Physics of planetary atmospheres

Lecture 5: Opacities in planetary atmospheres (Heng Ch. 5)

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Opacity

- Absorption cross section per unit mass as a function of wavelength or wavenumber $\kappa(\tilde{\nu})$ due to atoms and molecules present in the atmosphere
- Needed to compute transmission functions, fluxes, and spectra of planetary atmospheres
- $\kappa(\tilde{\nu})$ also depends on temperature and pressure, and so is needed as input to calculate temperature-pressure profile using radiative equilibrium (energy conservation)
- In practice this is done by iterating until convergence.

This lecture

- Discuss the calculation of the opacity function, in particular the *strengths and shapes of spectral lines*, in order to get to know the inputs required for a radiative transfer solver
- Molecules in planetary atmospheres give rise to huge numbers of spectral lines (e.g. more than 500 million for water).
- To make computations possible on human time scales, *distribution functions* of opacity are used, which significantly reduce the number of opacity points that need to be sampled.

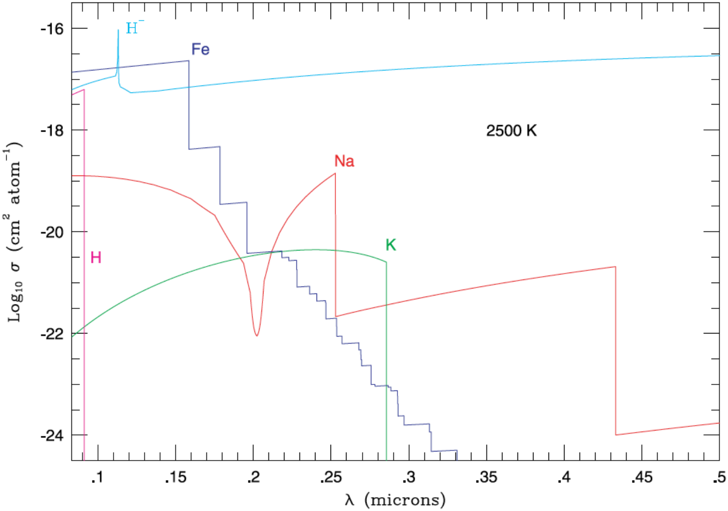
Continuous and line opacity

- *Continuous* opacity arises from processes with arbitrary changes in energy: bound-free transitions, free-free transitions, collision-induced absorption, grain absorption.
- *Line* opacity arises from processes with discrete changes in energy: spectral lines or bound-bound transitions.
- In atmospheres of rocky planets, line opacity is most important, while in gas giants there can be some contribution from continuous opacity.

Continuous opacity

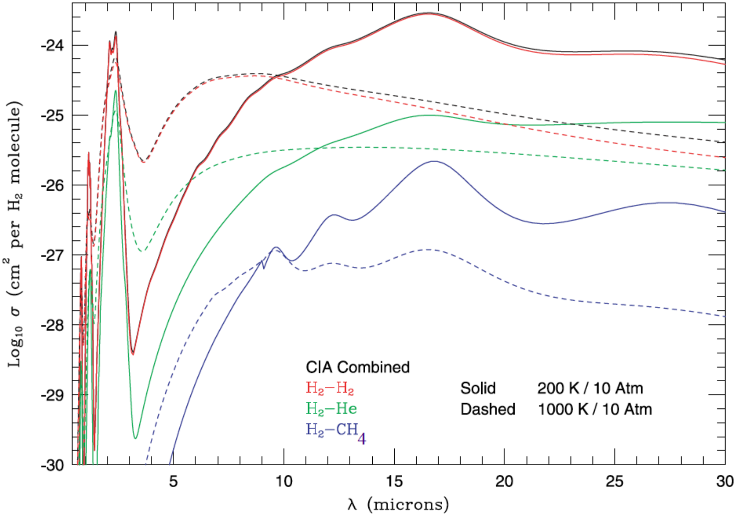
- Bound-free absorption
  - Photoionization of an electron from an atom, ion, or molecule, and photodissociation of molecules
  - $T \gtrsim 1500$ K: free atomic hydrogen → Lyman continuum in the ultraviolet; H^- → broad range; Fe
  - $T \gtrsim 1000$ K: Na (low ionization energy, longer wavelengths), K (incomplete data)
- Collision-induced absorption: Induced dipole-dipole absorption by collisions of H_2 with H_2, He, or CH_4
- Grain opacities
  - Scattering and absorption caused by solid and liquid particles (clouds)
  - Cross-sections calculated using Mie theory, from complex index of refraction, particle radius, photon wavelength

