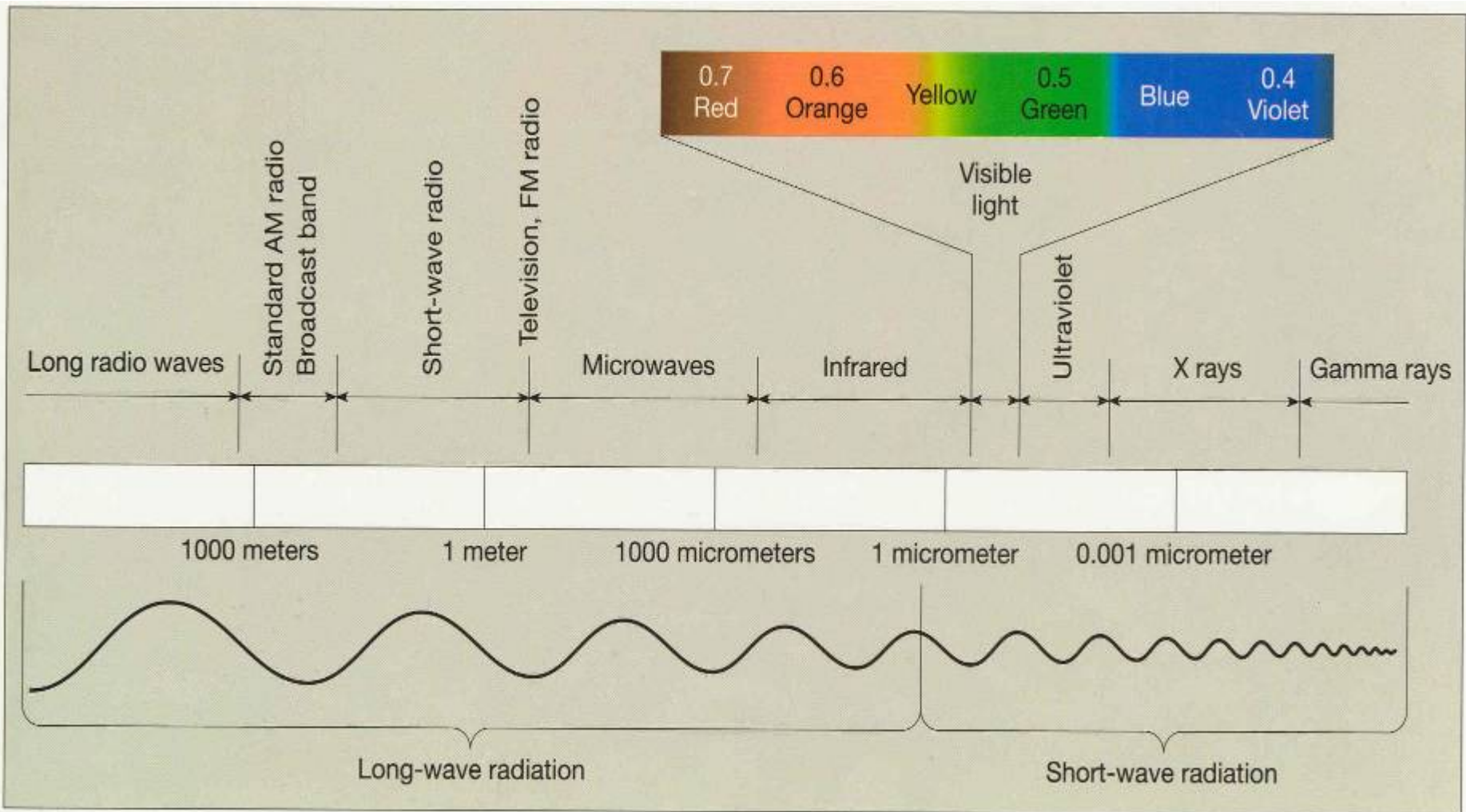


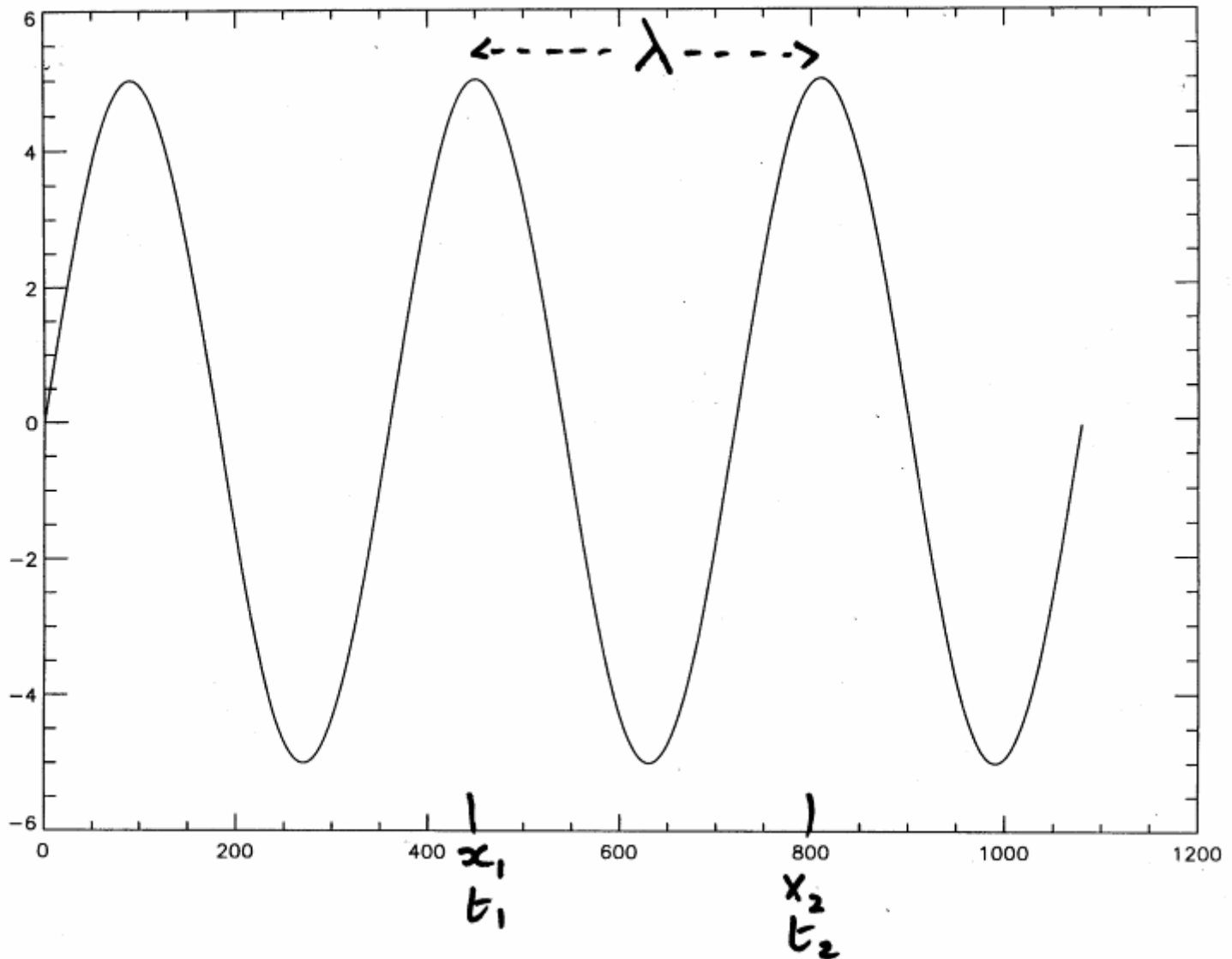
# Introduction to radiative transfer

Robert Hudson

# Electromagnetic spectrum



# Schematic of a wave



# WAVELENGTH

- **DISTANCE BETWEEN SUCCESSIVE PEAKS**
- **GIVEN THE SYMBOL  $\lambda$**
- **MANY UNITS USED :**
  - **(A) MICRON,  $10^{-6}$  METERS**
  - **(B) NANOMETER,  $10^{-9}$  METERS**
  - **(C) ANGSTROM,  $10^{-10}$  METERS**

# FREQUENCY

Defined as the number of maxima that pass an observer per second

Given the symbol  $\tilde{\nu}$

$$c = \lambda \tilde{\nu}$$

The term wave number is also used. It is the reciprocal of the wavelength. It is usually given the symbol  $\nu$ .

Caution - the use of  $\nu$  and  $\tilde{\nu}$  are reversed in many textbooks.

