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# Approximate Methods of Calculating Transmission by Bands of Spectral Lines

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PREFACE

The topic for this paper was suggested by Chris Chaloner when he was a research student in the Department of Atmospheric Physics at Oxford University. He felt that the treatment of this subject in the standard textbook (Goody, 1964) was a little out of date and perhaps too difficult for the average research student. I promised to try to remedy the situation, but I did not find time to do so until I spent a sabbatical year at NCAR. I am grateful to the Advanced Study Program and the Upper Atmosphere Project for giving me this opportunity.

The paper is based on various lecture series that I have given in the past, and in particular on the lectures I gave to the NCAR Summer Colloquium in 1975. The topic covered is the calculation by approximate methods of the transmission or absorption of radiation by bands of spectral lines in the laboratory and the atmosphere. Calculation of transmission by exact methods is extremely time consuming and is still uncertain in some aspects. The main application is in radiative transfer in planetary atmospheres for such things as energy balance studies and remote sounding.

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ABSTRACT

This paper describes approximations that have been found useful in calculating the transmission of molecular gases in planetary atmospheres. This includes the use of band models and empirical models, but not the more complex "line by line" methods. A variety of techniques are described for dealing with the case of transmission through an atmospheric path which is inhomogeneous in the distribution of temperature, pressure and absorber concentration.

An extensive bibliography is included.



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## 1. INTRODUCTION

This paper is intended for research students in Atmospheric Physics as an introduction to a variety of practical methods whereby the transmission of atmospheric gases may be estimated or calculated. It is hoped that it will be of value in helping the student to choose a method appropriate to the problem in hand, so that he will neither use too simple a method and hence obtain inaccurate results, nor use too complex a method, and hence waste large quantities of both computer time and his own time. It is also hoped that the student will develop an insight and intuition for the properties of transmission functions which will enable him to know what to expect from his calculations.

We will assume that the basic physics is well understood. This paper concerns approximations, their accuracy and their limits of validity, as well as numerical methods in certain cases. The transmission,  $T(\nu)$ , of a band of spectral lines may be written as

$$T(\nu) = \exp \left( - \sum_{i,j} \int_{x_1}^{x_2} S_{ij}(x) f_{ij}(\nu - \nu_{ij}, x) \rho_j(x) dx \right) \quad (1.1)$$

where  $\nu$  is wavenumber,  $S_{ij}(x)$  is the strength of the  $i$ 'th line of the  $j$ 'th absorbing gas in the path from position  $x_1$  to  $x_2$ ,  $f_{ij}(\nu - \nu_{ij}, x)$  is the line shape factor,  $\nu_{ij}$  is the position of the line centre, and  $\rho_j(x)$  is the density of absorbing gas. Line strengths and positions may be calculated using quantum mechanics; this will not be discussed in detail here. Line strengths are temperature dependent in a well known way, depending on the population of the lower state. Line shapes depend on

the details of molecular collisions and motions, and are, therefore, temperature and pressure dependent. It has been assumed in Eq. (1.1) that when lines overlap their individual contributions to the optical depth simply add together. There are circumstances when this is not the case, and in the limit of very high pressures the phenomenon of "band narrowing" may be of significance.

Tabulations of positions and intensities of spectral lines of some atmospheric gases are available from a variety of sources. These should be used with caution, as some molecules are still quite poorly understood. Transmission calculation methods should always be validated against laboratory measurements when those are available.

## 2. SHAPES OF SPECTRAL LINES

There are two basic mechanisms that determine the shapes of lines of interest to the atmospheric physicist, namely Doppler broadening and collision broadening. Other mechanisms such as natural broadening and Stark broadening are usually insignificant.

Doppler broadening is a consequence of Doppler shift due to motions of the emitting molecule. If the component of its velocity towards the observer is  $u$ , and it is emitting at wavenumber  $\nu_0$  in its own frame of reference, then the Doppler shift in wavenumber is

$$(\nu - \nu_0) = \frac{u}{c} \nu_0 \quad (2.1)$$

If the distribution of velocities is Maxwellian:

$$P(u) \propto \exp(-mu^2/2kT) \quad (2.2)$$

where  $m$  is the molecular mass, then the line shape is proportional to the distribution of Doppler shifts:

$$\begin{aligned} f_D(\nu - \nu_0) &\propto \exp(-mc^2(\nu - \nu_0)^2 / 2kT \nu_0^2) \\ &= \frac{1}{\alpha_D \sqrt{\pi}} \exp(-(\nu - \nu_0)^2 / \alpha_D^2) \end{aligned} \quad (2.3)$$

where

$$\alpha_D = v_0 \sqrt{\frac{2kT}{mc^2}} = 4.301 \times 10^{-7} v_0 \sqrt{\frac{T}{M}},$$

M is molecular weight, and T is in degrees K. The factor  $\alpha_D \sqrt{\pi}$  is required to ensure that  $\int f_D(v) dv = 1$ . The Doppler line shape factor is shown in Fig. 1. The quantity  $\alpha_D$  is called the Doppler width of the line. The same symbol is sometimes used for a slightly different quantity, the half width at half height, which is smaller by a factor of  $\sqrt{\log 2}$ .

This derivation assumes that the molecule does not change its velocity by collision while it is emitting. If it does then the mean velocity and therefore the mean Doppler shift will be smaller and the line will be narrower. However, the phenomenon of collision narrowing is of little significance for most atmospheric gases (Rodgers, 1976) because it is masked by collision broadening. When molecules collide, not only are their velocities changed, but their internal energy levels are disturbed, and the frequency of the emitted radiation is changed. The theory of line broadening according to Quantum Mechanics is extremely complex, as it involves the details of interactions between molecules averaged over all possible collision trajectories, and averaged over all possible states of both colliding molecules. The simple classical theory due to Lorentz (1906) and Michelson assumes that the phase of the wave being emitted is randomized on collision, and results in the Lorentz line shape