Bound-free absorption



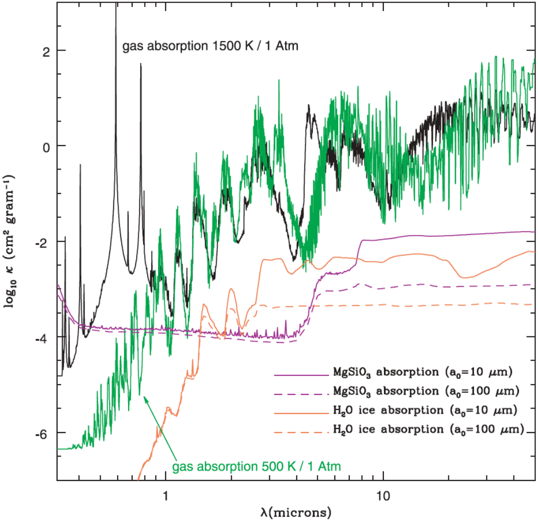
Sharp and Burrows 2007, ApJS 168, 140, Fig. 14

Collision-induced absorption



Sharp and Burrows 2007, ApJS 168, 140, Fig. 15

Grain absorption



Sharp and Burrows 2007, ApJS 168, 140, Fig. 16

Line opacity – line profile I

- General shape of spectral line: combination of Lorentz profile (damping profile, dispersion function) and Doppler profile (Gaussian)
- *Lorentz profile* = *natural broadening* caused by finite lifetime of upper and lower energy levels (+ uncertainty principle)

$$\Phi_{\mathrm{L}}(\Delta\tilde{\nu}) = \frac{\Gamma_{\mathrm{L}}/\pi}{(\tilde{\nu}-\tilde{\nu}_0)^2+\Gamma_{\mathrm{L}}^2}$$

$\tilde{\nu}_0$ … wavenumber at line center, $\Delta\tilde{\nu} = \tilde{\nu} - \tilde{\nu}_0$

Γ_{L} … HWHM, $\rightarrow 2\Gamma_{\mathrm{L}}$ is natural line width

Line opacity – line profile II

For gas temperature T atoms and molecules of mass m have a characteristic speed, the *thermal speed* (maximum or most probable speed of a Maxwell distribution):

$$v_{\mathrm{th}} = \left(\frac{2k_{\mathrm{B}}T}{m}\right)^{1/2}$$

→ *Doppler profile*: a Gaussian distribution with dispersion $\Delta\tilde{\nu}_{\mathrm{D}}$

$$\Phi_{\mathrm{D}}(\Delta\tilde{\nu}) = \frac{1}{\pi^{1/2}\Delta\tilde{\nu}_{\mathrm{D}}} e^{-(\tilde{\nu}-\tilde{\nu}_0)^2/\Delta\tilde{\nu}_{\mathrm{D}}^2}$$

$$\Delta\tilde{\nu}_{\mathrm{D}} = \frac{v_{\mathrm{th}}}{c}\tilde{\nu}_0$$

Line opacity – Voigt profile

Effects of natural and Doppler broadening are superimposed
→ total profile given by convolution of Lorentz and Doppler profiles
= *Voigt profile*, expressed in terms of *H-function*
(named after paper by F. Hjerting, 1938)

$$\Phi_{\mathrm{V}}(\Delta\tilde{\nu}) = \int_{-\infty}^{\infty} \Phi_{\mathrm{L}}(\Delta\tilde{\nu} - \Delta\tilde{\nu}')\, \Phi_{\mathrm{D}}(\Delta\tilde{\nu}')\, d\Delta\tilde{\nu}' = \frac{1}{\pi^{1/2}\Delta\tilde{\nu}_{\mathrm{D}}} H(x, a_0)$$

$$H(x, a_0) = \frac{a_0}{\pi} \int_{-\infty}^{\infty} \frac{e^{-x'^2}}{(x - x')^2 + a_0^2} dx'$$

$$x = \frac{\Delta\tilde{\nu}}{\Delta\tilde{\nu}_{\mathrm{D}}}, a_0 = \frac{\Gamma_{\mathrm{L}}}{\Delta\tilde{\nu}_{\mathrm{D}}} \ \ldots \text{damping parameter}$$