# VELOCITY

- **WAVE VELOCITY IS DEFINED AS THE DISTANCE A PEAK MOVES IN ONE SECOND.**
- **IN VACUO THE WAVE VELOCITY OF AN ELECTROMAGNETIC WAVE IS  $2.997925 \times 10^8$  METERS PER SECOND**
- **FOR THOSE OF YOU WHO PREFER ENGLISH UNITS, THE VELOCITY OF LIGHT IS  $1.80262 \times 10^{12}$  FURLONGS PER FORTNIGHT.**
- **THE WAVE VELOCITY IS GIVEN THE SYMBOL  $c$ .**

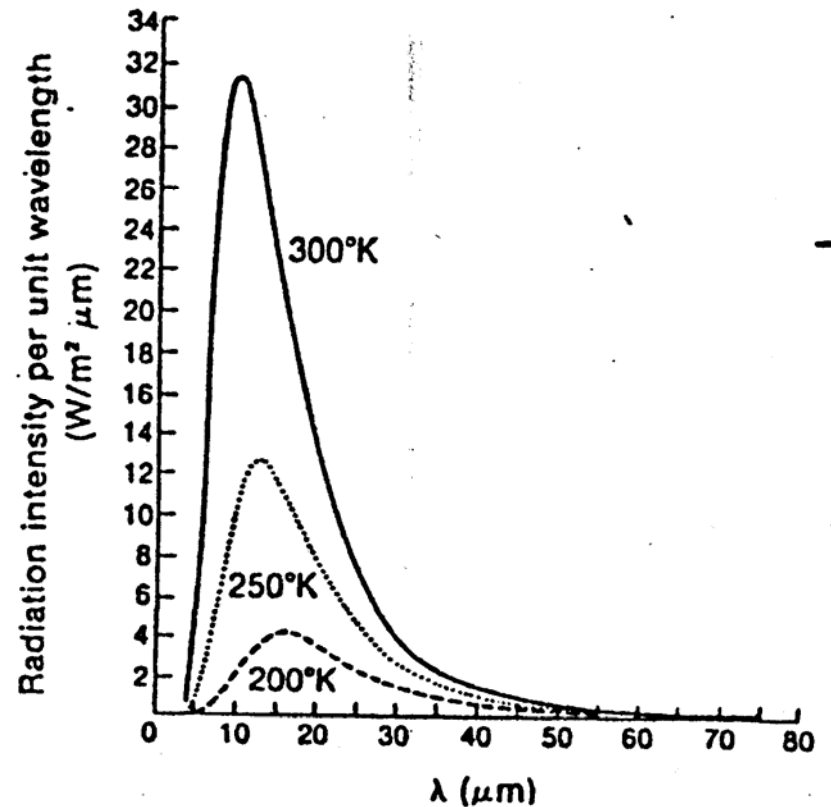
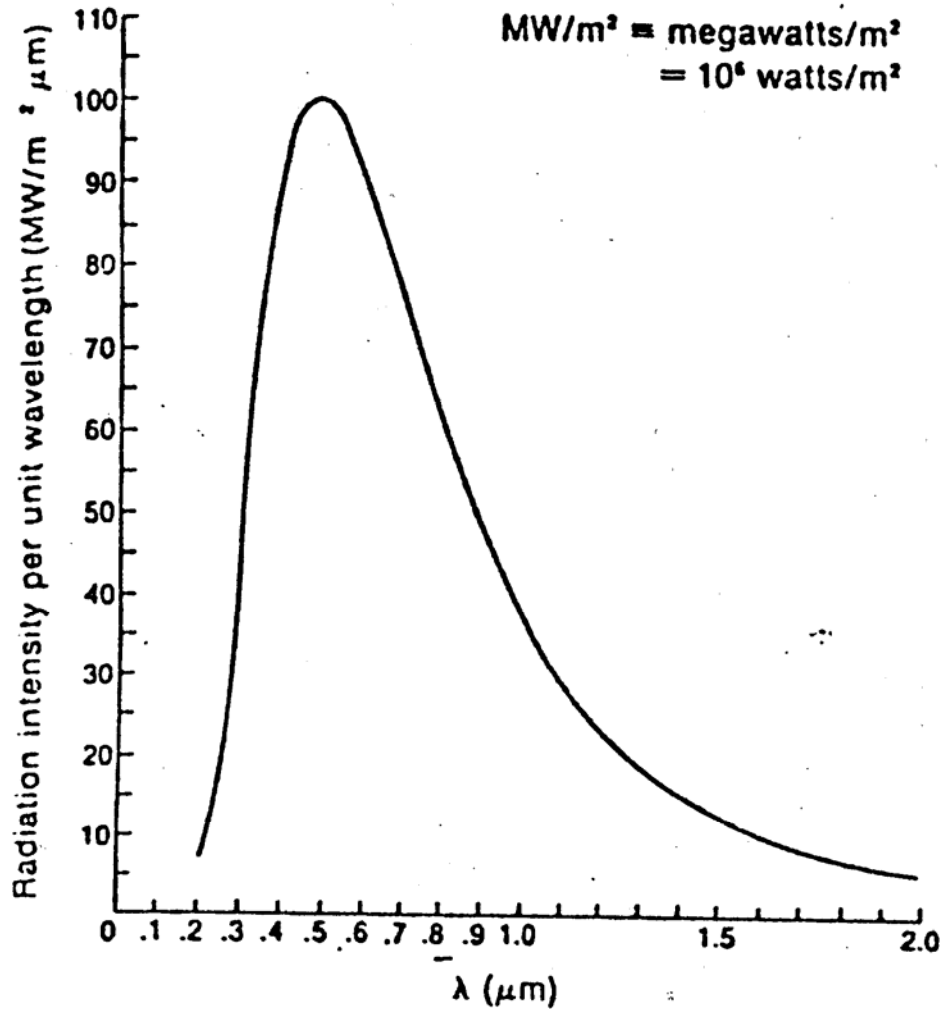
# Planck's spectral distribution law

- Planck introduced in 1901 his hypothesis of quantized oscillators in a radiating body.
- He derived an expression for the hemispherical blackbody spectral radiative flux

$$F_{\nu}^{BB} = \frac{m_r^2}{c^2} \frac{2\pi h \nu^3}{[\exp(h\nu/k_B T) - 1]}$$

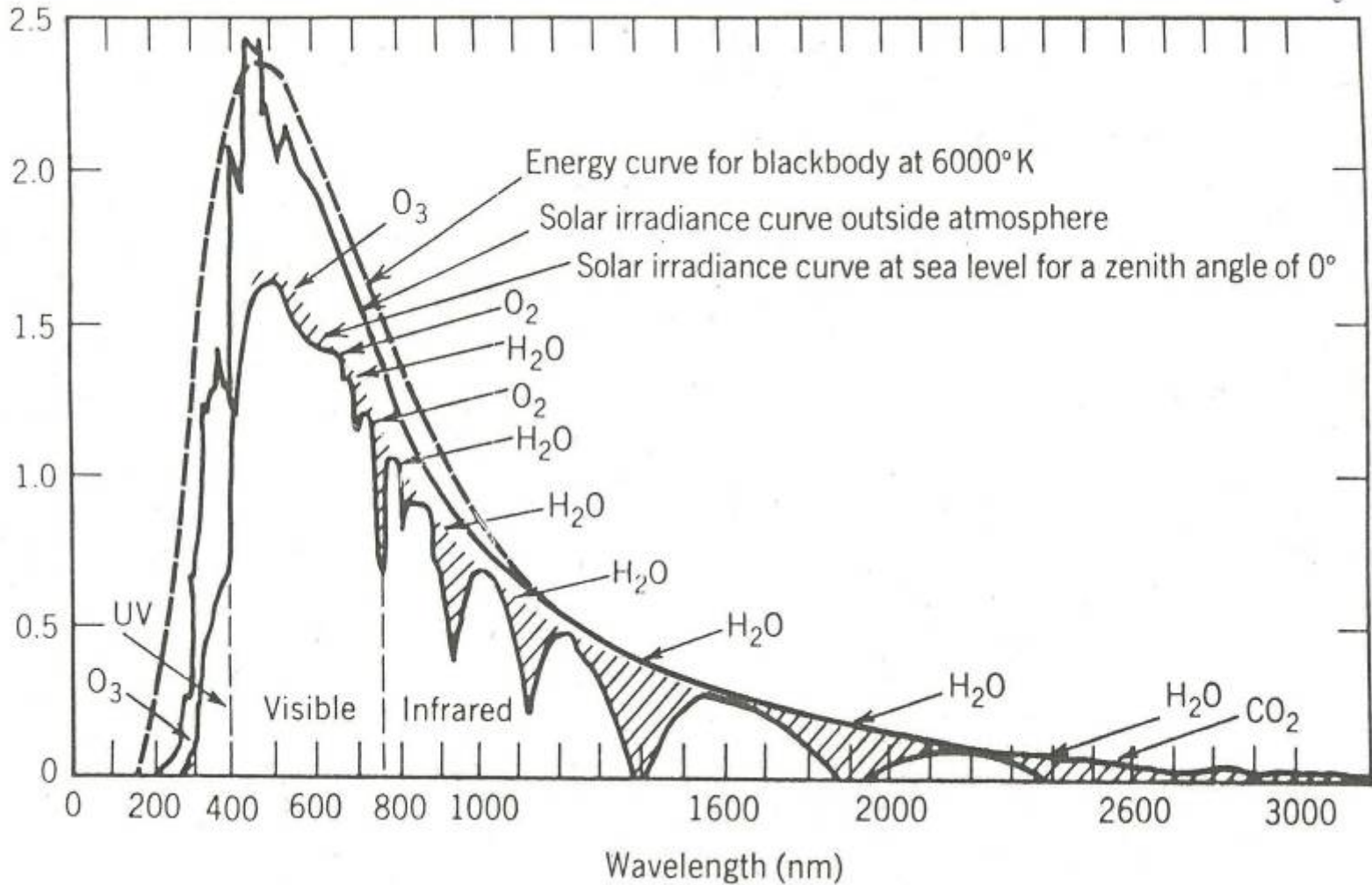
Where  $h$  is Planck's constant,  $m_r$  is the real index of refraction,  $k_B$  is Boltzmann's constant

