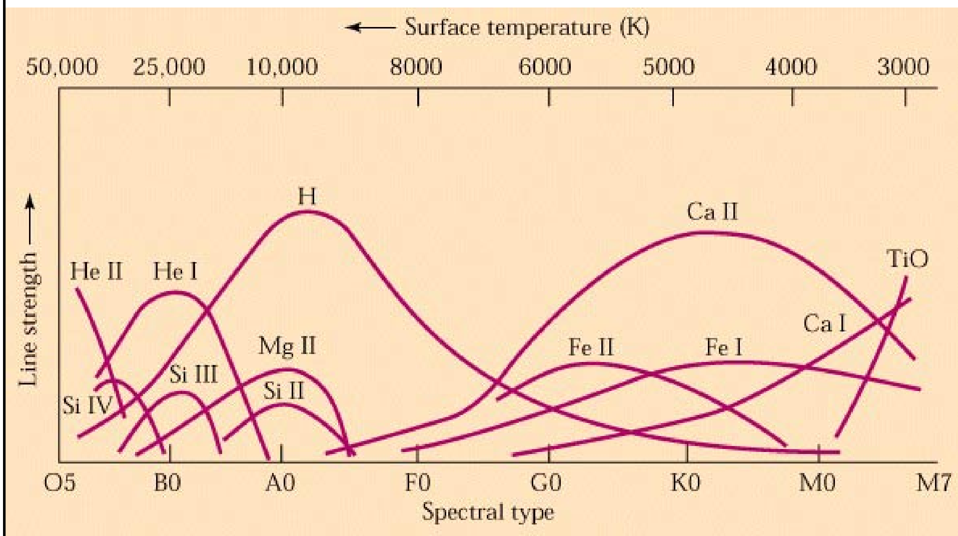
$$\frac{N_{\mathrm{j}}}{N_{\mathrm{J}}} = \frac{N_{\mathrm{j}}}{N_{\mathrm{j+1}}} \cdot \frac{N_{\mathrm{j+1}}}{N_{\mathrm{j+2}}} \cdot \ldots \cdot \frac{N_{\mathrm{J\text{-}1}}}{N_{\mathrm{J}}}$$

$$N = \sum_{\mathrm{j=1}}^{\mathrm{J}} N_{\mathrm{j}} = N_{\mathrm{J}} \sum_{\mathrm{j=1}}^{\mathrm{J}} \frac{N_{\mathrm{j}}}{N_{\mathrm{J}}} = N_{\mathrm{J}} \left[1 + \frac{N_{\mathrm{J\text{-}1}}}{N_{\mathrm{J}}} + \frac{N_{\mathrm{J\text{-}1}}}{N_{\mathrm{J}}} \cdot \frac{N_{\mathrm{J\text{-}2}}}{N_{\mathrm{J\text{-}1}}} + \ldots + \frac{N_{\mathrm{J\text{-}1}}}{N_{\mathrm{J}}} \cdots \frac{N_1}{N_2} \right]$$

$$\frac{N_{\mathrm{j}}}{N} = \frac{N_{\mathrm{j}}}{N_J} \frac{N_{\mathrm{J}}}{N} = \frac{\dfrac{N_{\mathrm{j}}}{N_{\mathrm{j+1}}} \cdot \dfrac{N_{\mathrm{j+1}}}{N_{\mathrm{j+2}}} \cdot \ldots \cdot \dfrac{N_{\mathrm{J\text{-}1}}}{N_{\mathrm{J}}}}{1 + \dfrac{N_{\mathrm{J\text{-}1}}}{N_{\mathrm{J}}} + \dfrac{N_{\mathrm{J\text{-}1}}}{N_{\mathrm{J}}} \cdot \dfrac{N_{\mathrm{J\text{-}2}}}{N_{\mathrm{J\text{-}1}}} + \ldots + \dfrac{N_{\mathrm{J\text{-}1}}}{N_{\mathrm{J}}} \cdots \dfrac{N_1}{N_2}}$$

$$\boxed{\frac{N_{\mathrm{j}}}{N} = \frac{\prod_{\mathrm{k=j}}^{\mathrm{J\text{-}1}} n_{\mathrm{e}} \Phi_{\mathrm{k}}(T)}{1 + \sum_{\mathrm{m=1}}^{\mathrm{J}} \prod_{\mathrm{k=m}}^{\mathrm{J\text{-}1}} n_{\mathrm{e}} \Phi_{\mathrm{k}}(T)}}$$

Ionization fractions



Summary: Emission and Absorption

- Line absorption and emission coefficients (bound-bound)

$$\kappa_{\text{lu}}(\nu)=\frac{\pi e^2}{mc} f_{\text{lu}}\left(n_{\text{low}}-\frac{g_{\text{low}}}{g_{\text{up}}} n_{\text{up}}\right)\varphi(\nu) \qquad \eta_{\text{lu}}(\nu)=\frac{2h\nu_0^3}{c^2}\frac{\pi e^2}{mc} f_{\text{lu}}\frac{g_{\text{low}}}{g_{\text{up}}} n_{\text{up}}\varphi(\nu)$$

$\varphi(\nu)=$ profile function, e.g., Voigtprofile $V(a,\mathrm{v})=\frac{1}{\Delta\nu_D\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{e^{-y^2}}{(\mathrm{v}-y)^2+a^2}dy$

- Continuum (bound-free)

$$\kappa(\nu)=\sigma_\nu\left[n_{\text{low}}-n_{\text{up}}\left(\frac{n_{\text{up}}}{n_{\text{low}}}\right)^{*} e^{-h\nu/kT}\right] \qquad \eta_\nu(\nu)=\frac{2h\nu}{c^3}\sigma_\nu n_{\text{up}}\left(\frac{n_{\text{up}}}{n_{\text{low}}}\right)^{*} e^{-h\nu/kT}$$

- Continuum (free-free), always in LTE

$$\kappa^{\text{ff}}(\nu)=\sigma_{\text{ff}}(\nu)n_e n_k\left(1-e^{-h\nu/kT}\right) \qquad \eta^{\text{ff}}(\nu)=\kappa^{\text{ff}}(\nu)n_e n_k B_\nu(\nu,T)$$

- Scattering (Compton, on free electrons) $\kappa=n_e\sigma_e \qquad \eta_\nu(\nu)=n_e\sigma_e J_\nu$

Total opacity and emissivity add up all contributions, then source function $S_\nu=\eta_\nu/\kappa(\nu)$

Excitation and ionization in LTE

$$\frac{n_{low}}{n_{up}} = \frac{g_{low}}{g_{up}} e^{-(E_{low}-E_{up})/kT}$$ Boltzmann

$$\frac{n_{\mathrm{up}}}{n_{\mathrm{low}}} = \frac{2}{n_{\mathrm{e}}} \left(\frac{2\pi m_{\mathrm{e}} kT}{h^3} \right)^{3/2} \frac{g_{\mathrm{up}}}{g_{\mathrm{low}}} e^{-(E_{\mathrm{up}}-E_{\mathrm{low}})/kT}$$ Saha