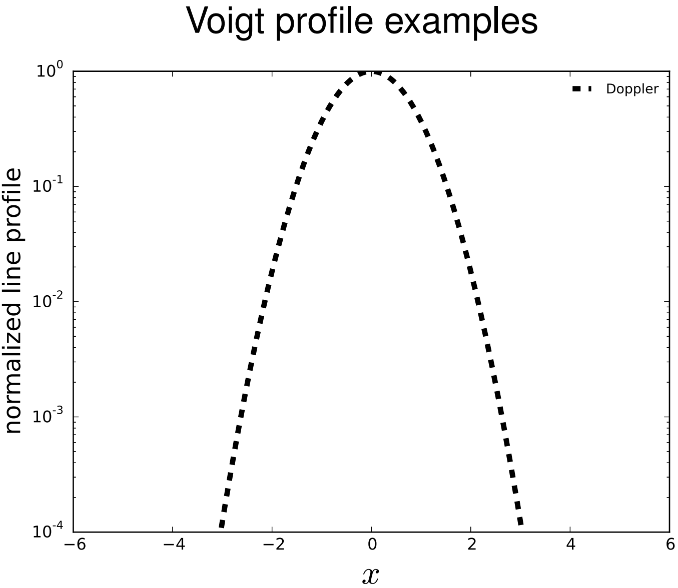


Figure 5.2: Doppler profile

Voigt profile examples

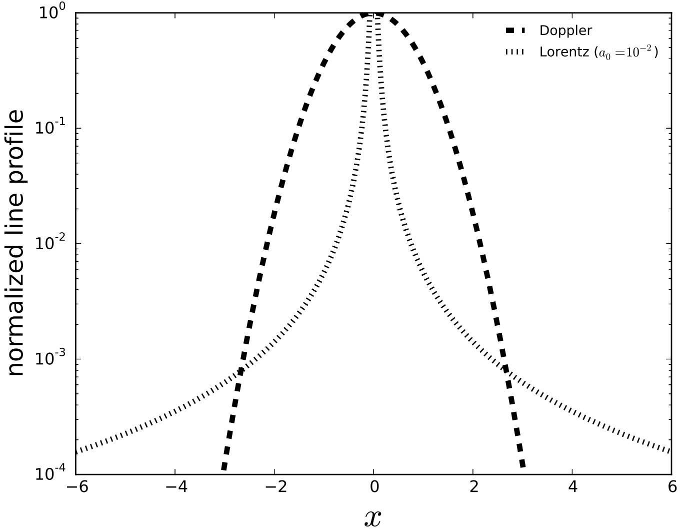


Figure 5.2: Lorentz profile – small damping parameter

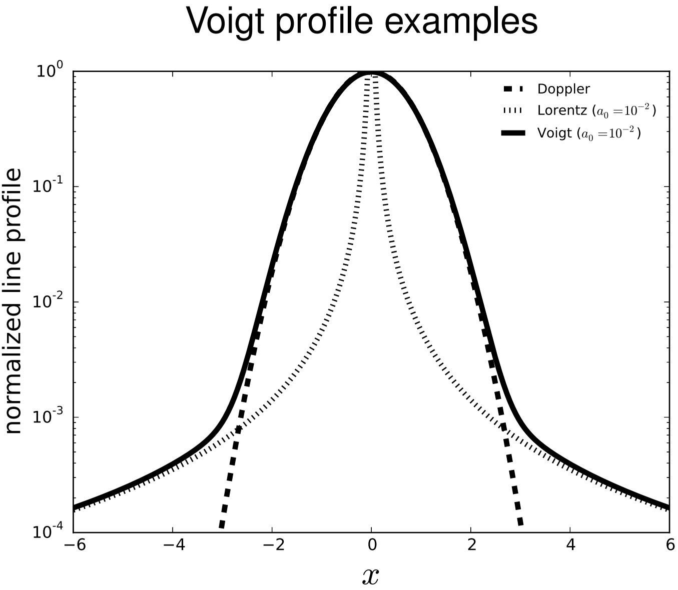


Figure 5.2: Voigt profile - small damping parameter

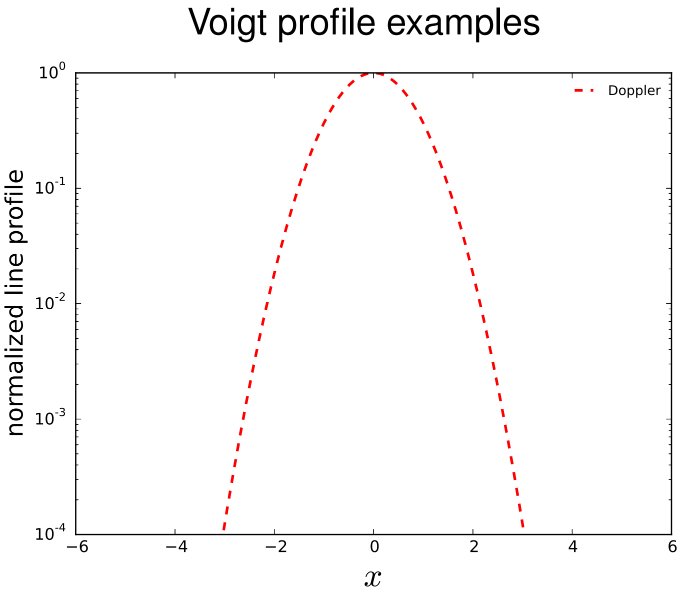


Figure 5.2: Doppler profile

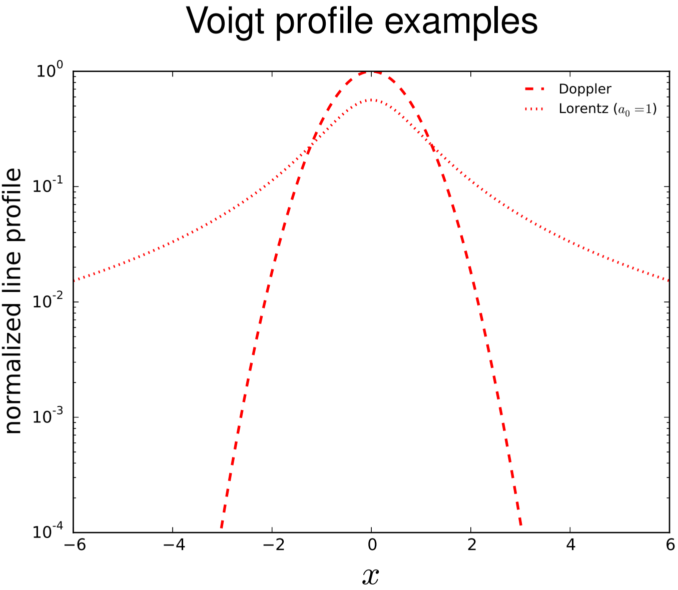


Figure 5.2: Lorentz profile – large damping parameter

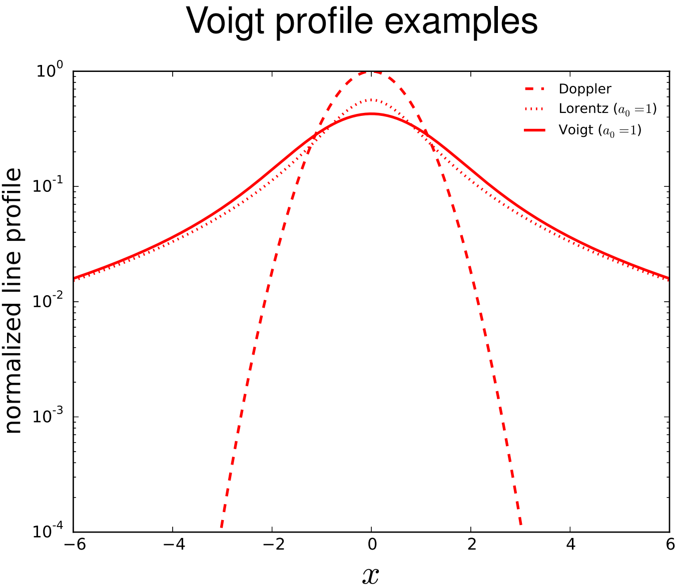


Figure 5.2: Voigt profile – large damping parameter

Line opacity – line strength I

- Opacity is obtained by multiplying Voigt profile by *integrated line strength* $\mathcal{S}$
- $\mathcal{S}$ is calculated from quantum mechanics and statistical mechanics for different species, and *tabulated for a reference temperature* in spectroscopic databases, e.g. HITEMP by Rothman et al. 2010, JQSRT 111, 2139
- Use an analytical *scaling relation* to obtain $\mathcal{S}$ for any other temperature

Line opacity – line strength II

Line strength is related to transition probability between lower energy level 1 and upper energy level 2, e.g. probability for spontaneous emission given by *Einstein A-coefficient* A_{21} (Eq. 5.13 using Eq. 5.12 and ideal gas law $P = nk_\mathrm{B}T$):

$$\mathcal{S} = \frac{h\tilde{\nu}}{mn}\frac{n_2 A_{21}}{\mathcal{E}}$$

