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**

\[ h\nu + E_i \rightarrow E_u \]

**Emission**

- **Spontaneous** (isotropic)
  \[ E_u \rightarrow E_i + h\nu \]

- **Stimulated** (direction of incoming photon)
  \[ h\nu + E_u \rightarrow E_i + 2h\nu \]
A. Line transitions

Einstein coefficients

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

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

- $B_{lu}$: Einstein coefficient for absorption
- $I_\nu(\omega)$: probability that no. of incident photons
- $\varphi(\nu)$: absorption profile
- Probability $\nu \in (\nu, \nu + d\nu)$
- Probability $\omega \in (\omega, \omega + d\omega)$
Einstein coefficients

similarly for stimulated emission

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

\( B_{ul} \): Einstein coefficient for stimulated emission

and for spontaneous emission

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

\( A_{ul} \): Einstein coefficient for spontaneous emission
Absorption and emission coefficients are a function of Einstein coefficients, occupation numbers and line broadening.
Relations between Einstein coefficients

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

We can assume TE:

\[ S_\nu = \frac{\epsilon_\nu^L}{k_\nu^L} = B_\nu(T) \]

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

From the Boltzmann formula:

\[ \frac{n_u}{n_l} = \frac{g_u}{g_l} e^{-\frac{h\nu}{kT}} \]

for \( \frac{h\nu}{kT} \ll 1: \)

\[ \frac{n_u}{n_l} = \frac{g_u}{g_l} \left( 1 - \frac{h\nu}{kT} \right), \quad B_\nu(T) = \frac{2\nu^2}{c^2} kT \]

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

for \( T \rightarrow \infty \)

\[ g_l B_{lu} = g_u B_{ul} \]
Relations between Einstein coefficients

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

\[ g_l B_{lu} = g_u B_{ul} \]

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

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

for \( T \to \infty \)

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

\[ A_{ul} = \frac{2 h \nu^3}{c^2} B_{ul} \]

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

\[ \epsilon^L_{\nu} = \frac{h \nu}{4\pi} \varphi(\nu) n_u \frac{g_l}{g_u} \frac{2h \nu^3}{c^2} B_{lu} \]

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.

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:

\[ H_{\text{atom}} |\psi_l> = E_l |\psi_l> \quad H_{\text{atom}} = \frac{p^2}{2m} + V_{\text{nucleus}} + V_{\text{shell}} \]

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:

\[ V(t) = e \sum_{i=1}^{N} E \cdot r_i = E \cdot d \quad \text{d: dipol operator} \]

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

with transition probability

\[ \sim | <\psi_l|d|\psi_u>|^2 \]
Oscillator strength

The result is

\[ \frac{h\nu}{4\pi} B_{lu} = \frac{\pi e^2}{m_e c} f_{lu} \]

\( f_{lu} \): oscillator strength (dimensionless)

classical result from electrodynamics

= 0.02654 cm²/s

Classical electrodynamics

electron quasi-elastically bound to nucleus and oscillates within outer electric field as \( E \).

Equation of motion (damped harmonic oscillator):

\[ \ddot{x} + \gamma \dot{x} + \omega_0^2 x = \frac{e}{m_e} E \]

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

resonant (natural) frequency
\( \nu_0 = 2\pi \nu_0 \)

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:

\[ \int \kappa_{\nu}^{L,cl} d\nu = n_l \frac{\pi e^2}{m_ec} = n_l \sigma_{\text{tot}}^{cl} \]

\[ \varphi(\nu) d\nu = \frac{1}{\pi} \frac{\gamma/4\pi}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2} \]

[ Lorentz (damping) line profile]

Oscillator strength \( f_{lu} \) is quantum mechanical correction to classical result

(Effective number of classical oscillators, \( \approx 1 \) for strong resonance lines)

From \( \kappa_{\nu}^{L} = \frac{\hbar \nu}{4\pi} \varphi(\nu) n_l B_{lu} \) (neglecting stimulated emission)
Oscillator strength

\[
\frac{\hbar \nu}{4\pi} \varphi(\nu) B_{lu} = \frac{\pi e^2}{m_e c} \varphi(\nu) f_{lu} = \sigma_{lu}(\nu)
\]

absorption cross section; dimension is cm\(^2\)/s

\[
f_{lu} = \frac{1}{4\pi} \frac{m_e c}{\pi e^2} \frac{\hbar \nu}{B_{lu}}
\]

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

\[
f_{lu} = \frac{2^5}{3^{3/2} \pi i^5 u^3} \left( \frac{1}{l^2} - \frac{1}{u^2} \right)^{-3}
\]
g: Gaunt factor
H\(\alpha\): f=0.6407
H\(\beta\): f=0.1193
H\(\gamma\): 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 $\rightarrow$ line width

**Natural Line Broadening or Radiation Damping**

$$\tau = 1 / A_{ul} \quad (\approx 10^{-8} \text{ s in H atom } 2 \rightarrow 1): \text{ finite lifetime with respect to spontaneous emission}$$

$$\Delta E \tau \geq h/2\pi \quad \text{uncertainty principle}$$

**Line Broadening**

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

Lorentzian profile

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

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

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

Ha: $\Delta \lambda_{1/2} = 4.6 \times 10^{-4}$ A
The natural damping profile is described by the equation:

\[ \Gamma = A_{u1} \]

Where \( \Gamma \) is the natural line broadening, and \( A_{u1} \) is the natural line width.