# Comparison of solar and earth's blackbody intensity

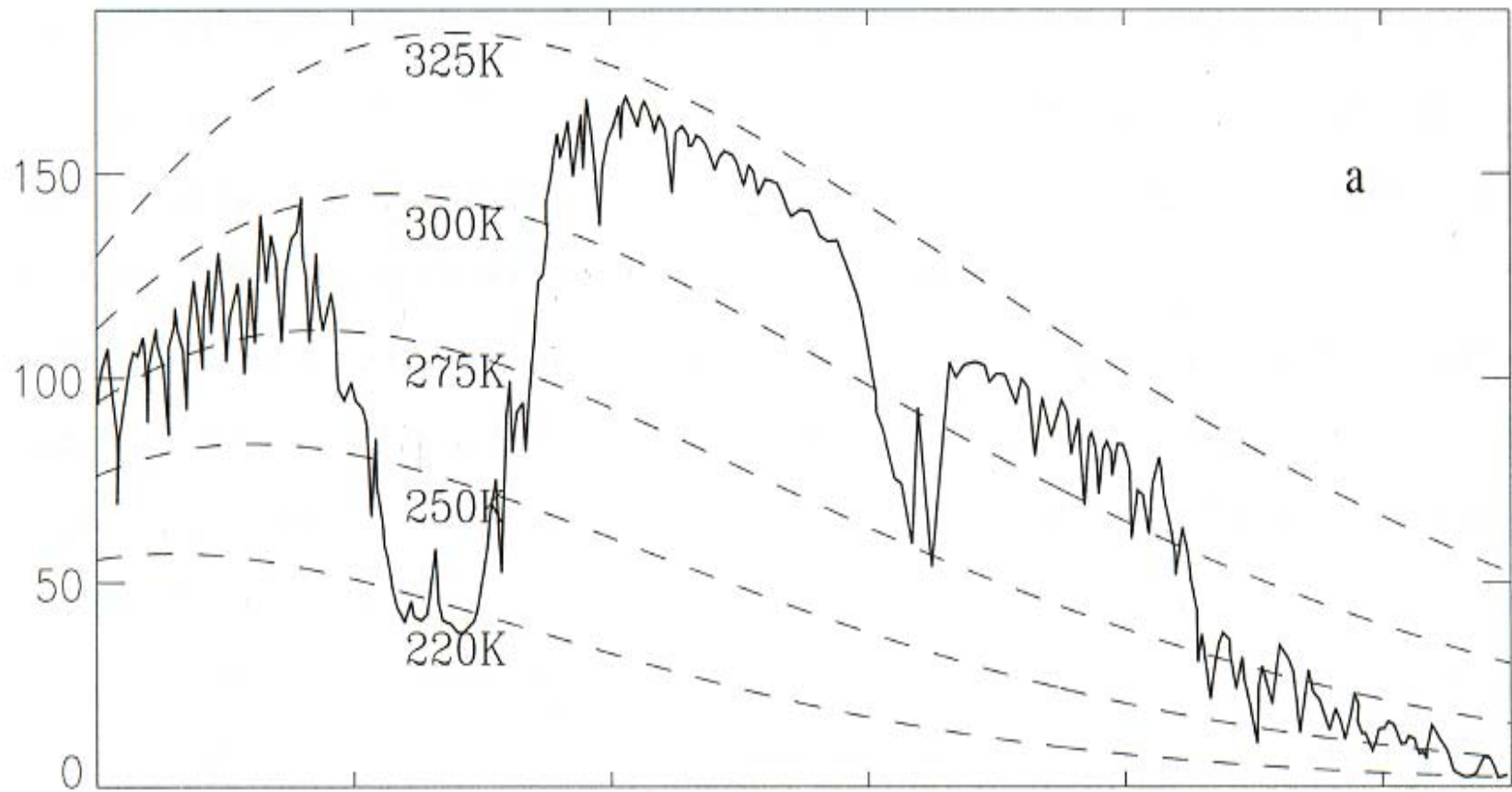




# UV-VISIBLE SOLAR SPECTRUM



# INFRARED FLUX FROM EARTH SAHARA



# Absorption in molecular lines and bands

- Molecules have three types of energy levels - electronic, vibrational, and rotational
- Transitions between electronic levels occur mainly in the ultraviolet
- Transitions between vibrational levels - visible/near IR
- Transitions between rotational levels - far IR/mm wave region
- $O_2$  and  $N_2$  have essentially no absorption in the IR
- 4 most important IR absorbers  $H_2O$ ,  $CO_2$ ,  $O_3$ ,  $CH_4$

# Vibrational levels

- Consider a diatomic molecule. The two atoms are bound together by a force, and can oscillate along the axis of the molecule.
- The force between the two atoms is given by

$$F = -k.x = m \frac{d^2 x}{dt^2}$$

- The solution of which is

$$x = x_0 \sin( 2 \pi \nu_0 t + \phi )$$

# Vibrational levels

- $\nu_0$  is known as the vibrational frequency

$$\nu_0 = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

- theoretically  $\nu_0$  can assume all values
- However in quantum mechanics these values must be discrete

$$E_v = h\nu_0(v + 1/2)$$

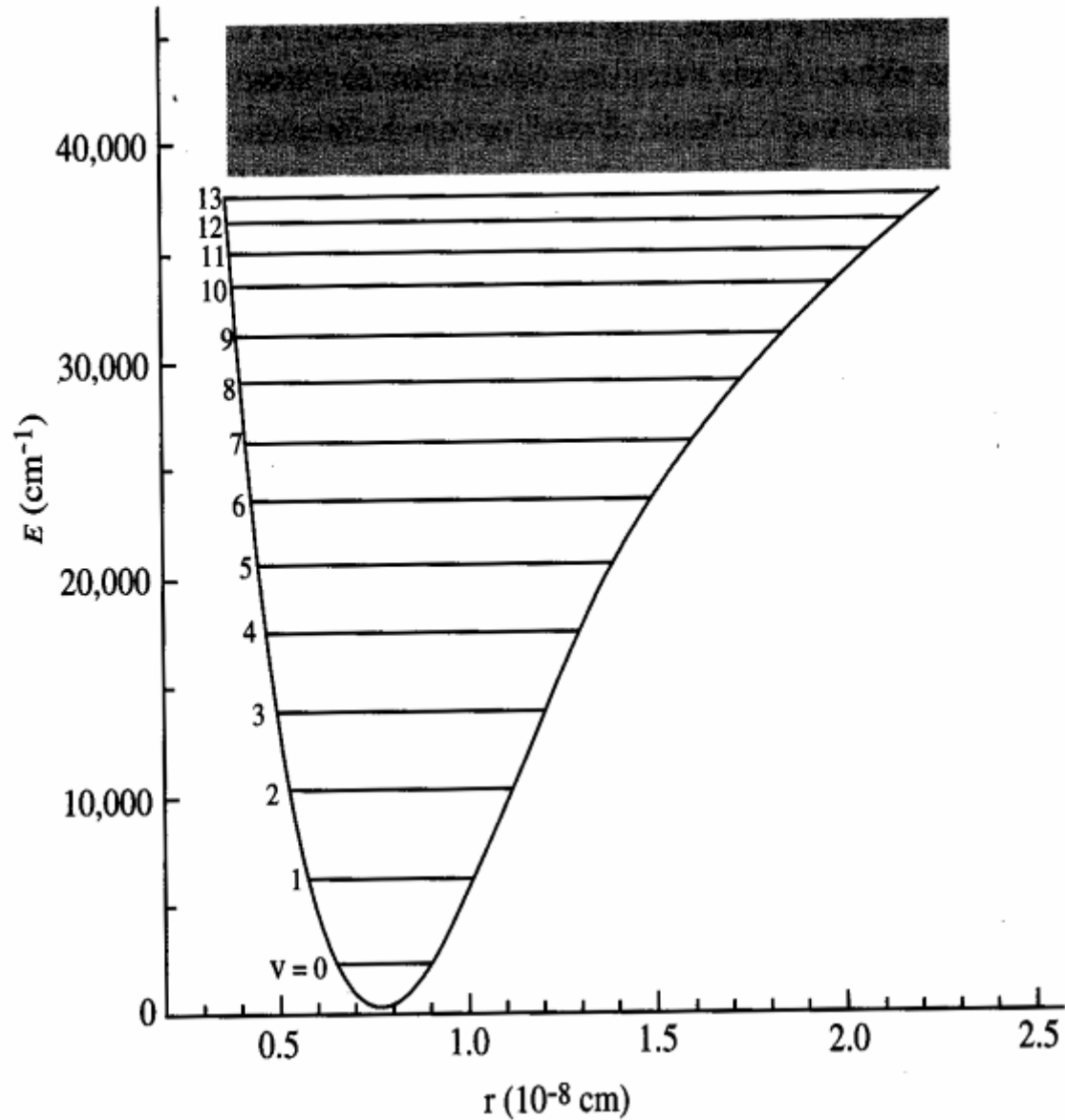
- $v$  is the vibrational quantum number