n . . . total number density of species with mass m

n_2 . . . population of energy level 2

$\mathcal{E}$ . . . energy density per unit wavenumber

Line opacity – line strength III

In local thermodynamic equilibrium (LTE):
Boltzmann – Saha – Planck (Eqs. 5.14 – 5.17)

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} e^{-\Delta E/k_\mathrm{B}T}$$

$$\frac{n_1}{n} = \frac{g_1}{Q(T)} e^{-E_1/k_\mathrm{B}T}$$

$$\mathcal{E} = \frac{4\pi B}{c}, \quad B = 2hc^2\tilde{\nu}^3(e^{h\tilde{\nu}c/k_\mathrm{B}T} - 1)^{-1}$$

$$\Delta E = E_2 - E_1 = h\tilde{\nu}c$$

$Q(T) = \sum g_i e^{-E_i/k_\mathrm{B}T}$ … partition function

Line opacity – line strength IV

$$\mathcal{S} = \frac{h\tilde{\nu}}{mn}\frac{n_2 A_{21}}{\mathcal{E}}$$

$$\mathcal{S} = \frac{h\tilde{\nu}\ A_{21}}{m\ n_1/g_1 Q(T) e^{E_1/k_\mathrm{B}T}}\ n_1 \frac{g_2}{g_1} e^{-\Delta E/k_\mathrm{B}T}\ \frac{c\ (e^{h\tilde{\nu}c/k_\mathrm{B}T} - 1)}{4\pi\ 2hc^2\tilde{\nu}^3}$$

$$\mathcal{S} = \frac{\cancel{h}\cancel{\tilde{\nu}}\ A_{21}}{m\ \cancel{n_1}/\cancel{g_1} Q(T) e^{E_1/k_\mathrm{B}T}}\ \cancel{n_1} \frac{g_2}{\cancel{g_1}} e^{-\Delta E/k_\mathrm{B}T}\ \frac{\cancel{c}\ (e^{h\tilde{\nu}c/k_\mathrm{B}T} - 1)}{4\pi\ 2\cancel{h}c^{\cancel{2}}\tilde{\nu}^{\cancelto{2}{3}}}$$

$$\mathcal{S} = \frac{g_2 A_{21}}{8\pi\ c\tilde{\nu}^2\ m\ Q(T)} e^{-E_1/k_\mathrm{B}T}\ \left(1 - e^{-h\tilde{\nu}c/k_\mathrm{B}T}\right)$$