The line broadening is given by:

\[ \Gamma_u = \sum_{i<u} A_{ui} \]

\[ \Gamma_l = \sum_{i<l} A_{li} \]

The total line broadening is the sum of the upper and lower components:

\[ \Gamma = \Gamma_u + \Gamma_l \]

Natural line broadening is important for strong lines (resonance lines) at low densities (no additional broadening mechanisms).

For example, Ly \( \alpha \) 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

$$\Delta E(t) = h \Delta \nu = C/r^n(t)$$  \hspace{1cm} r: distance to perturbing atom

\textit{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 \textit{Lorentzian profile} is obtained (but with larger total \( \Gamma \) than only natural damping)

\textit{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** $\Delta E \gg F$

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

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

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

important for H I lines, 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)

**n = 3  resonance broadening**

atom A perturbed by atom A’ of same species

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

$\rightarrow \Delta E \gg 1/r^3$
Collisional broadening

\begin{itemize}
  \item \textbf{n = 4} \quad \textit{quadratic Stark effect} \quad \Delta E \sim F^2 \\
      field strength \( F \sim 1/r^2 \) \\
      \quad \rightarrow \Delta E \sim 1/r^4 \quad \text{(no dipole moment)} \\
      important for metal ions broadened by \( e^- \) in hot stars \rightarrow \text{Lorentz profile with } \gamma_e \sim n_e
\end{itemize}

\begin{itemize}
  \item \textbf{n = 6} \quad \textit{van der Waals broadening} \\
      atom A perturbed by atom B \\
      important in cool stars, e.g. Na perturbed by H in the Sun
\end{itemize}
Quasi-static approximation

\[ t_{\text{perturbation}} \gg \tau = 1/A_{ul} \]

→ 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 \( \Delta E = h \Delta v \))
→ field strength distribution function
→ line broadening

Linear Stark effect of H lines can be approximated to 0\(^{\text{st}}\) 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.

\[ W(F) \, dF: \text{probability that field seen by radiating atom is } F \]

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

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 \((r,r+dr)\)

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

probability for no particle in \((0,r)\)

Relative probability for particle in shell \((r,r+dr)\)

\(N\): total uniform particle density

Integral equation for \(W(r)\)

we find solution by differentiating

\[\Rightarrow\] differential equation

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

Differential equation

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

Normalized solution
Quasi-static approximation

Mean interparticle distance:

\[ r_0 = \left( \frac{4}{3} \pi N \right)^{-1/3} \]

Normal field strength: \[ F_0 = \frac{e}{r_0^2} \]

(Linear Stark)

Define:

\[ \beta = \frac{F}{F_0} = \left\{ \frac{r_0}{r} \right\}^2 \]

Note: at high particle density \( \rightarrow \) large \( F_0 \)

\( \rightarrow \) stronger broadening

From \( W(r) \, dr \rightarrow W(\beta) \, d\beta \):

\[ W(\beta) \, d\beta = \frac{3}{2} \beta^{-5/2} e^{-\beta^{-3/2}} \, d\beta \]

\[ W(\beta) \sim \beta^{-5/2} \quad \text{for} \quad \beta \rightarrow \infty \]

\[ \Delta \nu \sim \beta \quad \rightarrow \quad \varphi(\Delta \nu) \sim \Delta \nu^{-5/2} \]

Stark broadened line profile in the wings, not \( \Delta \lambda^2 \) as for natural or impact broadening
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)

\[
W(\beta) = \frac{2\beta \delta^{4/3}}{\pi} \int_{0}^{\infty} e^{-\delta g(y)} y \sin(\delta^{2/3} \beta y) dy
\]

\[
g(y) = \frac{2}{3} y^{3/2} \int_{y}^{\infty} (1 - z^{-1} \sin z) z^{-5/2} dz
\]

\[
D = 4.8 \frac{T^{1/2}}{n_e} \text{ cm}
\]