# Vibrational levels

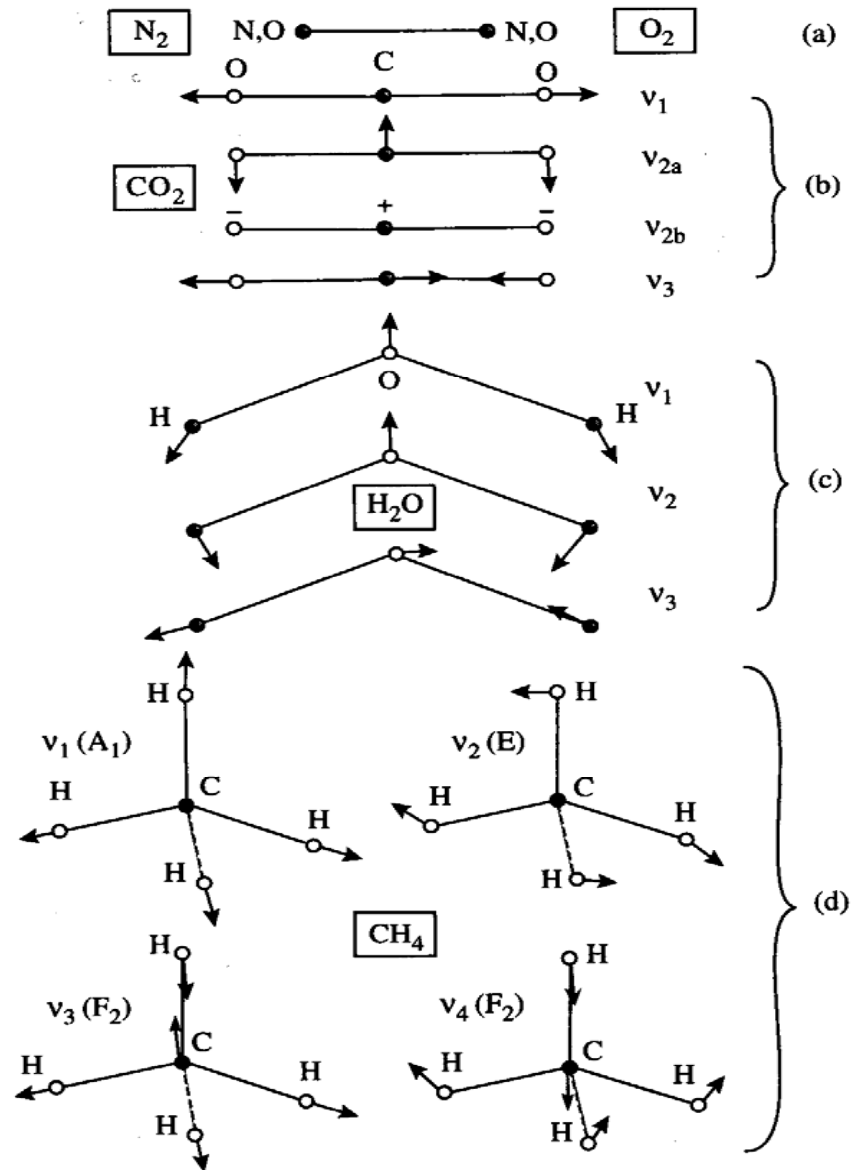
- In general  $k$  depends on the separation of the atoms and we have an 'anharmonic oscillator'

$$E_v = hc\omega_e(v+1/2) + hc\omega_e x_e(v+1/2)^2 + hc\omega_e y_e(v+1/2)^3$$

# Schematic of vibrational levels



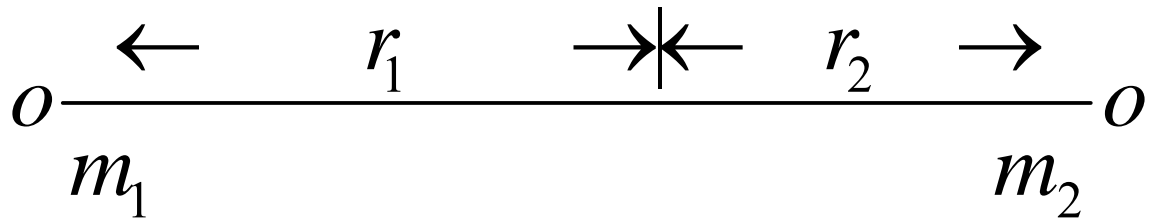
# Various forms of molecular vibration





# Rotational levels

- Consider a diatomic molecule with different atoms of mass  $m_1$  and  $m_2$ , whose distance from the center of mass are  $r_1$  and  $r_2$  respectively



- The moment of inertia of the system about the center of mass is:

$$I = m_1 r_1^2 + m_2 r_2^2$$

# Rotational levels

- The classical expression for energy of rotation is

$$E_r = \frac{I\omega^2}{2} = \frac{L^2}{2I} \text{ where } L = \text{angular momentum}$$

$$L^2 \rightarrow \left(\frac{h}{2\pi}\right)^2 J(J+1)$$

- where  $J$  is the rotational quantum number

$$E(J) = \frac{1}{2I} \left(\frac{h}{2\pi}\right)^2 J(J+1) = h c B_v J(J+1)$$

$$B_v = \frac{h}{8\pi^2 c I} \text{ the rotational constant}$$

# Vibrating Rotator

- If there were no interaction between the rotation and vibration, then the total energy of a quantum state would be the sum of the two energies. But there is, and we get

$$\frac{E(v, J)}{hc} = \omega_0(v + 1/2) + \omega_0 x_e (v + 1/2)^2$$

$$+ B_v J(J + 1) - D_v J^2 (J + 1)^2$$

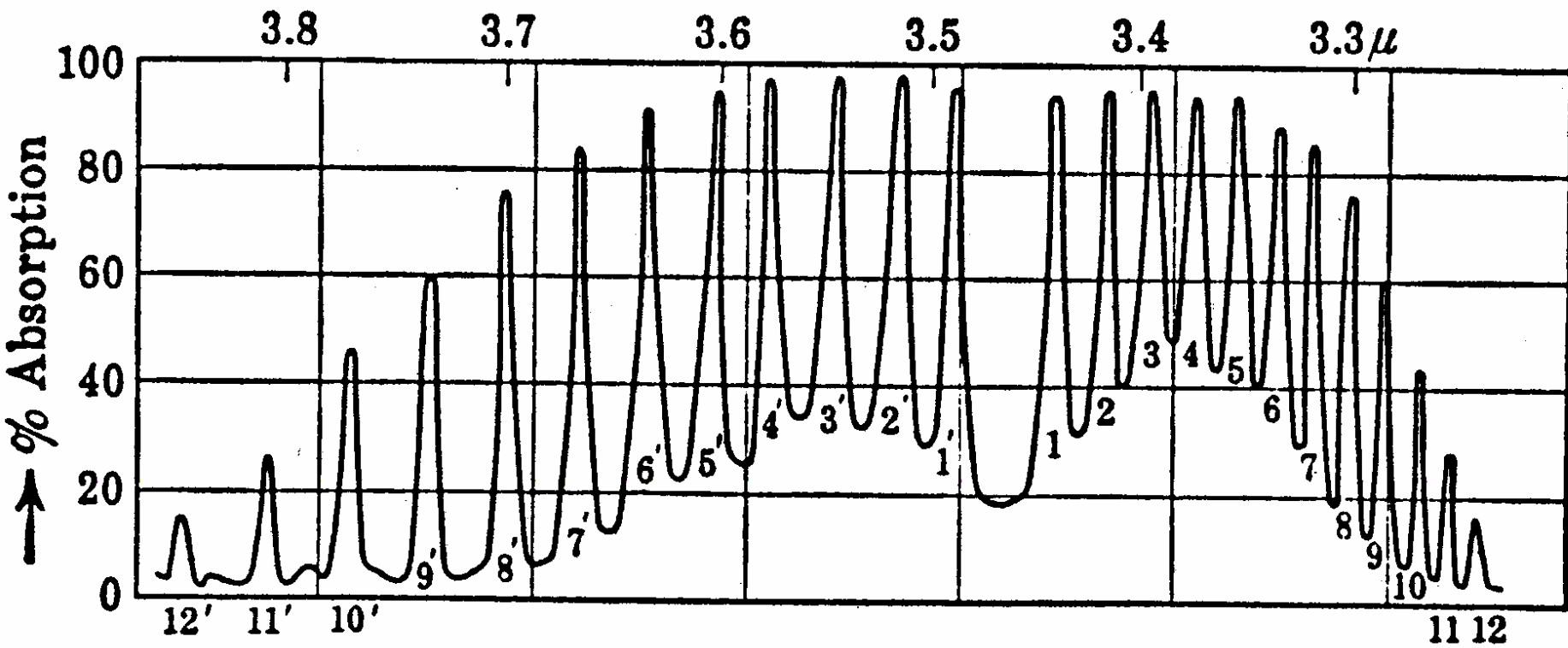
- The wavenumber of a spectral line is given by the difference of the term values of the two states