Note that $\mathcal{S}$ depends only on T, not on n (or P)!

Line opacity – line strength V

To use database value $\mathcal{S}(T_0)$ at reference temperature T_0:

$$\frac{\mathcal{S}(T)}{\mathcal{S}(T_0)} = \frac{Q(T_0)}{Q(T)} e^{-E_1/k_\mathrm{B}T + E_1/k_\mathrm{B}T_0} \; \frac{1 - e^{-h\tilde{\nu}c/k_\mathrm{B}T}}{1 - e^{-h\tilde{\nu}c/k_\mathrm{B}T_0}}$$

Line opacity – pressure broadening

- In addition to natural and thermal broadening, spectral lines are broadened by collisions between particles, described by a Lorentz profile.
- Increased Lorentz line width (empirical formula), with parameters given in databases at reference pressure P_0:

$$\Gamma_{\mathrm{L}}' = \Gamma_{\mathrm{L}} + \left(\frac{T}{T_0}\right)^{-n_{\mathrm{coll}}} \left[\frac{\alpha_{\mathrm{air}}(P - P_{\mathrm{self}})}{P_0} + \frac{\alpha_{\mathrm{self}} P_{\mathrm{self}}}{P_0}\right]$$

- Accounts for
  - Broadening by “air”: collisions with molecules of the dominating gas in the atmosphere
  - Self-broadening: collisions with molecules of the same species as the absorbing species
- This treatment is incorrect in the far line wings.
  This error plays a role in wavelength regions with millions of lines, and has to be dealt with by using a “cutoff” for the line wings when calculating the total opacity.

Line opacity: water at T = 1500 K, P = 1 atm

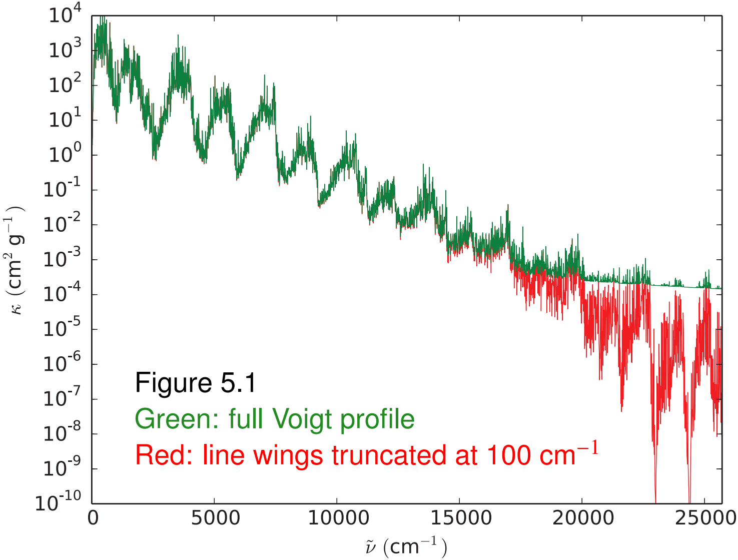
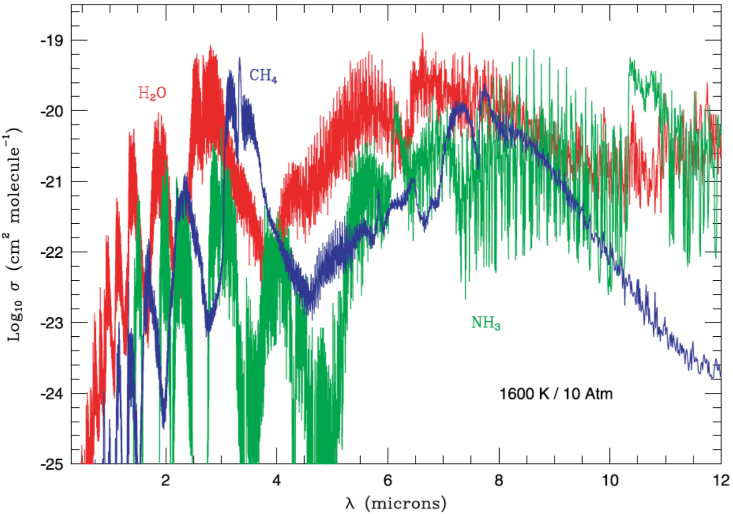