Debye length, field of ion vanishes beyond D

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

number of particles inside Debye sphere
3. Doppler broadening

Radiating atoms have thermal velocity

**Maxwellian distribution:**

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

**Doppler effect:** Atom with velocity \( v \) emitting at frequency \( \nu' \), observed at frequency \( \nu \):

\[
\nu' = \nu - \nu \frac{v \cos \theta}{c}
\]
Doppler broadening

Define the velocity component along the line of sight: $\xi$

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

if $v/c << 1$ \rightarrow $(v' - v)/v << 1$:

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

Line profile for \( v = 0 \) \( \Rightarrow \) profile for \( v \neq 0 \) \( v \rightarrow v' \)

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

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
Doppler broadening: sharp line approximation

\[ \varphi^{\text{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \varphi(\nu - \nu_0 - \nu_0 \frac{\xi_0}{c} \frac{\xi}{\xi_0}) e^{-\left(\frac{\xi}{\xi_0}\right)^2} \frac{d\xi}{\xi_0} \]

\[ \Delta \nu_D: \text{Doppler width of the line} \]

\[ \Delta \nu_D = 4.301 \times 10^{-7} \nu \left(\frac{T}{\mu}\right)^{1/2} \]

\[ \Delta \lambda_D = 4.301 \times 10^{-7} \lambda \left(\frac{T}{\mu}\right)^{1/2} \]

\[ \xi_0 = \left(2kT/m\right)^{1/2} \text{ thermal velocity} \]

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

\[ \varphi(\nu - \nu_0) \approx \delta(\nu - \nu_0) \text{ delta function} \]
Doppler broadening: sharp line approximation

\[
\varphi_{\text{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \delta(\nu - \nu_0 - \Delta \nu_D) \frac{\xi}{\xi_0} e^{-\left(\frac{\xi}{\xi_0}\right)^2} \frac{d\xi}{\xi_0}
\]

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

\[
\varphi_{\text{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \delta\left(\frac{\nu - \nu_0}{\Delta \nu_D} - \frac{\xi}{\xi_0}\right) e^{-\left(\frac{\xi}{\xi_0}\right)^2} \frac{d\xi}{\Delta \nu_D \xi_0}
\]

Gaussian profile – valid in the line core
Doppler broadening: Voigt function

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

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

\[
\varphi_{\text{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2} \Delta \nu_D} \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{(\frac{\Delta \nu}{\Delta \nu_D} - y)^2 + a^2} dy \quad a = \frac{\Gamma}{4\pi \Delta \nu_D}
\]

\[
\varphi_{\text{new}}(\nu - \nu_0) = \frac{1}{\pi^{1/2} \Delta \nu_D} H \left( a, \frac{\nu - \nu_0}{\Delta \nu_D} \right)
\]

Voigt function (Lorentzian * Gaussian): calculated numerically
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.
The Voigt function normalization is given by:

\[ \int_{-\infty}^{\infty} H(a, v) \, dv = \sqrt{\pi} \]

Usually, \( \alpha \ll 1 \)

Max at \( v=0 \):

\[ H(\alpha, v=0) \approx 1 - \alpha \]

Unsoeld, 68
**B. Continuous transitions**

1. **Bound-free and free-free processes**

- **bound-bound:** spectral lines
- **bound-free**
- **free-free**

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

**e.g. Hydrogen**

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

$R = \text{Rydberg constant} = 1.0968 \times 10^5 \text{ cm}^{-1}$
b-f and f-f processes

Hydrogen

<table>
<thead>
<tr>
<th>Transition $i \rightarrow u$</th>
<th>Wavelength (Å)</th>
<th>Edge</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1 \rightarrow 1$</td>
<td>912</td>
<td>Lyman</td>
</tr>
<tr>
<td>$2 \rightarrow 1$</td>
<td>3646</td>
<td>Balmer</td>
</tr>
<tr>
<td>$3 \rightarrow 1$</td>
<td>8204</td>
<td>Paschen</td>
</tr>
<tr>
<td>$4 \rightarrow 1$</td>
<td>14584</td>
<td>Brackett</td>
</tr>
<tr>
<td>$5 \rightarrow 1$</td>
<td>22790</td>
<td>Pfund</td>
</tr>
</tbody>
</table>

Wavelengths for transitions:
- Lyman: 912 Å
- Balmer: 3646 Å
- Paschen: 8204 Å
- Brackett: 14584 Å
- Pfund: 22790 Å

Graph showing transitions and wavelengths for Lyman, Balmer, Paschen, and Brackett series.
b-f and f-f processes

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

- for all transitions:
  \[ \kappa_{\nu}^{b-f} = \sum_{\text{elements, ions}} \sum_{l} n_l \sigma_{lk}(\nu) \]

for hydrogenic ions
  \[ \sigma_{lk}(\nu) = \sigma_0(n) \left( \frac{\nu_l}{\nu} \right)^3 g_{bf}(\nu) \]