# Energy levels of a vibrating rotator

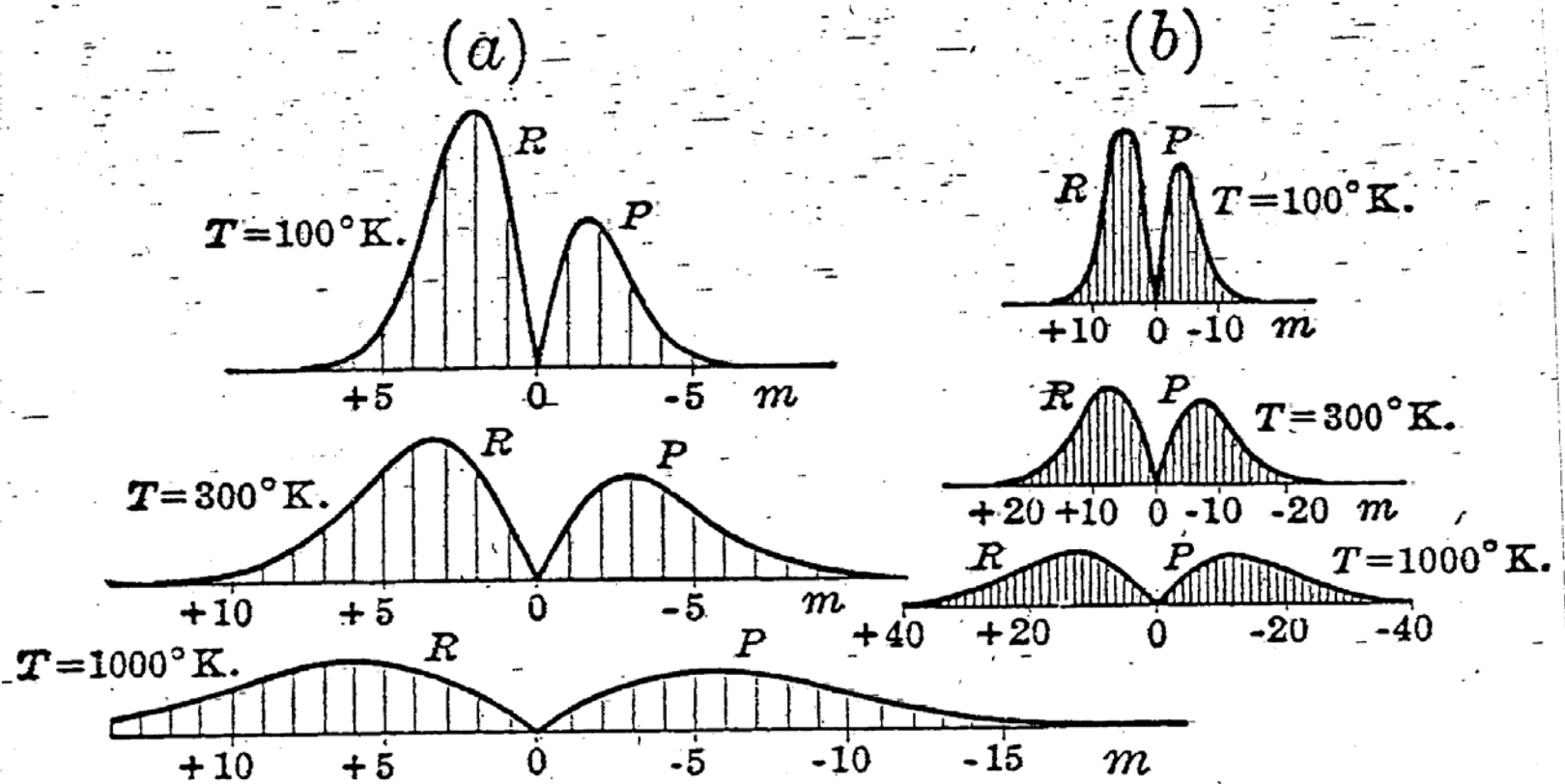


FIG. 53. Energy Levels of the Vibrating Rotator. For each of the first five vibrational levels, a number of rotational levels are drawn (short horizontal lines).

# Fine structure in HCl



# Intensity distribution in bands of HCl



# Line broadening

- Classical theory leads to the following equation for the shape of a line (transition). It is called the Lorentz profile

$$\Phi_L(\nu) = \frac{\gamma / 4\pi}{\pi \left[ (\nu_0 - \nu)^2 + (\gamma / 4\pi)^2 \right]}$$

Since the Lorentz profile is normalized we find by integrating over all frequencies

$$\int_0^{\infty} d\nu \sigma_n^{res}(\nu) = \frac{e^2}{4m_e \epsilon_0 c}$$

# Line broadening

- The line width (full width at half maximum) of the Lorentz profile is the damping parameter,  $\gamma$ .
- For an isolated molecule the damping parameter can be interpreted as the inverse of the lifetime of the excited quantum state.
- This is consistent with the Heisenberg Uncertainty Principle

$$\Delta E \Delta t \approx \frac{h}{2\pi} \quad \Delta t \approx \frac{h}{2\pi \cdot h \Delta \nu} \approx \frac{1}{2\pi \Delta \nu}$$

- If absorption line is dampened solely by the natural lifetime of the state this is natural broadening



# Pressure broadening

- For an isolated molecule the typical natural lifetime is about  $10^{-8}$  s,  $5 \times 10^{-4}$   $\text{cm}^{-1}$  line width
- Collisions between molecules can shorten this lifetime
- These collisions can be viewed as ‘billiard ball’ reactions, or as the overlapping of the potential fields of the two molecules.
- The collision process leads to a Lorentz line shape.

# Pressure broadening

- Clearly the line width will depend on the number of collisions per second, i.e. on the number density of the molecules (Pressure) and the relative speed of the molecules (the square root of the temperature)

$$\alpha_L \approx \alpha_L(STP) \frac{n v_{rel}}{n_L v_{rel}(STP)} = \alpha_L(STP) \frac{n \sqrt{T}}{n_L \sqrt{T_0}}$$

# Doppler broadening

- Second major source of line broadening
- Molecules are in motion when they absorb. This causes a change in the frequency of the incoming radiation as seen in the molecules frame of reference (Doppler effect)
- Let the velocity be  $v$ , and the incoming frequency be  $\nu$ , then

$$\nu' = \nu + \frac{v \cos \theta}{\lambda} = \nu + \frac{v \nu \cos \theta}{c} = \nu \left(1 + \frac{v}{c} \cos \theta\right)$$

# Doppler broadening

- In the atmosphere the molecules are moving with velocities determined by the Maxwell Boltzmann distribution

$$f(v_X)dv_X = \left( \frac{m}{2\pi k_B T} \right)^{1/2} \exp(-v_X^2 / v_0^2) dv_X$$

$$\text{where } v_0 = \sqrt{2k_B T / m}$$

# Doppler broadening

- The cross section at a frequency  $\nu$  is the sum of all line of sight components

$$\begin{aligned}\sigma_n(\nu) &= \int_{-\infty}^{+\infty} dv_x f(v_x) \sigma_n[\nu(1 + v_x/c)] \\ &= \left(\frac{m}{2\pi k_B T}\right)^{1/2} \int_{-\infty}^{+\infty} dv_x \exp(-v_x^2/v_0^2) \sigma_n(\nu + v_x/c) \\ &= S \left(\frac{m}{2\pi k_B T}\right)^{1/2} \exp\left[-c^2(\nu - \nu_0)^2 / v_0^2 \nu_0^2\right]\end{aligned}$$