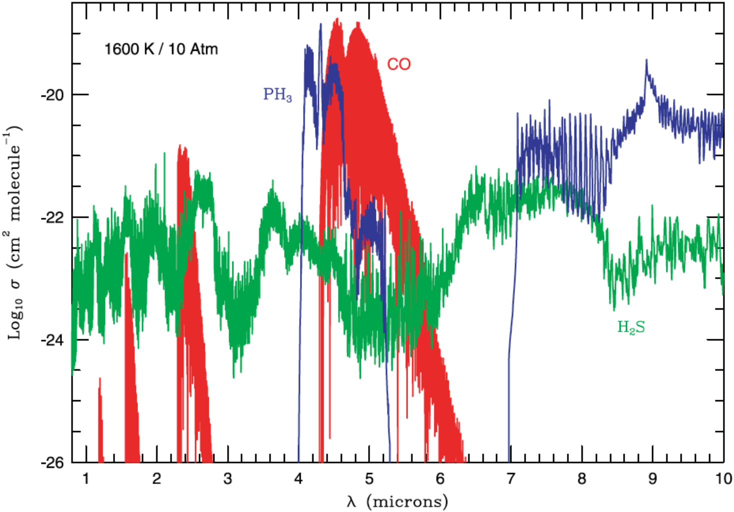
Figure 5.1

Line opacity: water, methane, ammonia



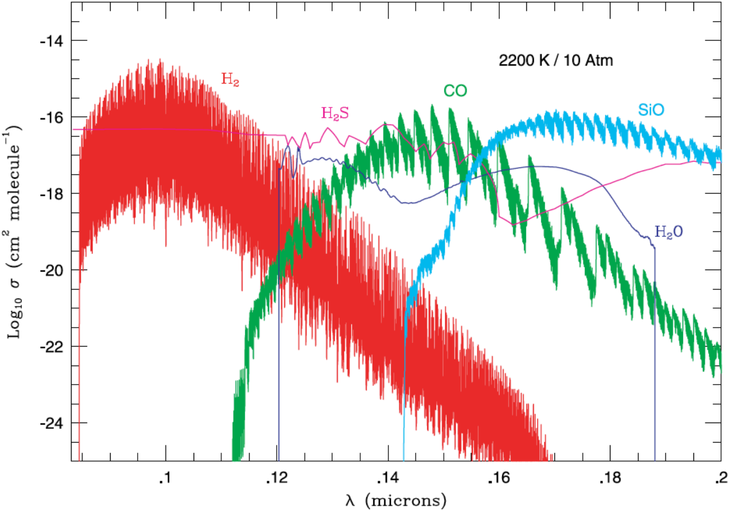
Sharp and Burrows 2007, ApJS 168, 140, Fig. 1

Line opacity: CO



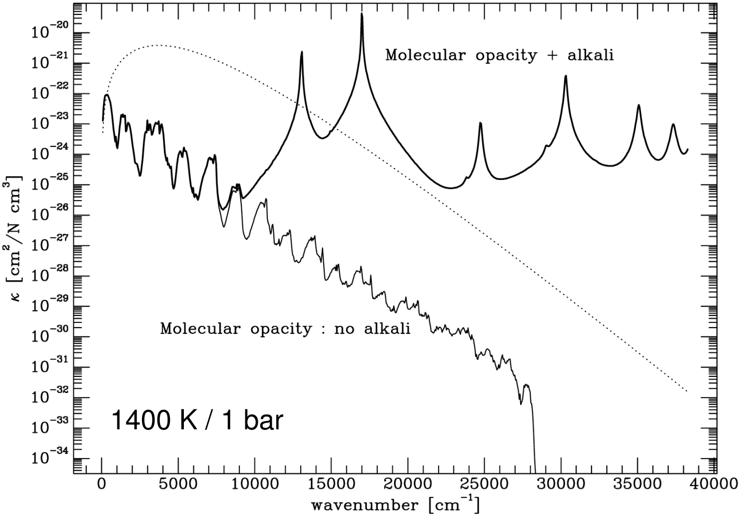
Sharp and Burrows 2007, ApJS 168, 140, Fig. 3

Line opacity: ultraviolet absorption



Sharp and Burrows 2007, ApJS 168, 140, Fig. 11

Line opacity: Alkali atoms – Na, K



Freedman, Marley, and Lodders 2008, ApJS 174, 504, Fig. 4

Line opacity in practice

- Each molecule gives rise to a large number of spectral lines, depending on temperature, e.g. water on Earth $\sim 10^5$ lines, on exoplanets with 1000 K $\sim 10^8$ lines.
- In principle, opacity function needs to be calculated at a number of wavelength points larger than the number of lines, to resolve all lines = *line-by-line* calculation.
- To be repeated $\sim$100 times for a model, at different temperatures, pressures, abundances.
- Line-by-line calculations are infeasible in practice
  → two approaches:
  - *Opacity sampling* – select a smaller number of points
  - The *k-distribution method* – use cumulative distribution function of opacity function