$$f_L(v) = \frac{\alpha_L / \pi}{(v - v_0)^2 + \alpha_L^2} \quad (2.4)$$

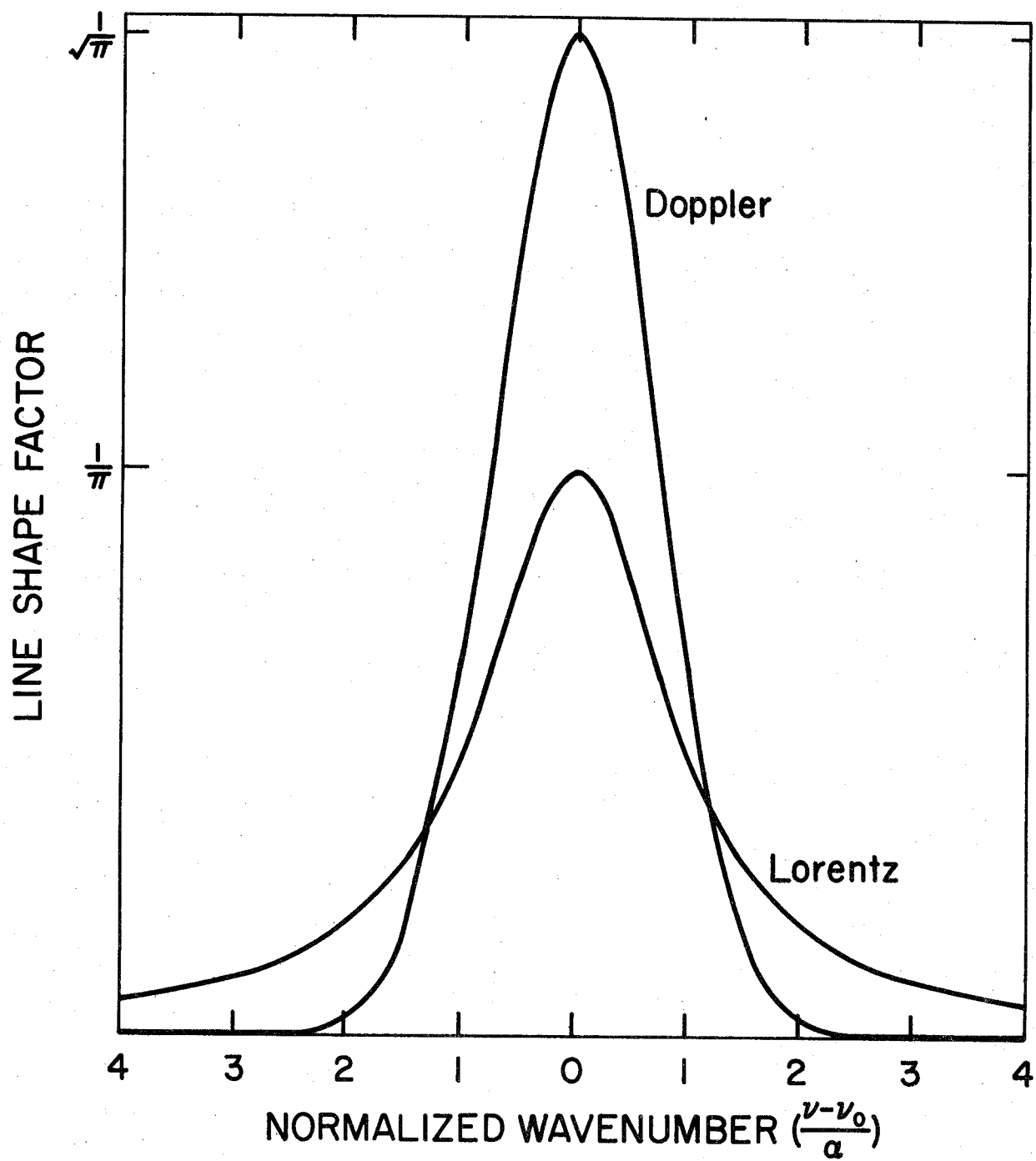


Fig. 1 Doppler and Lorentz line shapes.

where  $\alpha_L = 1/2\pi c\tau$ , and  $\tau$  is the mean time between collisions. The Lorentz line shape is shown in Fig. 1 in comparison with the Doppler shape. A semiclassical theory due to Lindholm (1946) and Foley (1946) assumes that there is a phase shift in the emitted wave which depends on the "impact parameter," or distance of closest approach. In this case the line shape is Lorentzian but shifted:

$$f_L(\nu) = \frac{\alpha/\pi}{(\nu-\nu_0-\delta)^2 + \alpha^2} \quad (2.5)$$

where  $\alpha$  and  $\delta$  depend on the phase shift function. For reasonable phase shifts,  $|\delta/\alpha| \lesssim 0.5$ .

The simplest quantum mechanical theory is that of Anderson (1949). It appears to be adequate for  $\text{CO}_2$ , and probably for  $\text{H}_2\text{O}$ , so that the more modern theories (e.g., Baranger, 1962; Greim, 1964) do not add a great deal. Most theories lead to the same algebraic form as the Lindholm theory, but with different means of evaluating  $\alpha$  and  $\delta$  from the physics of the interaction.

When both Doppler and collision broadening are significant, the detailed line shape depends on the nature of the collisions. The limits of "hard" and "soft" collisions have been treated by Rautian and Sobelman (1967) and by Galatry (1961). However, for most atmospheric gases the Voigt line shape is entirely adequate. In this approximation the processes that determine Doppler broadening and collision broadening are assumed to be uncorrelated, and collision narrowing is ignored. The line shape is then found by averaging Doppler shifted Lorentz lines weighted with the distribution of velocities, so that it is a convolution

of the Doppler and Lorentz shapes:

$$f_v(v') \propto \int_{-\infty}^{\infty} \frac{e^{-v^2/\alpha_D^2} dv}{(v-v'+v_0)^2 + \alpha_L^2} \quad (2.6)$$

Numerical methods for evaluating this function have been discussed by several authors, for example, Armstrong (1967), Harstad (1972), Kielkopf (1973), Whiting (1968).



### 3. HOMOGENEOUS PATHS

The most important special case of Eq. (1.1) is when pressure and temperature do not vary along the optical path because this applies to laboratory paths, and may be used as an approximation to the atmosphere in certain situations (Section 4.3). In this case the integral with respect to  $x$  is trivial and transmission can be written

$$T(\nu) = \exp\left(- \sum_{ij} S_{ij} f_{ij}(\nu) m_j\right), \quad (3.1)$$

where  $m_j = \rho_i(x_2 - x_1)$  is the amount of absorber  $j$  per unit area, and  $S_{ij}$  and  $f_{ij}$  are evaluated at the temperature and pressure of the absorbing path.

#### 3.1 INDEPENDENT LINES

The simplest situation that we can consider is the case of a single spectral line. The results of this section can be used as a transmission model in the case where spectral lines do not overlap significantly.

We define equivalent width<sup>1</sup>  $W$  of a spectral line as the spectrally integrated absorption:

$$W = \int_{-\infty}^{\infty} \left\{ 1 - T(\nu) \right\} d\nu = \int_{-\infty}^{\infty} \left\{ 1 - \exp(-Sf(\nu)m) \right\} d\nu. \quad (3.2)$$

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<sup>1</sup>The term "equivalent width" derives from the astrophysical literature. It is simply the width of a square sided line that would have the same integrated absorption as the line in question.

We have dropped suffices  $i$  and  $j$  for clarity. The infinite range of integration is purely arbitrary, as all of the significant absorption takes place within a small region near the line centre.

In the limits of "strong" absorption and "weak" absorption, most line shapes have simple expressions for their equivalent widths. The limits are determined by the asymptotic behavior as the optical depth at the line centre,  $Sf(\nu_0)m$ , tends to zero or infinity. The weak limit is independent of the line shape because as  $Sf(\nu_0)m \rightarrow 0$ ,

$$W = \int \left\{ 1 - e^{-Sf m} \right\} d\nu \rightarrow \int Sf(\nu) m d\nu = Sm \quad (3.3)$$

3.1.1 The equivalent width of a Lorentz line is

$$W_L = \int_{-\infty}^{\infty} \left\{ 1 - \exp \left( - \frac{Sm \alpha_L / \pi}{\nu^2 + \alpha_L^2} \right) \right\} d\nu = 2\pi\alpha_L L \left( \frac{Sm}{2\pi\alpha_L} \right) \quad (3.4)$$

We have moved the zero of the frequency scale to the line centre for convenience.

$L(y)$  is known as the Ladenburg-Reiche function, and can be expressed explicitly in terms of Bessel functions (Ladenburg and Reiche, 1911):

$$L(y) = ye^{-y} (I_0(y) + I_1(y)) \quad (3.5)$$

The strong limit is determined by  $Sm/\pi\alpha \rightarrow \infty$ , and may be obtained from the limit of the Bessel functions  $I_0$  and  $I_1$  as  $y \rightarrow \infty$ . However, it is physically more meaningful to obtain it from Eq. (3.4) as follows.

When  $Sm/\pi\alpha \rightarrow \infty$ , the line is black in the centre, and ignoring the  $\alpha_L^2$

will make no difference to Eq. (2) near the line centre. Far from the line centre  $v^2 \gg \alpha_L^2$ , and we can still ignore the  $\alpha_L^2$ . Therefore

$$\begin{aligned}
 W_L &\rightarrow \int_{-\infty}^{\infty} 1 - \exp\left(-\frac{Sm\alpha_L/\pi}{v^2}\right) dv \\
 &= \sqrt{Sm\alpha_L/\pi} \int_{-\infty}^{\infty} \left\{1 - \exp\left(-\frac{1}{x^2}\right)\right\} dx \\
 &= 2 \sqrt{Sm\alpha_L}
 \end{aligned} \tag{3.6}$$

A useful simple approximation to the equivalent width of a single Lorentz line is

$$W_L \simeq Sm (1 + Sm/4\alpha_L)^{-1/2} \tag{3.7}$$

This has the same strong and weak limits, and deviates by less than 8% for all values of the parameters. Another simple approximation due to Goldman (1968) is

$$W_L \simeq Sm \left(1 + \{Sm/4\alpha_L\}^{5/4}\right)^{-2/5} \tag{3.8}$$

which has a smaller maximum error of about 1%, but is a little more complicated. Figure 2 shows how the error in these approximations varies with  $Sm/\pi\alpha$ . A numerical approximation of higher accuracy can be found in Rodgers and Williams (1974).