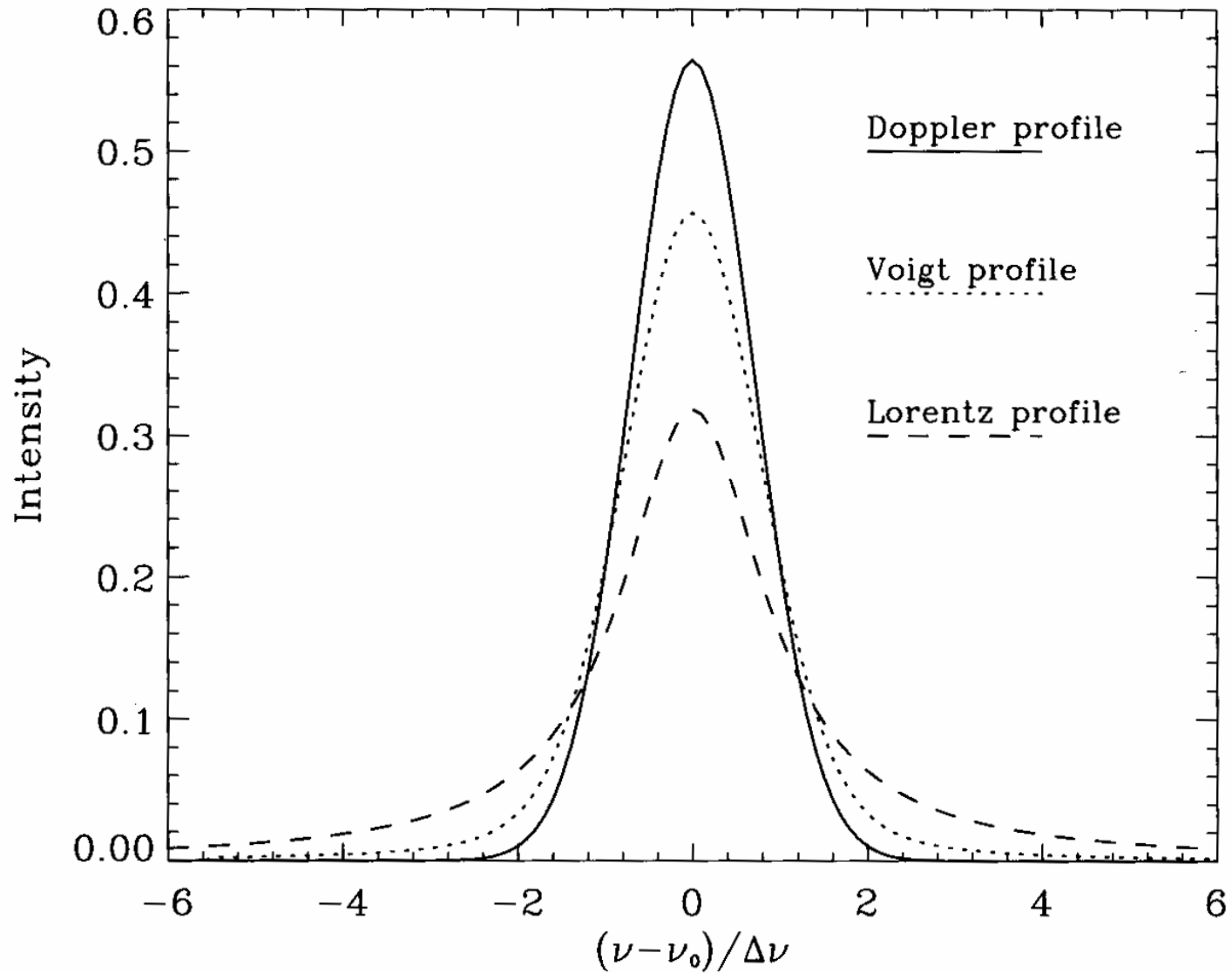
# Doppler broadening

- We now define the Doppler width as

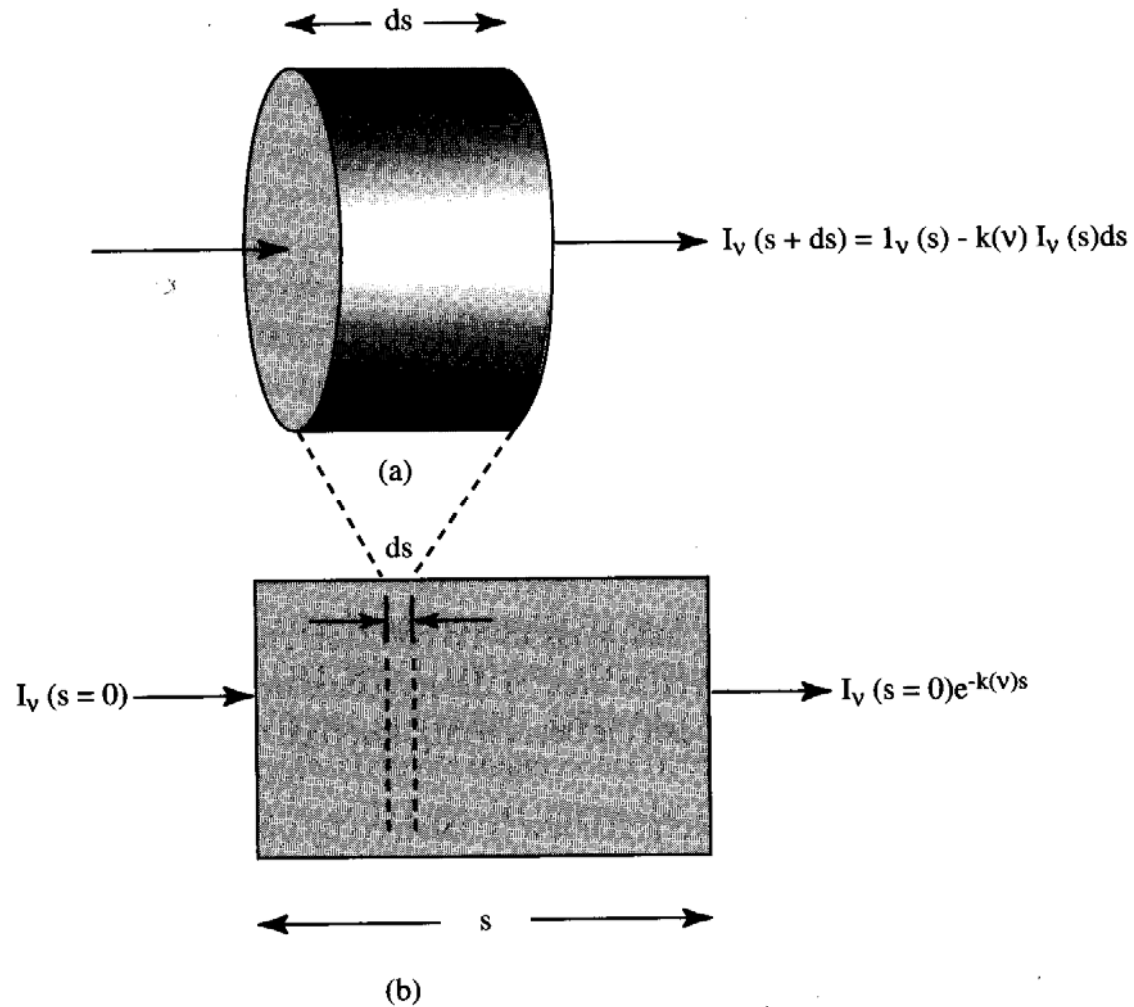
$$\alpha_D = v_0 v_0 / c$$

$$\sigma_n(\nu) = S \Phi_D(\nu) = \frac{S}{\sqrt{\pi\alpha_D}} \exp\left[-(\nu - \nu_0)^2 / \alpha_D^2\right]$$

# Comparison of line shapes



# The extinction law





# Extinction Law

- The extinction law can be written as

$$dI_{\nu} = -k(\nu) I_{\nu} ds$$

- The constant of proportionality is defined as the extinction coefficient.  $k$  can be defined by the length of the absorbing path with the gas at one atmosphere pressure

$$k(\nu) = \frac{dI_{\nu}}{I_{\nu} ds} \quad (m^{-1})$$

# Optical depth

- Normally we are interested in the total extinction over a finite distance (path length)

$$\tau_s(\nu) = \int_0^s ds' k(\nu) = \int_0^s ds' k_m(\nu) \rho = \int_0^s ds' k_n(\nu) n$$

Where  $\tau_s(\nu)$  is the extinction optical depth

- The integrated form of the extinction equation becomes

$$I_\nu(s, \bar{\Omega}) = I_\nu(0, \bar{\Omega}) \exp[-\tau_s(\nu)]$$

# Extinction = scattering + absorption

- Extinction really consists of two distinct processes, scattering and absorption, hence

$$\tau_s(\nu) = \tau_{sc}(\nu) + \tau_a(\nu)$$

where

$$\tau_{sc}(\nu) = \sum_i \int_0^s ds^i \sigma^i(\nu, s')$$

$$\tau_a(\nu) = \sum_i \int_0^s ds^i \alpha^i(\nu, s')$$

# Differential equation of radiative transfer

- We must now add the process called emission.
- We introduce an emission coefficient,  $j_\nu$
- Combining the extinction law with the definition of the emission coefficient

$$dI_\nu = -k(\nu)I_\nu ds + j_\nu ds$$

noting that

$$k(\nu)ds = d\tau_s$$

$$\frac{dI_\nu}{d\tau_s} = -I_\nu + \frac{j_\nu}{k(\nu)}$$

# Differential equation of radiative transfer

- The ratio  $j_\nu/k(\nu)$  is known as the source function,

$$S_\nu = \frac{j_\nu}{k(\nu)}$$

$$\frac{dI_\nu}{d\tau_s} = -I_\nu + S_\nu$$

This is the differential equation of radiative transfer

# Scattering

- Two types of scattering are considered – molecular scattering (Rayleigh) and scattering from aerosols (Mie)
- The equation for Rayleigh scattering can be written as

$$\sigma_n^{RAY}(\lambda) = \frac{8\pi}{3} \left( \frac{2\pi}{\lambda} \right)^4 \alpha_p^2$$

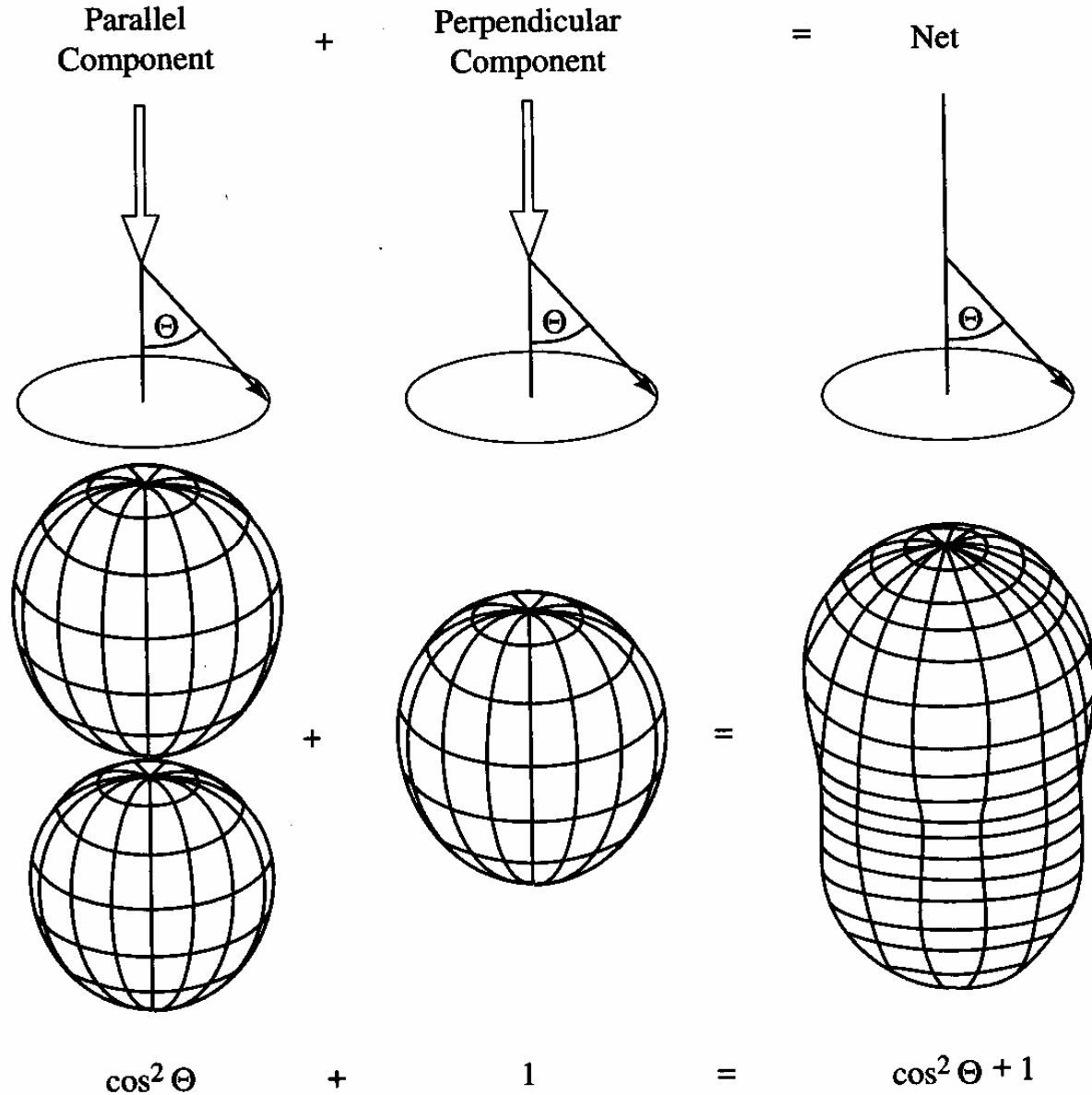
- Where  $\alpha$  is the polarizability

# Rayleigh scattering

$\lambda$ , nm	$\sigma$ , cm <sup>2</sup>	$\tau$ , surface	Exp(- $\tau$ )
300	6.00 E-26	1.2	0.301
400	1.90 E-26	0.38	0.684
600	3.80 E-27	0.075	0.928
1000	4.90 E-28	0.0097	0.990
10,000	4.85 E-32	9.70 E-7	0.999

- Sky appears blue at noon, red at sunrise and sunset - why?