K-distribution method

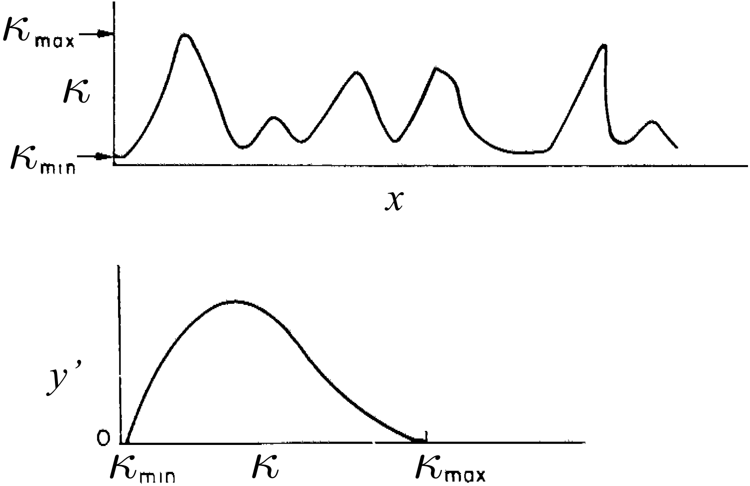
- Structure of atmosphere is determined by integrals that depend not so much on the details of the spectrum but more on its average properties
- We do not need to know the opacity explicitly at every frequency
- Adopt a line-absorption distribution function, which is a smooth and monotonically increasing function that can be sampled at few points
- Compute distribution functions for a grid of temperatures, pressures, and chemical abundances and interpolate between pre-tabulated grid points during model calculations

Construction of opacity distribution function

- Start from finely sampled opacity function $\kappa(x)$, where x is the wavenumber normalized by the entire range considered
- Choose an interval for which we want an “average” opacity
- Distribution function y' is the fraction of the interval that has opacity between κ and $\kappa + \Delta\kappa$
- Cumulative distribution function y is the fraction of the interval that has opacity κ or less:

$$y(\kappa) = \int_0^{\kappa} y'(\kappa')d\kappa', \quad y(\kappa_{\min}) = 0, \quad y(\kappa_{\max}) = 1$$

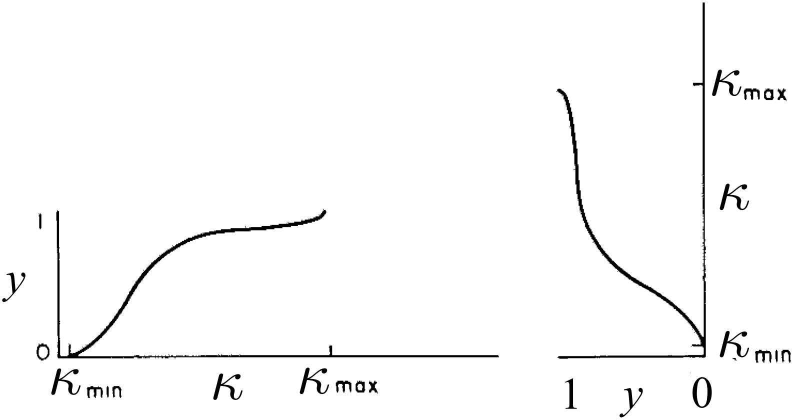
Opacity distribution function



Adapted from R.L. Kurucz 1970, SAO Special Report No. 309, p. 93

Opacity distribution function

$y(\kappa)$ can be inverted to get something that looks like a line profile: $\kappa(y)$, with $\kappa(0) = \kappa_{\min}$ and $\kappa(1) = \kappa_{\max}$



Adapted from R.L. Kurucz 1970, SAO Special Report No. 309, p. 93

Opacity and k-distribution function

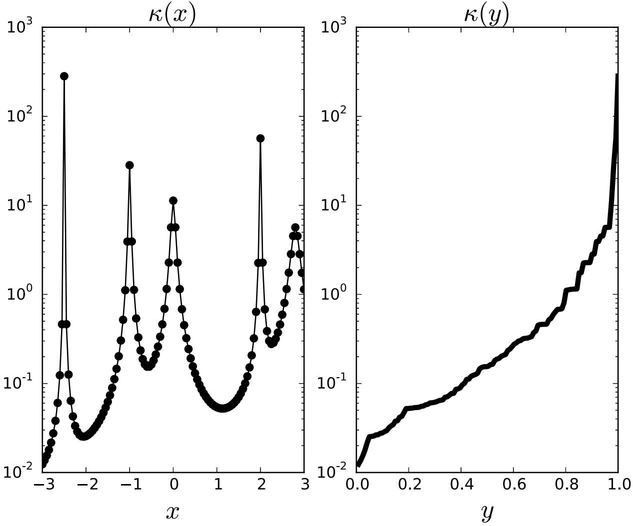


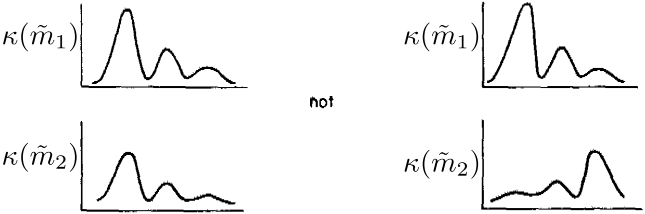
Figure 5.3

Application of k-distribution function

- Wavelength-integrated transmission function (cf. Eq. 3.36):