3.1.2 The equivalent width of a Doppler line is given by

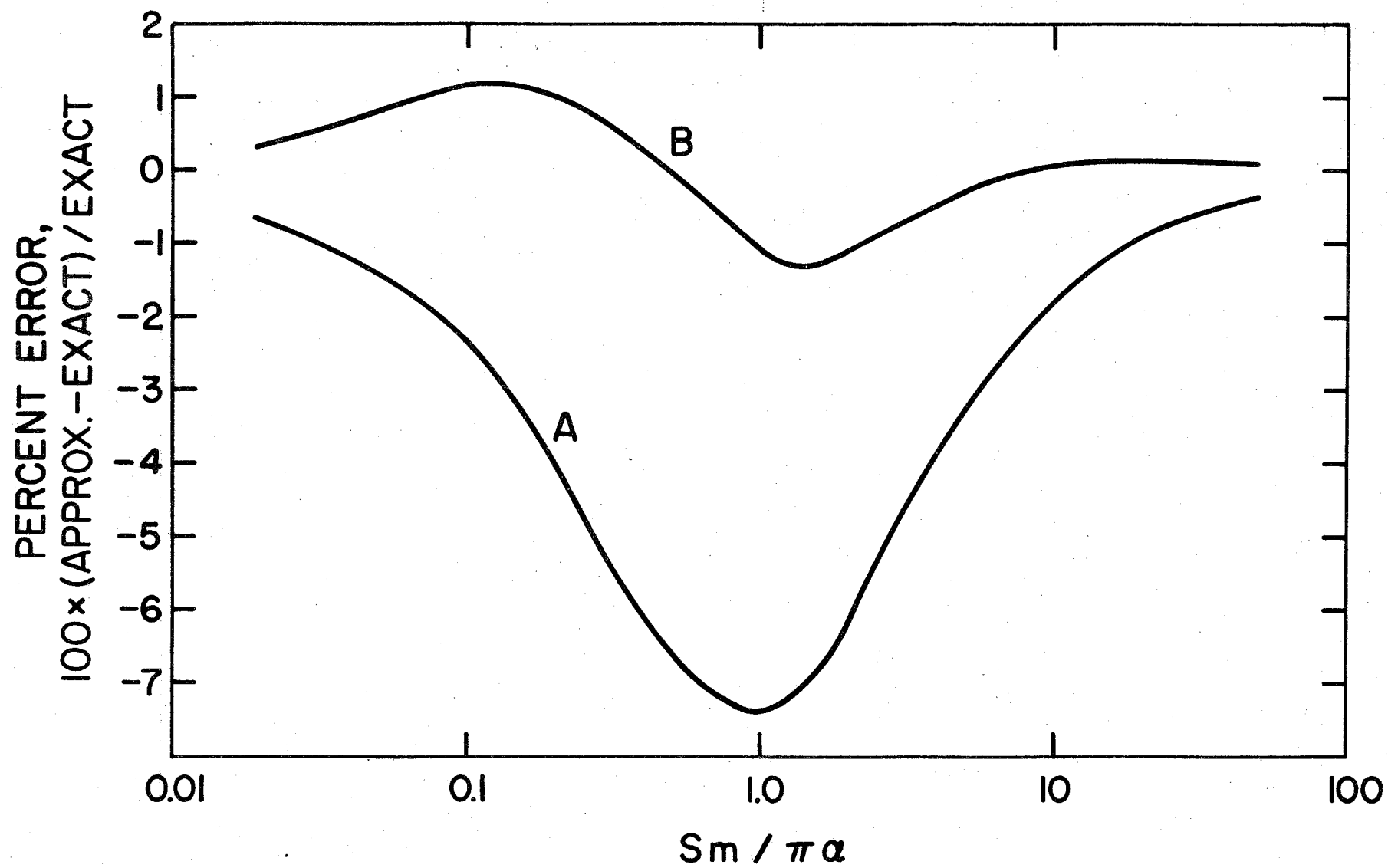


Fig. 2 Errors in simple approximations to the Ladenburg-Reiche function.  
 A - Eq. (3.7). B - Eq. (3.8).

$$W_D = \int_{-\infty}^{\infty} 1 - \exp \left( - \frac{Sm}{\alpha_D \sqrt{\pi}} e^{-v^2/\alpha_D^2} \right) dv \quad (3.9)$$

This expression cannot be integrated explicitly in terms of standard functions, but it can be written in terms of a function of a single variable

$$W_D = \alpha_D F_D \left( \frac{Sm}{\alpha_D \sqrt{\pi}} \right) \text{ where } F_D(y) = \int_{-\infty}^{\infty} 1 - \exp(-ye^{-x^2}) dx \quad (3.10)$$

The strong limit of  $W_D$  as  $Sm/\alpha_D \sqrt{\pi} \rightarrow \infty$  is of the form

$$W_D = 2 \alpha_D [\log (Sm/\alpha_D \sqrt{\pi})]^{1/2}. \quad (3.11)$$

A numerical approximation for  $F_D(y)$  can be found in Rodgers and Williams (1974).

3.1.3 The equivalent width of a Voigt line requires a function of two variables, e.g.,  $\alpha_L/\alpha_D$  and  $Sm/\alpha_D$ . It cannot be written in terms of elementary functions, and to the author's knowledge no efficient numerical approximations exist. However, it has been tabulated by several authors, and a contour plot is given in Fig. 3. It may be approximated by

$$W_V^2 = W_L^2 + W_D^2 - (W_L W_D / Sm)^2 \quad (3.12)$$

with a maximum error of about 8% (Rodgers and Williams, 1974).

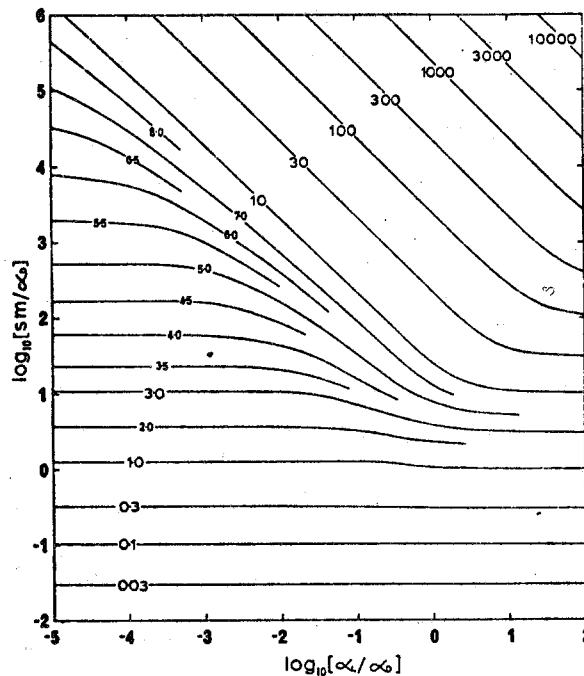


Fig. 3 Contours of equivalent width of a Voigt line divided by  $\alpha_D$ , the Doppler width (Rodgers and Williams, 1974).

#### 3.1.4 Accuracy of Single Line Models

A single line model may be used to approximate transmission when lines do not overlap appreciably. In this case the transmission of a spectral interval  $\Delta\nu$  can be written

$$T = 1 - (\sum W_i / \Delta\nu) \quad (3.13)$$

where the sum is over all lines in the interval  $\Delta\nu$ . The errors involved in this are best assessed relative to a more accurate model, and if we use a random model (see 3.2.2.1) we can show that the absolute error in  $T$  will be of order  $(\sum W_i / \Delta\nu)^2$ , or the relative error in  $1-T$  will be order  $1-T$ .

### 3.2 OVERLAPPING LINES

We may distinguish two kinds of overlapping lines; for the lack of better words we will call them

(a) strongly overlapping  $\alpha > \delta$

(b) weakly overlapping  $W > \delta$

where  $\delta$  is the spacing between the lines and  $W$  is the equivalent width of any one line. The case of weakly overlapping lines simply implies that single line models cannot be used; the rest of section 3.2 concerns this case. The case of strongly overlapping lines may be much more difficult to treat correctly, because it is possible that the several resonant frequencies may mix at the quantum mechanical level, with the consequence that the lines become shifted and may change in strength in a way which depends on pressure. This is the phenomenon of "band narrowing" referred to earlier. At high pressures (~100 atm) it is possible for all the lines in a single rotation-vibration band to merge into one strong line located near the band centre. This overlap effect will be ignored in this paper.

#### 3.2.1 Regular model

The first case of overlapping lines to be considered was the "Elsasser Model," which uses an array of equally spaced identical Lorentz lines, as in Fig. 4 (Elsasser, 1938).