# Phase diagram for Rayleigh scattering

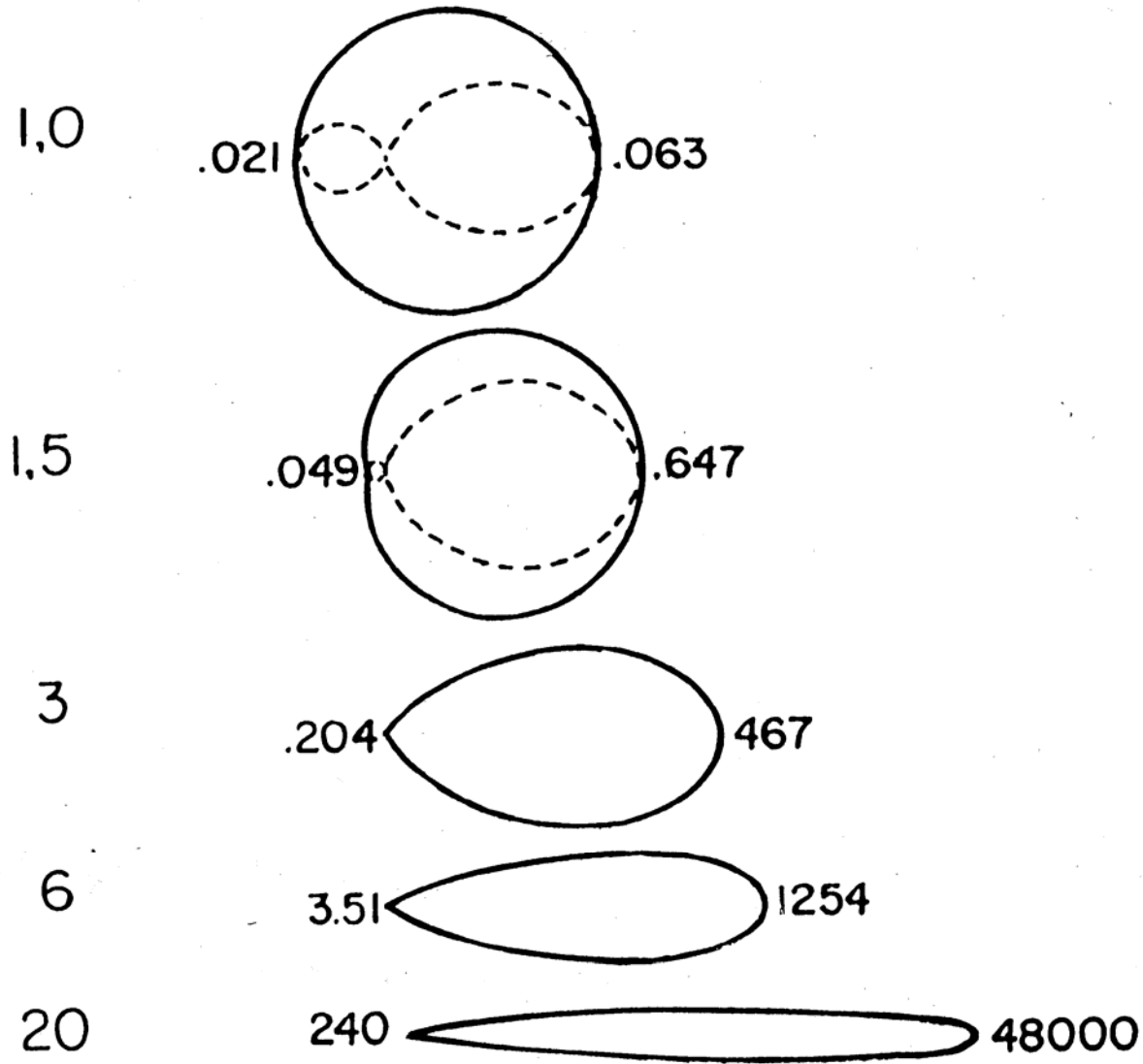




# Mie-Debye scattering

- For particles which are not small compared with the wavelength one has to deal with multiple waves from different molecules/atoms within the particle
- Forward moving waves tend to be in phase and this gives a large resultant amplitude.
- Backward waves tend to be out of phase and this results in a small resultant amplitude
- Hence the scattering phase function for a particle has a much larger forward component (forward peak) than the backward component

# Phase diagrams for aerosols



# Differential Equation of Radiative Transfer

- Introduce two additional parameters.  $B$ , the Planck function, and  $a$ , the single scattering albedo (the ratio of the scattering cross section to the extinction coefficient).
- The complete time-independent radiative transfer equation which includes both scattering and absorption is

$$\frac{dI_\nu}{d\tau_s} = -I_\nu + [1 - a(\nu)]B_\nu(T) + \frac{a(\nu)}{4\pi} \int_{4\pi} d\omega' p(\hat{\Omega}', \hat{\Omega}) I_\nu$$

# Solution for Zero Scattering

- If there is no scattering, e.g. in the thermal infrared, then the equation becomes

$$\frac{dI_{\nu}}{d\tau_s} = -I_{\nu} + B_{\nu}(T)$$

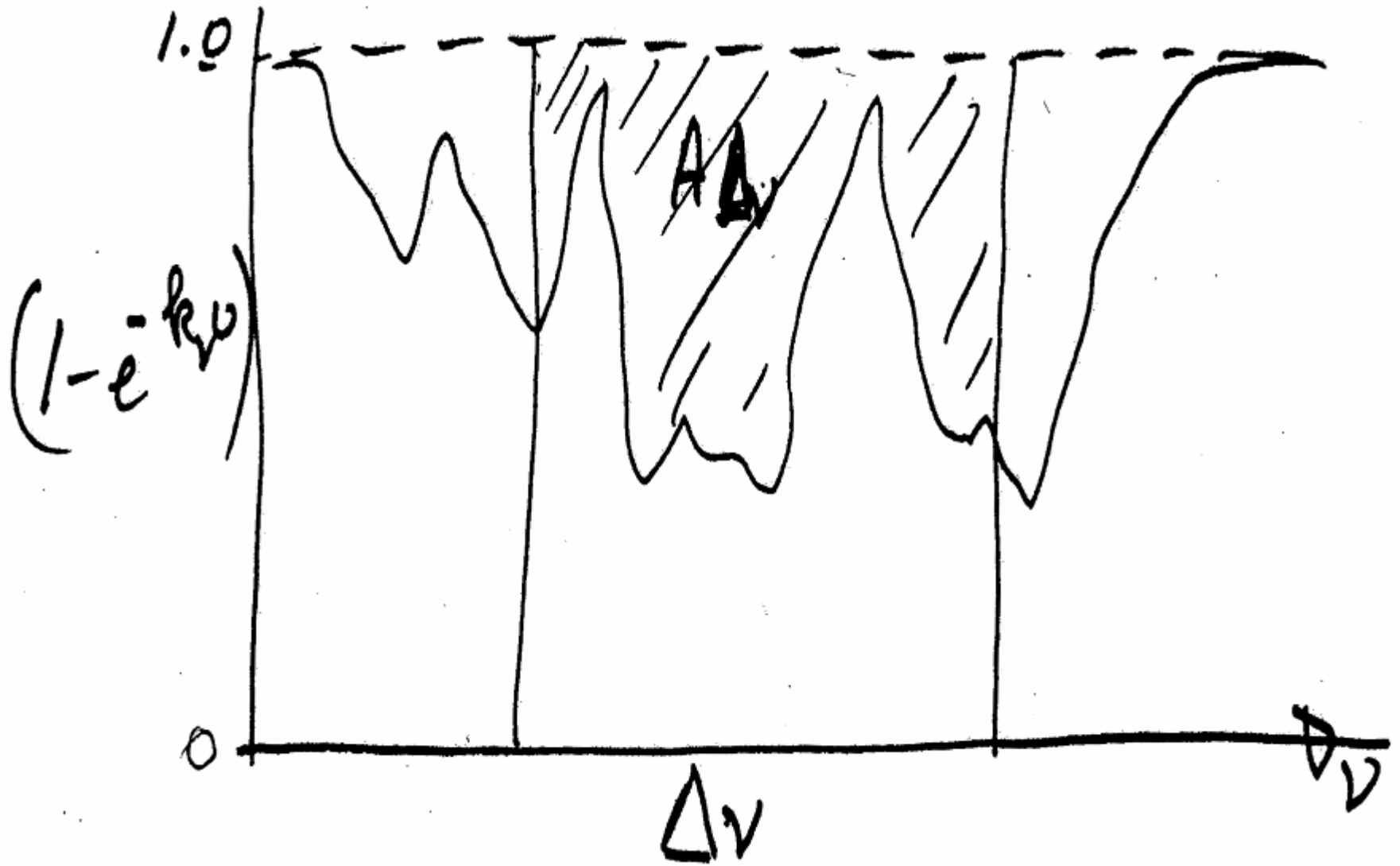
# Transmittance

- For monochromatic radiation the transmittance,  $T$ , is given simply by

$$T(\tau; \mu) = e^{-\tau/\mu}$$

- But now we must consider how to deal with radiation that is not monochromatic. In this case the integration must be made over all frequencies.
- Absorption cross section at high spectral resolution are available in tabular form – HITRAN.
- But usually an average value over a frequency interval is used.