$$\mathcal{T} = \int_0^\infty e^{-\kappa(x)\tilde{m}} dx = \int_0^1 e^{-\kappa(y)\tilde{m}} dy$$

- **Assumption**: opacity function has the same relative shape at all column masses $\tilde{m}$ → k-distribution is independent of depth = *correlated-k approximation*



Adapted from R.L. Kurucz 1970, SAO Special Report No. 309, p. 96

Atmospheric chemical composition

- If there is more than one molecule in the atmosphere, one needs to compute the *total opacity function* by adding the opacities of the various molecules, weighted by their relative abundances (see lecture on atmospheric chemistry), *before* constructing the k-distribution function.
- The opposite case of adding the k-distribution functions of different molecules corresponds to assuming that the lines of the two molecules are correlated, i.e. they populate the same wavenumber regions.
- Limiting cases for distribution of spectral lines: *perfectly-uncorrelated*, *perfectly-correlated*, *disjoint* lines effect on transmission function → Problem 5.6.6 (home work)

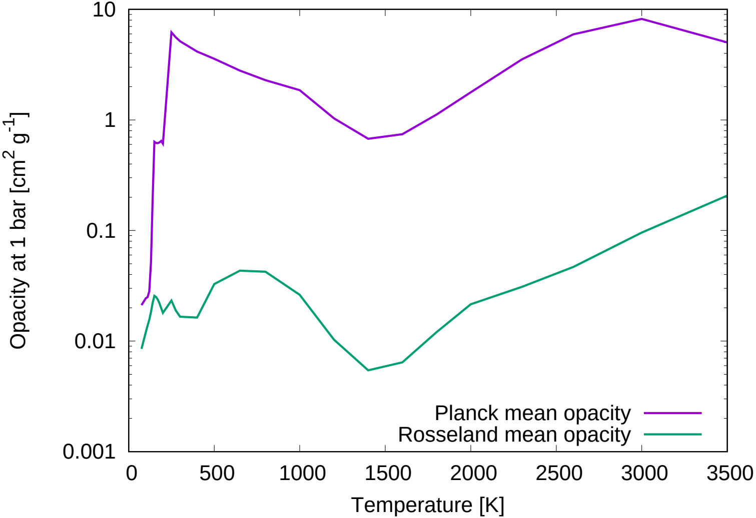
Low-temperature, low-pressure limit

- At low temperatures and low pressures the opacity function can be expressed as the product of two functions, one only dependent on wavenumber, the other only dependent on temperature.
- In that case, the k-distribution method with correlated-k approximation is exact.
- Low-temperature limit: $T_{\text{limiting}} = hc\tilde{\nu}/k_{\text{B}}$, $T \ll T_{\text{limiting}}$
- Examples: assume T is at most 1% of T_{limiting}
  ($hc/k_{\text{B}} \approx 0.014$ K/m):
  Optical – $\lambda = 400$ nm, $\tilde{\nu} = 25000$ cm^{-1} $\rightarrow T \sim 360$ K
  Infrared – $\lambda = 2\,\mu$m, $\tilde{\nu} = 5000$ cm^{-1} $\rightarrow T \sim 70$ K
- In general, the uncertainty due to opacity treatment needs to be evaluated by comparing distribution-function calculations to line-by-line calculations.

Mean opacities

- Mean opacities integrated over all wavenumbers are sometimes needed, e.g. for computing temperature-pressure profiles
- *Planck mean opacity*: $\kappa_\mathrm{P} = \dfrac{\int \kappa B d\tilde{\nu}}{\int B d\tilde{\nu}}$
  arithmetic mean weighted by Planck function,
  applicable at $\tau \sim 1$, strong lines important for radiative transfer
- *Rosseland mean opacity*: $\kappa_\mathrm{R} = \left(\dfrac{\int \frac{1}{\kappa} \frac{\partial B}{\partial T} d\tilde{\nu}}{\int \frac{\partial B}{\partial T} d\tilde{\nu}} \right)^{-1}$
  harmonic mean weighted by gradient of Planck function, applicable at large optical depths, weak lines important for radiative transfer

Mean opacities



Freedman, Marley, and Lodders 2008, ApJS 174, 504, Table 1

Home work

- 5.6.6 Atmospheres with two molecules: uncorrelated, correlated and disjoint spectral lines (Hint: if the solution is not obvious, draw figures for each of the three cases)