It can be shown that the line contour is given by

$$f_E(\nu) = \frac{1}{8} \frac{\sinh(2\pi\alpha/\delta)}{\cosh(2\pi\alpha/\delta) - \cos(2\pi\nu/\delta)} \quad (3.14)$$

The corresponding transmission is

$$T_E = \frac{1}{\delta} \int_{\delta} \exp(-S f_E(v)m) dv, \quad (3.15)$$

and cannot be integrated in terms of elementary functions. However, it is tabulated as a function of  $u = Sm/2\pi\alpha$  and  $y = \alpha/\delta$  in several places, for example Goody (1964). There are several limits which yield simple expressions. Let  $W_E$  be the equivalent width in an interval of width  $\delta$ .

1. Independent Lines  $W_E = W_L$ , Ladenberg-Reiche function

This is valid for the case  $W_E \ll \delta$ , which also includes overlapping weak lines.

2. Strong Lines  $\frac{Sm}{\pi\alpha} \gg 1$   $W_E/\delta = \operatorname{erf} \left\{ \frac{1}{\delta} (\sqrt{Sm\pi\alpha}) \right\}.$
3. Weak Lines  $\frac{Sm}{\pi\alpha} \ll 1$   $W_E = Sm$  as usual.

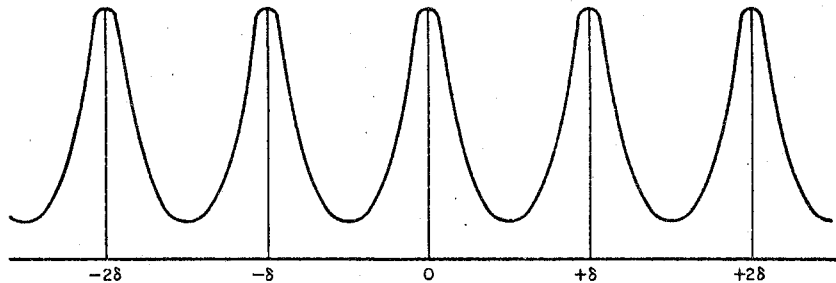


Fig. 4 Line shape for the Elsasser model (after Goody, 1964).



### 3.2.2 Random Models

The concept of a random band model is of considerable importance, and a glance at the spectrum of a gas such as water vapor (Fig. 5) will show the reader why such models were developed. The positions and intensities of the spectral lines appear to be quite random. Of course they are not, because they may be calculated in a non-random manner using quantum mechanics.

The basic concept of all random models is that the transmission of a spectral interval can be approximated by the transmission averaged over all rearrangements of line positions. This averaging over rearrangements leads to the very useful "multiplication property." We know that monochromatically we may multiply transmissions due to independent absorption mechanisms, but it is not correct in general to multiply transmissions which have been averaged over finite spectral intervals. However, if we make the randomness hypothesis, we may multiply spectrally averaged transmissions.

The multiplication property. Consider a spectral interval  $\Delta\nu$  having transmission  $T_0(\nu)$ , and therefore an average transmission given by

$$\bar{T}_0 = \frac{1}{\Delta\nu} \int_{\Delta\nu} T_0(\nu) d\nu. \quad (3.16)$$

If we introduce a spectral line at position  $\nu'$  having by itself a transmission  $T_1(\nu-\nu')$ , such that its equivalent width is  $\ll \Delta\nu$ , then the frequency averaged transmission will become

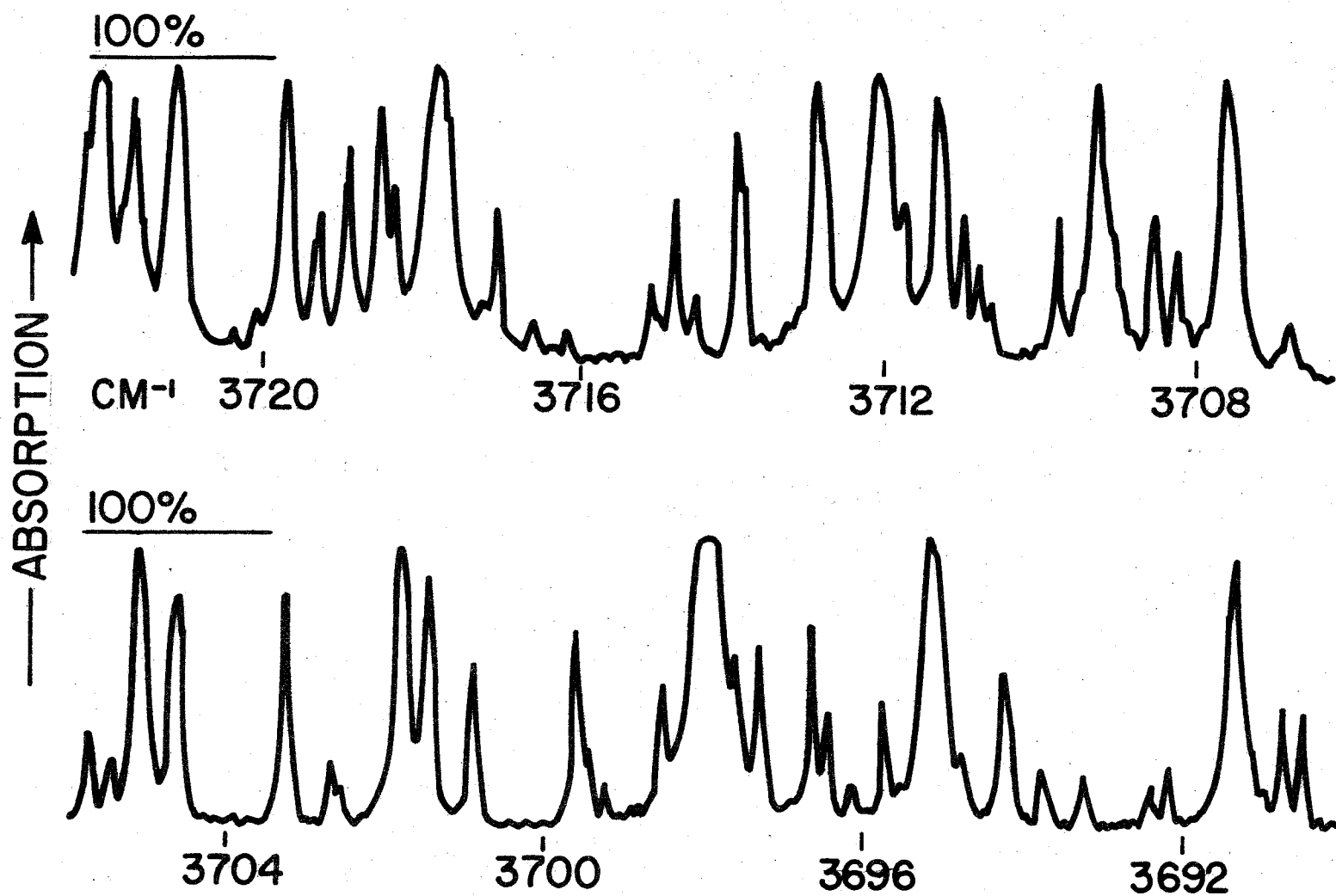


Fig. 5 A laboratory spectrum of part of the 2.7 $\mu$  water vapor band (Fraley, Rao and Jones, 1969).

$$\frac{1}{\Delta\nu} \int_{\Delta\nu} T_0(\nu) T_1(\nu-\nu') d\nu \quad (3.17)$$

We now average this over all possible positions of the new line, and we obtain for the average transmission

$$\bar{T} = \frac{1}{\Delta\nu} \int_{\Delta\nu} d\nu' \left\{ \frac{1}{\Delta\nu} \int_{\Delta\nu} T_0(\nu) T_1(\nu-\nu') d\nu \right\} \quad (3.18)$$

If we perform the  $\nu'$  integral first we easily obtain

$$\boxed{\bar{T} = \bar{T}_0 \bar{T}_1} \quad (3.19)$$

where  $\bar{T}_1$  is the frequency averaged transmission of the new line. Thus we may say loosely that if lines are placed randomly then we may multiply frequency averaged transmissions.

### 3.2.2.1 The general random model

A single line whose equivalent width is  $W_i$  has a transmission in spectral interval  $\Delta\nu$  given by

$$T_i = 1 - W_i/\Delta\nu \simeq \exp(-W_i/\Delta\nu) \quad (3.20)$$

provided that  $W_i \ll \Delta\nu$ . Using the multiplication property, the transmission of  $N$  lines in the interval  $\Delta\nu$ , averaged over all rearrangements of position is

$$T = \prod_{i=1}^N \exp(-W_i/\Delta\nu) = \exp(-\sum_{i=1}^N W_i/\Delta\nu) \quad (3.21)$$

Thus the general random model may be written

$$T = \exp(-W/\Delta\nu) \quad (3.22)$$

where  $W$  is the total equivalent width in the interval  $\Delta\nu$ . This derivation requires that  $W_i \ll \Delta\nu$ . However it is possible to derive the same expression for  $T$  in the more general circumstance, provided that surrounding spectral intervals are statistically similar to the one under consideration. Qualitatively, absorption outside  $\Delta\nu$  due to the wings of lines inside  $\Delta\nu$  will be compensated for by absorption inside  $\Delta\nu$  due to wings of lines outside  $\Delta\nu$ .