Kramers 1923

for H:
  \[ \sigma_0 = 7.9 \times 10^{-18} \text{ n} \]
  \[ \nu_l = 3.29 \times 10^{15} / \text{n}^2 \]

extinction per particle →
**b-f and f-f processes**

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

peaks increase with $n$:

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

$$\quad \Rightarrow \nu^{-3} \rightarrow n^6$$

for non-H-like atoms no $\nu^{-3}$ dependence

peaks at resonant frequencies

free-free absorption much smaller
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:
b-f and f-f processes: Einstein-Milne relations

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

\[
\begin{align*}
\text{line transitions} \\
\sigma_{lu}(\nu) &= \frac{h\nu}{4\pi} \varphi(\nu) B_{lu} \\
g_l B_{lu} &= g_u B_{ul} \\
A_{ul} &= \frac{2h\nu^3}{c^2} B_{ul}
\end{align*}
\]

b-f transitions

\[
\kappa_{\nu}^{b-f} = \sum_{\text{elements}} \sum_{\text{ions}} \sigma_{ik}(\nu) \left[ n_i - n_e n_{\text{Ion}} \frac{g_i}{2g_1} \left( \frac{h^2}{2\pi mkT} \right)^{3/2} e^{E_{i\text{Ion}}/kT} e^{-\nu/kT} \right] n_i^* \\
\text{stimulated b-f emission}
\]

LTE occupation number
2. Scattering

In scattering events photons are not destroyed, but redirected and perhaps shifted in frequency. In free-free process photon interacts with electron in the presence of ion’s potential. For scattering 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): *Klein-Nishina* formula (Q.E.D.)
- high energy photons (electrons): *Compton (inverse Compton)* scattering
- low energy (< 12.4 kEV $\approx$ 1 Angstrom): *Thomson* scattering
Thomson scattering

**THOMSON SCATTERING**: important source of opacity in hot OB stars

\[ \sigma_e = \frac{8\pi}{3} \cdot r_0^2 = \frac{8\pi}{3} \cdot \frac{e^4}{m_e^2 c^4} = 6.65 \times 10^{-25} \text{cm}^2 \]

independent of frequency, isotropic

**Approximations:**
- angle averaging done, in reality: \( \sigma_e \rightarrow \sigma_e (1+\cos^2 \phi) \) for single scattering
- neglected velocity distribution and Doppler shift (frequency-dependency)
**Rayleigh Scattering**: line absorption/emission of atoms and molecules far from resonance frequency: \( \nu << \nu_0 \)

from classical expression of cross section for oscillators:

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

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

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

\[
\sigma(\omega) \sim \omega^4 \sim \lambda^{-4}
\]

important in cool G-K stars
for strong lines (e.g. Lyman series when H is neutral) the \( \lambda^{-4} \) 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**

Ionization potential = 0.754 eV

→ \( \lambda_{\text{ion}} = 16550 \) Angstroms

H⁻ b-f peaks around 8500 A

H⁻ f-f \( \sim \lambda^3 \) (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

Gray, 92
Additional continuous absorbers

**Hydrogen**

$H_2$ molecules more numerous than atomic H in M stars

$H_2^+$ absorption in UV

$H_2$ f-f absorption in IR

**Helium**

He$^+$ f-f absorption for cool stars

**Metals**

C, Si, Al, Mg, Fe: b-f absorption in UV
Examples of continuous absorption coefficients

Unsoeld, 68

\[ T_{\text{eff}} = 5040 \, \text{K} \]

\[ B0: \ T_{\text{eff}} = 28,000 \, \text{K} \]
Total opacity

\[
\kappa_\nu = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sigma^\text{line}_{ij}(\nu) \left( n_i - \frac{g_i}{g_j} n_j \right) \quad \text{(line absorption)}
\]

\[
+ \sum_{i=1}^{N} \sigma_{ik}(\nu) \left( n_i - n_i^* e^{-\hbar \nu / kT} \right) \quad \text{(bound-free)}
\]

\[
+ n_e n_p \sigma_{kk}(\nu, T) \left( 1 - e^{-\hbar \nu / kT} \right) \quad \text{(free-free)}
\]

\[
+ n_e \sigma_e \quad \text{(Thomson scattering)}
\]
Total emissivity

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

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
Summary

• Modern model atmosphere codes include:

  millions of spectral lines

  all bf- and ff-transitions of hydrogen helium and metals

  contributions of all important negative ions

  molecular opacities
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
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**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


accurate radiative/collisional data to 10% on the mean
Confrontation with Reality

Photoionization

\[ h\nu + O \rightarrow O^{2+} + e^- \]


Electron Collision

\[ S^2+ \rightarrow S^4+ \]


✓ high-precision atomic data ✓
Improved Modelling for Astrophysics

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