# Schematic for A



# Transmission in spectrally complex media

- transmittance

$$T_{\Delta\nu} = 1 - \langle \alpha_{\Delta\nu} \rangle = \frac{1}{\Delta\nu} \left( \int_{\Delta\nu} e^{-k_\nu u} d\nu \right)$$

# Statistical Band Model (Goody)

- Goody studied the water-vapor bands and noted the apparent random line positions and band strengths.
- Let us assume that the interval  $\Delta\nu$  contains  $n$  lines of mean separation  $d$ , i.e.  $\Delta\nu=nd$
- Let the probability that line  $i$  has a line strength  $S_i$  be  $P(S_i)$  where

$$\int_0^{\infty} P(S_i) dS = 1$$

- $P$  is normally assumed to have a Poisson distribution



# Statistical Band Model (Goody)

assuming a Lorentz line shape, one gets

$$T = \exp \left[ - \frac{\bar{S}u}{d} \left( 1 + \frac{\bar{S}u}{\pi\alpha_L} \right)^{-1/2} \right]$$

where  $\bar{S}$  is the mean line strength.

# Statistical Band Model (Goody)

- We have reduced the parameters needed to calculate  $T$  to two

$$\frac{\bar{S}}{d} \quad \text{and} \quad \frac{\pi\alpha_L}{d}$$

- These two parameters are either derived by fitting the values of  $T$  obtained from a line-by-line calculation, or from experimental data.

weak line

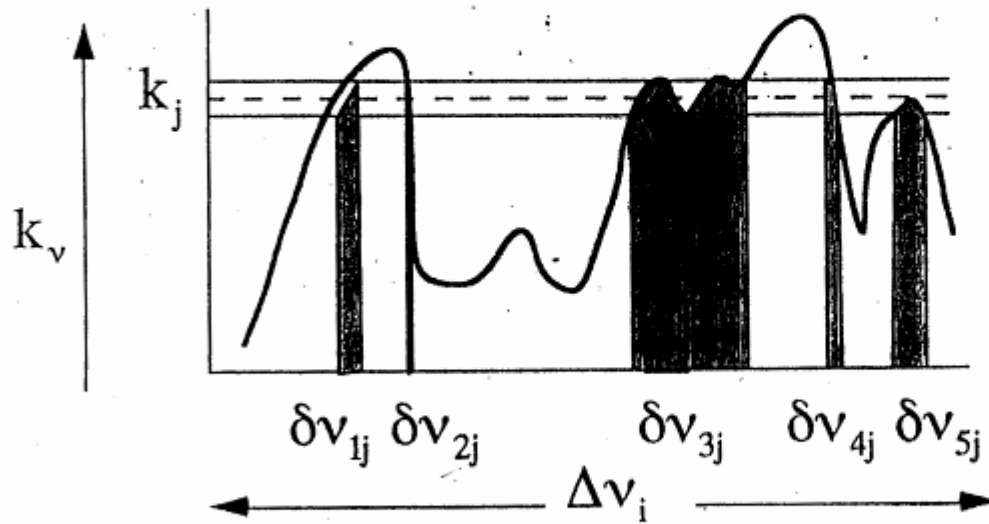
strong line

$$T = \exp\left(-\frac{\bar{S}u}{d}\right) \quad T = \exp\left(-\frac{\sqrt{\pi\alpha_L\bar{S}u}}{d}\right)$$

# K distribution technique

$$I_i \equiv \frac{1}{\Delta\nu_i} \int I_\nu d\nu$$

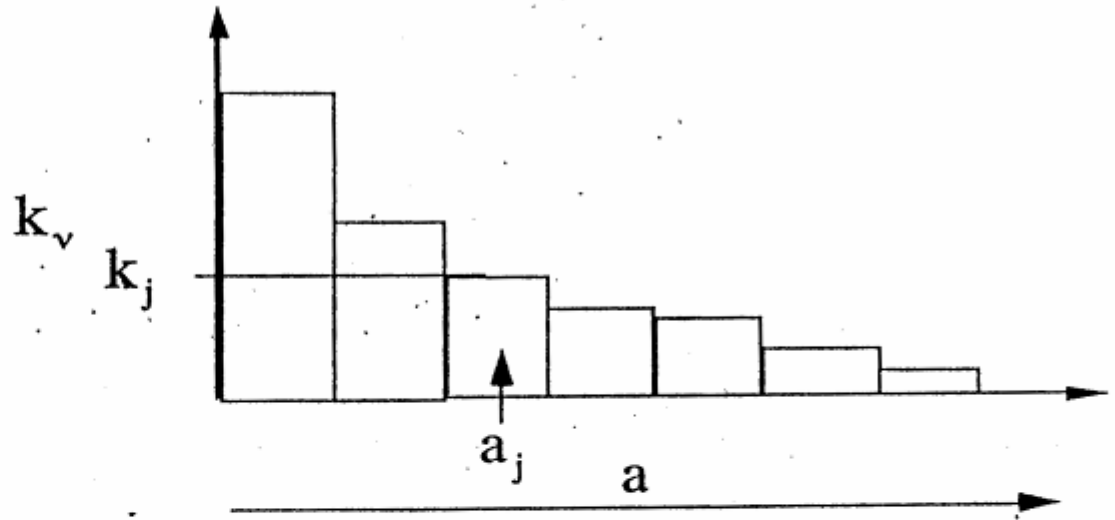
Since  $B_\nu$  is  $\approx$  constant in an interval,  
 $I_\nu$  is the same when  $k_\nu$  is the same



$$a_j = \sum_k \frac{\delta\nu_{kj}}{\Delta\nu} = \text{fraction of } \Delta\nu_i \text{ for which } k_\nu \approx k_j$$

# K distribution technique

Rearrange  $k_v$  as a probability histogram



Now we need only solve  $M$  monochromatic problems

$$I_i = \sum_{j=1}^M a_j I(k_v = k_j)$$

**One can obtain the histogram from:**

**(a) line-by-line calculations**

**(b) exponential sum fitting of band model transmission functions**

# Two-stream Approximation- Isotropic Scattering

- Although anisotropic scattering is more realistic, let's look at isotropic scattering i.e.  $p=1$
- The radiative transfer equations are

$$\mu \frac{dI^+(\tau, \mu)}{d\tau} = I^+(\tau, \mu) - \frac{a}{2} \int_0^1 d\mu' I^+(\tau, \mu') - \frac{a}{2} \int_0^1 d\mu' I^-(\tau, \mu') - (1-a)B$$

# Two-stream Approximation- Isotropic Scattering

$$-\mu \frac{dI^-(\tau, \mu)}{d\tau} = I^-(\tau, \mu) - \frac{a}{2} \int_0^1 d\mu' I^+(\tau, \mu') - \frac{a}{2} \int_0^1 d\mu' I^-(\tau, \mu') - (1-a)B$$

- In the two-stream approximation we replace the angular dependent quantities  $I$  by their averages over each hemisphere. This leads to the following pair of coupled differential equations

# Two-stream Approximation- Isotropic Scattering

$$\bar{\mu}^+ \frac{dI^+(\tau)}{d\tau} = I^+(\tau) - \frac{a}{2} I^+(\tau) - \frac{a}{2} I^-(\tau) - (1-a)B$$

$$-\bar{\mu}^- \frac{dI^-(\tau)}{d\tau} = I^-(\tau) - \frac{a}{2} I^+(\tau) - \frac{a}{2} I^-(\tau) - (1-a)B$$

If the medium is homogeneous then  $a$  is constant. One can now obtain analytic solutions to these equations.  $\mu$  in the above equations is the cosine of the average polar angle. It generally differs in the two hemispheres

# Discrete Ordinate Method – Isotropic Scattering

- The solution of the isotropic scattering problem involves the following integral over angle

$$\int_{-1}^1 du I(\tau, u) = \int_0^1 d\mu I^+(\tau, u) + \int_0^1 d\mu I^-(\tau, u)$$

- In the two stream method we replaced the integration over  $\mu$  with the simple formula

$$\int_{-1}^1 du I = I^+(\tau) + I^-(\tau)$$



# Discrete Ordinate Method – Isotropic Scattering

- This is obviously a crude approximation. We can improve the accuracy by including more points in a numerical quadrature formula

$$\int_{-1}^1 du I(\tau, u) = \sum_{j=1}^m w'_j I(\tau, u_j)$$

- Where  $w'_j$  is a quadrature weight, and  $u_j$  is the discrete ordinate
- Most commonly used radiative transfer computer codes is DISORT – DIScreteOrdinateRadiativeTransfer