### 3.2.2.2 Simplified random models

The general random model requires a sum over all spectral lines in a particular interval, which may be a formidable task. A further step of simplification is to make an assumption about the distribution of line strengths, namely that the number of lines in the interval with strengths between  $S$  and  $S+dS$  is some function  $N(S)dS$ . The distribution function should be chosen to be reasonably representative of the actual distribution of line strengths, but with some weight given to algebraic convenience. Three distributions have been found particularly useful, due to Goody (1952), Godson (1954) and Malkmus (1967).

The Goody Model.

$$N(S) = \frac{N_0}{k} e^{-S/k} \quad (3.23)$$

This distribution has a total of  $N_0$  lines with mean strength  $k$ , as may easily be verified. The total equivalent width  $W$  is given by

$$W = N_0 \bar{W} = \int_0^\infty N(S) W(S) dS = \int_0^\infty \frac{N_0}{k} e^{-S/k} \int_{-\infty}^\infty \left[ 1 - e^{-Sf(v)m} \right] dv dS \quad (3.24)$$

We may do the  $S$  integral first for any line shape  $f(v)$ , obtaining

$$W = N_0 \int_{-\infty}^\infty \frac{k m f(v)}{1 + k m f(v)} dv = N_0 \int_{-\infty}^\infty \frac{\tau(v)}{1 + \tau(v)} dv \quad (3.25)$$

where  $\tau(v)$  is the optical depth for a line of strength  $k$ . If we use a Lorentz line shape we obtain

$$W = \frac{N_0 k m}{\sqrt{1 + k m / \pi \alpha}} \quad (3.26)$$

The transmission for the Goody random model is usually written

$$T = \exp \left( \frac{-k m / \delta}{\sqrt{1 + k m / \pi \alpha}} \right) \quad (3.27)$$

where  $\delta = \Delta v / N_0$  is the mean line spacing.

The Godson model.

$$\begin{aligned}
 N(S) &= N_0/S & S < k \\
 &= 0 & S > k
 \end{aligned}
 \tag{3.28}$$

This distribution has an infinite number of lines, but  $N_0$  lines in each factor of  $e$  in strength. For the general line shape there is no simple expression for  $W$ . For the Lorentz line shape  $W$  can be written in terms of Bessel functions:

$$W = 2\pi\alpha N_0 \left\{ e^{-y} I_0(y) + 2 y e^{-y} [I_0(y) + I_1(y)] - 1 \right\} \tag{3.29}$$

where

$$y = \frac{km}{2\pi\alpha}$$

Malkmus model.

$$N(S) = \frac{N_0}{S} e^{-S/k} \tag{3.30}$$

This is the result of averaging Goody distributions according to the Godson distribution, and is more representative of reality than either.

The total equivalent width for a general line shape may be written

$$W = \int_0^\infty \frac{N_0}{S} e^{-S/k} \int_{-\infty}^\infty [1 - e^{-Sf(v)m}] dv dS \tag{3.31}$$

If we perform the S integral first we obtain

$$W = N_0 \int_{-\infty}^{\infty} \log (1 + \tau(v)) dv \quad \text{where } \tau(v) = kmf(v) \quad (3.32)$$

The actual derivation of this expression is left as a challenge to the reader. Integration by parts gives

$$W = N_0 \int_{-\infty}^{\infty} \frac{v}{1+\tau(v)} \frac{d\tau(v)}{dv} dv \quad (3.33)$$

In the case of a Lorentz line the integral can be performed to yield

$$\begin{aligned} W &= 2\pi\alpha N_0 \left\{ (1 + km/\pi\alpha)^{1/2} - 1 \right\} \\ &= 2N_0 km / \left\{ 1 + (1 + km/\pi\alpha)^{1/2} \right\} \end{aligned} \quad (3.34)$$

cf 3.26

### 3.2.2.3 Strong and weak limits and parameter fitting

The strong and weak limits of the equivalent width may be found either by putting  $km/\pi\alpha \rightarrow 0$  or  $\infty$  in the expressions for W or by putting the strong and weak limits for the single line W(S) in the equation for W:

$$W = \int_0^{\infty} N(S) W(S) dS \quad (3.35)$$

The limits are as follows:

| <u>Model</u> | <u>Weak</u>    | <u>Strong</u>                    |
|--------------|----------------|----------------------------------|
| General      | $\sum_i S_i m$ | $2 \sum_i \sqrt{S_i \alpha_i m}$ |
| Goody        | $N_0 km$       | $N_0 \sqrt{k\pi\alpha m}$        |
| Godson       | $N_0 km$       | $N_0 \sqrt{km\alpha}$            |
| Malkmus      | $N_0 km$       | $2 N_0 \sqrt{k\pi\alpha m}$      |

The best way of fitting line data to the simplified random models is not by attempting to match the model distributions of line strengths with the actual distributions (Fig. 6), but rather by matching the weak and strong limits with the general random model. For example, for the Malkmus model we would put

$$N_0 k = \sum_i S_i, \quad N_0 \sqrt{k\pi\alpha} = \sum_i \sqrt{S_i \alpha_i} \quad (3.36)$$

Note that although we have defined three parameters,  $N_0$ ,  $k$  and  $\alpha$ , we only have two equations. However, only two combinations of parameters are required in the expressions for transmission, so there are sufficient equations to determine them. If we define  $w$  (weak) and  $s$  (strong) by

$$w = \frac{1}{\Delta\nu} \sum_i S_i, \quad s = \frac{2}{\Delta\nu} \sum_i \sqrt{S_i \alpha_i} \quad (3.37)$$

then two of the models may be written:

$$\text{Goody} \quad T = \exp(-(w^{-2} + s^{-2})^{-1/2}) \quad (3.38)$$

$$\text{Malkmus} \quad T = \exp \left( -\frac{s^2}{2w} \left[ \left( 1 + \frac{4w^2}{s^2} \right)^{1/2} - 1 \right] \right) \quad (3.39)$$

and for the Godson model put  $\frac{2\pi\alpha N_0}{\Delta\nu} = \frac{2\pi s^2}{w}$  and  $y = 2\pi \frac{w^2}{s^2}$  in the Godson equation (3.29). The weak limit is valid when  $w \ll s$ , and the strong limit when  $w \gg s$ .



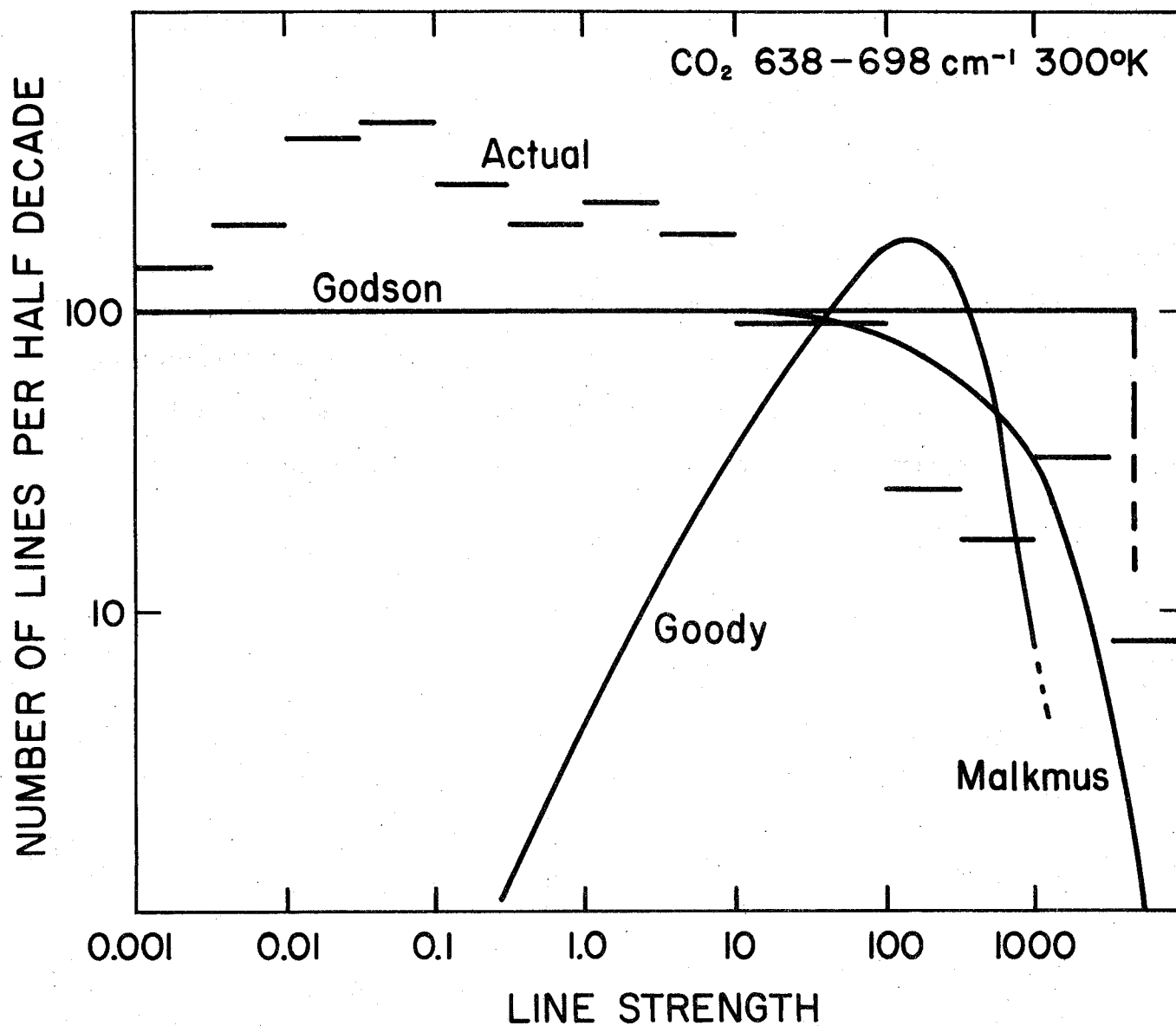


Fig. 6 Comparison of an actual distribution of line strengths with the three model distributions. The model distributions have not been fitted to the actual distribution.

### 3.2.3 Empirical Models

#### 3.2.3.1 Simple empirical models

A wide variety of empirical transmission models has been used for bands of lines. For example, the following is often used to represent the equivalent widths of complete bands measured in the laboratory:

$$\begin{aligned} W &= Au & W < W_0 \\ &= B + C \log u & W > W_0 \end{aligned} \quad (3.40)$$

where

$$u = mp^n$$

where A, B, C,  $W_0$  and n are empirical constants, m is absorber mass and p is pressure, corrected for self-broadening. Such fits are often found to be good almost within experimental error.

Goody and Belton (1967) have used a very similar form as a fit to a whole band of overlapping lines:

$$W = C \log \left( 1 + \frac{\sum W_i}{C} \right) \quad (3.41)$$

where C is an empirically adjusted constant, and  $\sum W_i$  is the sum of the individual equivalent widths. Yamamoto and Sasamori (1957) have pointed out that transmission is approximated by an expression of the form

$$T = F(\sum W_i) \quad (3.42)$$

for a wide range of band models, and have conjectured that this is a good empirical form to use in general, with the functional form  $F$  depending on the distribution of line positions and intensities. We may note that it is appropriate for all statistical models, and for some of the limits of the Elsasser model.

It should be pointed out that the strong limit of the random model is a useful general purpose first order approximation to the transmission of most atmospheric gases:

$$T = \exp(-\sqrt{\ell u}) \quad (3.43)$$

where  $u = mp$  or  $\int pdm$  is a scaled absorber amount and  $\ell$  is a generalized absorption coefficient. It is usually accurate to better than 10% when lines are strong.

### 3.2.3.2 Complex empirical models

The simple empirical models of the previous section may be regarded as simplifications of band models. It is also possible to make empirical generalizations of band models to try to fit laboratory data better.

From equation (3.38), we may rewrite the Goody random model transmission  $T$  in the form

$$(-\log T)^{-2} = (\log T_w)^{-2} + (\log T_s)^{-2} \quad (3.44)$$

where  $T_w$  is the transmission weak limit and  $T_s$  is the strong limit.

Zachor (1968a) generalizes this equation to

$$(-\log T)^{-2} = (\log T_w)^{-2} + (\log T_s)^{-2} + M(\log T_w \log T_s)^{-1}. \quad (3.45)$$

The extra term does not affect the weak and strong limits of the model, but adjustment of the empirical constant  $M$  allows the intermediate region to be fitted more closely. As a further generalization he does not use the strong limit of the Goody model for  $T_s$ , but a more general model of King (1964), for which

$$T_s = 1 - P(n, \{n\Gamma(u)(km\alpha)^{1/2}\}^{1/n}) \quad (3.46)$$

where  $\Gamma$  is the gamma function,  $P$  is the incomplete gamma function, and  $n$  is an adjustable constant. For  $n = 1$ , this gives the strong limit of the random model, and for  $n = 0.5$  it gives the strong limit of the Elsasser model. There are four parameters in Zachor's model which must be determined by least squares fitting to laboratory data. They are  $M$ ,  $n$ ,  $k$  and  $K$ , the constant for the weak limit  $K_m$ . Gibson and Pierluissi (1971) have further generalized the model by including another parameter multiplying the term  $(\log T_s)^{-2}$ . Applications of these models (Pierluissi, 1973; Zachor, 1968b) show that they are capable of fitting data to high accuracy.

A similar approach has been developed by Smith (1969), who has generalized the simple empirical model

$$T = \exp(-K_m^a p^b \theta^c) \quad (3.47)$$

to the form

$$\begin{aligned} \text{Log}(-\log T) &= \log K + a \cdot \log m + b \cdot \log p + c \cdot \log \theta \\ &+ \text{higher order terms,} \end{aligned} \quad (3.48)$$

where  $\theta$  is temperatures. With sufficient terms this model is also capable of high accuracy.

All empirical models should be used with caution. Unless they are soundly based in theory they are only applicable to the range of parameters for which they are fitted, and they cannot be used to extrapolate beyond the original data. This is of course true of any band model, but empirical models are likely to be the worst offenders.

#### 3.2.4 Sum of Exponentials and the Inverse Transmission Function

When the absorber is at a known constant pressure and temperature we may write its spectrally averaged transmission as

$$T(m) = \frac{1}{\Delta \nu} \int d\nu e^{-k(\nu)m} \quad (3.49)$$

where  $k(\nu)$  is the absorption coefficient and  $m$  is the absorber amount. This immediately suggests that we might use a sum of exponentials as a transmission model:

$$T(m) \approx \sum_i a_i e^{-k_i m} \quad (3.50)$$

This form is advantageous when doing calculations which involve scattering as well as absorption because we retain the multiplication property term by term, and this is almost essential for some types of scattering methods.

The form may be used in a more general way, for example when line absorption is in the strong region it depends on  $u = mp$  only, so we may approximate transmission by

$$T(u) \approx \sum_i a_i e^{-k_i u} \quad (3.51)$$

which may be used over paths where the pressure varies.

Determining the coefficients  $a_i$  and  $k_i$  is closely related to performing an inverse Laplace transform, and may be done in a variety of ways. Probably the simplest is to choose a set of  $k_i$  arbitrarily, and then find the  $a_i$  by least squares fitting. Wiscombe and Evans (1976) have developed a general method of fitting both  $a_i$  and  $k_i$  to give a fit with the smallest number of terms for a given accuracy.<sup>2</sup>

We may generalize these ideas and define the "inverse transmission function"  $f(k)$  such that its Laplace transform is the transmission:

$$T(m) = \int_0^{\infty} f(k) e^{-km} dk \quad (3.52)$$

Thus  $f(k)dk$  corresponds to  $a_i$  in the discrete version. Many inverse transmission functions may be found simply by consulting a table of inverse Laplace transforms. A discussion of this subject is given by Domoto (1974).

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<sup>2</sup>W. Wiscombe and J. Evans: An exponential sum fitting of transmission functions. Submitted to J. Atmos. Sci.

### 3.2.5 Models for Complete Bands

The models described so far are applicable to sections of molecular vibration-rotation bands containing lines which are distributed uniformly in some sense. They are known as "band models" although they do not describe absorption by complete bands. Models which do describe complete bands are often described by somewhat misleading names such as "band correlation functions," although they have little to do with correlation in the statistical sense.

Edwards and Menard (1964) have constructed a set of models based on the Goody random model in which the band parameters vary with frequency in each of three known ways, simulating the behavior of a rigid rotator, a nonrigid rotator, and the third having a mean line strength decreasing with frequency exponentially:

$$k(\nu) = k(\nu_0) \exp((\nu_0 - \nu)/A), \quad (3.53)$$

so that the integrated absorption of the whole band may be written

$$W = \int_{\nu_0}^{\infty} d\nu \left\{ 1 - \exp \left( \frac{-k(\nu)m/\delta}{\sqrt{1 + k(\nu)m/\pi\alpha}} \right) \right\} d\nu \quad (3.54)$$

A complete solution is not given to this integral, but three limits are:

|                    |                  |
|--------------------|------------------|
| linear region      | $W = am$         |
| square root region | $W = b\sqrt{mp}$ |

$$\text{logarithmic region} \quad \left\{ \begin{array}{ll} W = c \{\log(dmp)\}^{1/2} & \text{rigid rotator} \\ W = c \log(dm^2 p) & \text{nonrigid rotator} \\ W = c \log(dmp) & \text{exponential} \end{array} \right.$$

where  $a$ ,  $b$ ,  $c$  and  $d$  are constants which may be related to the band structure, or may be found by fitting experimental data. The first two limits correspond to the weak and strong limits of a single line, whilst the logarithmic limit occurs when the center of the band is black.

Edwards and Menard give a means of joining the limits together in four separate regions of the parameters which agrees reasonably well with the measured integrated absorption of some real bands. Cess and Tiwari (1972) have found a single function which satisfies all the limits and joins them in a reasonable manner for the case of the exponential distribution:

$$W = 2 \log \left\{ 1 + am / [2 + (am + bm/p)^{1/2}] \right\} \quad (3.55)$$

where  $a$  and  $b$  are parameters to be fitted.

Cess (1973) has developed a similar theory for the case of Doppler broadened lines.



#### 4. INHOMOGENEOUS PATHS

We must now return to deal with the situation in which pressure and temperature may vary along the optical path. The consequence is that line shape varies along the path and an extra integral is required. In general this means that there is an even smaller number of cases in which transmission can be expressed in terms of standard functions. We must either resort to numerical methods, or introduce further approximations, or both.

##### 4.1 CONSTANT MIXING RATIO

There is one case in which the algebra can be done, at least in part, namely the case of a constant temperature atmosphere with an absorbing gas of constant mixing ratio and pure Lorentz lines. In this case the optical depth  $\tau(\nu)$  can be written for one line as

$$\tau(\nu) = \int_{p_1}^{p_2} \frac{S}{\pi} \frac{\alpha_0 p}{\nu^2 + \alpha_0^2 p^2} dm. \quad (4.1)$$

For a constant mixing ratio we can put  $dm = adp$  where  $a$  is the total absorber mass between  $p = 0$  and  $p = 1$ . Thus

$$\begin{aligned} \tau(\nu) &= \frac{Sa}{\pi\alpha_0} \int \frac{p}{(\nu/\alpha_0)^2 + p^2} dp \\ &= \eta \left[ \log \left( \left( \frac{\nu}{\alpha_0} \right)^2 + p^2 \right) \right]_{p_1}^{p_2} \quad \eta = Sa/2\pi\alpha_0. \end{aligned} \quad (4.2)$$

And monochromatic transmission is

$$T(\nu) = e^{-\tau} = \left( \frac{\nu^2 + \alpha_1^2}{\nu^2 + \alpha_2^2} \right)^\eta \quad \alpha_1 = \alpha_0 p_1 \quad (4.3)$$

This is as far as we can go with this particular case, unless  $\eta$  happens to be an integer.

#### 4.2 SCALING APPROXIMATION

It has been found (see Section 3.2.3) that the integrated absorption of complete molecular bands can be represented approximately as a function of a scaled absorber amount:

$$u = mp^n \quad (4.4)$$

where  $n$  usually lies between about 0.5 and 1. This led to the use of a natural but theoretically unjustifiable extension to inhomogeneous paths:

$$u = \int p^n dm \quad (4.5)$$

In the time before electronic computers, such an approximation was necessary in order to be able to compute fluxes of thermal radiation by means of "radiation charts." (See e.g. Goody, 1964, for more on this subject.) Any justification of this approximation must be entirely empirical, and is likely to depend on the specific application. All that can be said theoretically is that the scaling approximation lies

"between" the weak and strong limits of  $\int dm$  and  $\int pdm$ . Unfortunately, many methods that treat scattering and molecular absorption require that the absorption be expressed as a function of one variable such as a scaled absorber amount.

#### 4.3 THE CURTIS-GODSON APPROXIMATION

The aim of the Curtis-Godson Approximation (CG) is to find a homogeneous path for which the transmission is approximately the same as for the given inhomogeneous path (Curtis, 1952; Godson, 1954). For the moment we will consider a constant temperature but varying pressure along the path. The corresponding homogeneous path will then be determined if we specify its pressure  $\bar{p}$  and absorber amount,  $\bar{m}$ . The criterion used to determine equivalence is that the equivalent widths of strong Lorentz lines and weak lines must be the same for the two paths. The weak line correspondence requires

$$\int S dm = S \bar{m} \quad (4.6)$$

and the strong Lorentz line limit requires

$$\int S \alpha dm = S \bar{\alpha} \bar{m}, \quad \text{where } \bar{\alpha} = \alpha_0 \bar{p} \quad (4.7)$$

We can eliminate  $S$  and  $\alpha_0$  to give the simplest form of the CG approximation.

$$\boxed{\bar{m} = \int dm, \quad \bar{m} \bar{p} = \int p dm} \quad (4.8)$$

i.e., the mass is the same in both paths, and the pressure required in the mass weighted mean pressure.

The accuracy of this approximation depends of course on the distribution of absorber amount with pressure. To give an order of magnitude we may calculate the equivalent width for the case discussed in section 4.1 and for the CG approximation to it. The percentage error in the CG approximation for  $p_1 = 0$ ,  $p_2 = 1$  is shown in Fig. 7 as a function of  $\eta$ . As we would expect the error is maximum when  $\eta \sim 0.5$ , which is in the intermediate region between strong and weak lines.

#### 4.4 FOUR PARAMETER APPROXIMATION

The next stage after CG is the four parameter approximation, in which we find two-homogeneous paths in series which approximate the given inhomogeneous path. To do this we match the first four moments of the mass distribution with respect to pressure:

$$\begin{aligned}
 m_1 + m_2 &= \int dm = u_0 \\
 m_1 p_1 + m_2 p_2 &= \int p dm = u_1 \\
 m_1 p_1^2 + m_2 p_2^2 &= \int p^2 dm = u_2 \\
 m_1 p_1^3 + m_2 p_2^3 &= \int p^3 dm = u_3
 \end{aligned}
 \tag{4.9}$$

The first two equations are the same as the CG approximation, and are required for the same reason, to match the weak and strong limits. The fourth equation follows from matching the second term in an expansion of the strong limit. An expansion of the weak limit gives a second term which is quite intractable, as it involves a double integral, so we use

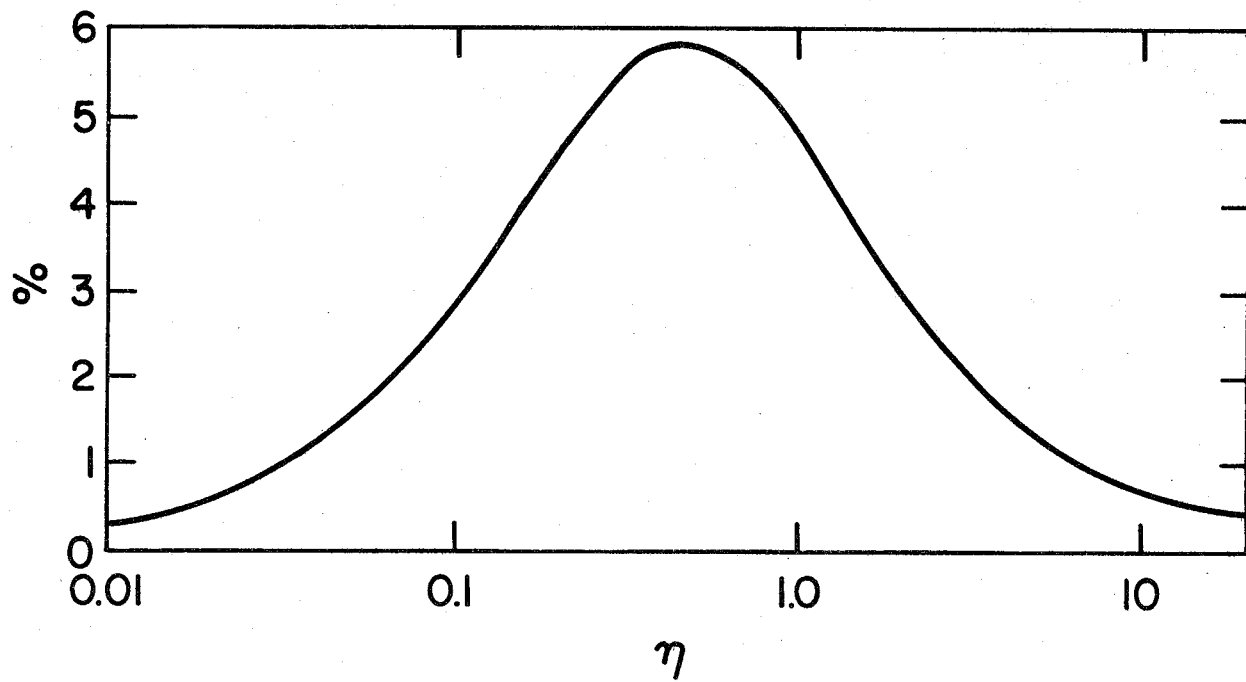


Fig. 7 Percent error in CG approximation for a single line and a constant mixing ratio between  $p = 0$  and  $p = 1$  atmos.

the equality of the second moment for the third equation quite arbitrarily, in order to make the equations easy to solve. It is easy to show that  $p_1$  and  $p_2$  are solutions of the quadratic

$$(u_1 p - u_2)^2 = (u_0 p - u_1)(u_2 p - u_3) \quad (4.10)$$

This two path equivalence is only of value if there is a transmission function which can be used with it. Fortunately two of the random models can be applied to this situation, namely the Goody model and the Malkmus model.

The optical depth for two paths in series is for a Lorentz line

$$\tau(\nu) = \frac{k}{\pi} \left\{ \frac{m_1 \alpha_1}{\nu^2 + \alpha_1^2} + \frac{m_2 \alpha_2}{\nu^2 + \alpha_2^2} \right\} \quad (4.11)$$

where  $\alpha_i = \alpha_0 p_i$ . The Goody and Malkmus models both require integrals of simple functions of  $\tau(\nu)$ , which can be performed analytically. We note that

$$1 + \tau(\nu) = \frac{(\nu^2 + \beta_1^2)(\nu^2 + \beta_2^2)}{(\nu^2 + \alpha_1^2)(\nu^2 + \alpha_2^2)} \quad (4.12)$$

where

$$2\beta_i^2 = \gamma_1 + \gamma_2 \pm [\{\gamma_1 - \gamma_2\}^2 + 4 u_1 u_2 \alpha_1^2 \alpha_2^2]^{1/2} \quad (4.13)$$

and

$$u_i = k_i m / \pi \alpha_i, \quad \gamma_i = \alpha_i^2 (1 + u_i) \quad (4.14)$$

For the Malkmus model, the mean equivalent width is

$$W_M = 2\pi(\beta_1 + \beta_2 - \alpha_1 - \alpha_2) \quad (4.15)$$

and for the Goody model it is

$$W_G = \pi \left[ \frac{\alpha_1 \alpha_2 (\gamma_1^u + \gamma_2^u)}{(1 + \gamma_1^u + \gamma_2^u)^{1/2}} + \gamma_1^u \alpha_1^2 + \gamma_2^u \alpha_2^2 \right] / (\beta_1 + \beta_2) \quad (4.16)$$

These expressions are to be inserted in Eq. (3.22) to obtain transmission.

#### 4.5 TEMPERATURE EFFECTS

The CG approximation may be extended to deal with paths in which the temperature varies with position (Godson, 1955a). Let us first consider a single Lorentz line. The strong and weak limits give the following relationships:

$$\begin{aligned} S(\theta_0) \bar{m} &= \int S(\theta(z)) \, dm \\ S(\theta_0) \alpha_0(\theta_0) \bar{p} \bar{m} &= \int S(\theta(z)) \alpha_0(\theta(z)) \, pdm \end{aligned} \quad (4.17)$$

so that

$$\bar{m} = \int \frac{S(\theta)}{S(\theta_0)} \, dm \quad \bar{p} \bar{m} = \int \frac{S(\theta) \alpha_0(\theta)}{S(\theta_0) \alpha_0(\theta_0)} \cdot pdm \quad (4.18)$$

where  $\theta_0$  is an arbitrarily chosen standard temperature. When we have several lines in an interval the situation is a little different. The weak limit gives

$$\sum_i S_i(\theta_0) \bar{m} = \int \sum_i S_i(\theta) dm \quad (4.19)$$

$$\text{i.e.} \quad \bar{m} = \int \frac{\sum_i S_i(\theta)}{\sum_i S_i(\theta_0)} dm = \int \Phi(\theta) dm \quad (4.20)$$

We note that this  $\bar{m}$  may be wrong for individual lines, but the errors will compensate.

The strong line limit requires

$$\sum_i (S_i(\theta_0) \alpha_{0i}(\theta_0) \bar{m})^{1/2} = \sum_i \left( \int S_i(\theta) \alpha_{0i}(\theta) pdm \right)^{1/2} \quad (4.21)$$

This equation requires us to do an integral for every spectral line in the interval, because the integral cannot be brought outside the square root. We would like an equation of the form

$$\bar{m} = \int \Psi(\theta) pdm \quad (4.22)$$

by analogy with the weak line limit. If this is to be any good at all, it must be valid in the simplest case - the strong limit of homogeneous paths of various temperatures. This requirement alone implies that

$$\Psi(\theta) = \left[ \frac{\sum_i S_i^{1/2}(\theta) \alpha_i^{1/2}(\theta)}{\sum_i S_i^{1/2}(\theta_0) \alpha_i^{1/2}(\theta_0)} \right]^2 \quad (4.23)$$



This is not strictly valid in general for paths with a variable temperature, but it is surprisingly good for realistic variations of temperature. It is exact in the strong limit in the case when all lines have the same temperature dependence.

## 5. ANGLE INTEGRATION

In a plane parallel atmosphere the transmission for the upward or downward compartments of flux may be obtained by integrating the intensity transmission over angle

$$\begin{aligned}
 T_f(\nu) &= 2 \int_0^{\pi/2} e^{-\tau(\nu)\sec\theta} \cos\theta \sin\theta \, d\theta \\
 &= 2 \int_1^{\infty} e^{-\tau(\nu)\mu} \frac{d\mu}{\mu^3}, \quad \text{where } \mu = \sec\theta \quad (5.1) \\
 &= 2 \operatorname{Ei}_3(\tau_\nu)
 \end{aligned}$$

where  $\operatorname{Ei}_3$  is the third exponential integral. There are several situations where the integral can be performed explicitly, although it cannot be done in the general case of the transmission of a finite spectral interval.

### 5.1 STRONG LIMIT OF RANDOM MODEL

In this case

$$T(m) = \exp(-(\ell m)^{1/2}) \quad (5.2)$$

and flux transmission is

$$\begin{aligned}
 T_f(m) &= 2 \int_1^{\infty} \exp(-(\ell m \mu)^{1/2}) d\mu / \mu^3 \\
 &= 4 \int_1^{\infty} \exp(-(\ell m)^{1/2} y) dy / y^5 \quad (5.3) \\
 &= 4 \operatorname{Ei}_5((\ell m)^{1/2})
 \end{aligned}$$

## 5.2 STRONG LIMIT OF A SINGLE LINE

We can define the equivalent width for flux by analogy with flux transmission. For a single Lorentz line in the strong limit,  $W(m) = (\ell_m)^{1/2}$  and  $W_f(m)$  is given by

$$\begin{aligned}
 W_f(m) &= 2 \int_1^{\infty} \sqrt{(\ell_m \mu)} \frac{d\mu}{\mu^3} \\
 &= \frac{4}{3} (\ell_m)^{1/2} \\
 &= W\left(\frac{16}{9} m\right)
 \end{aligned} \tag{5.4}$$

## 5.3 EMPIRICAL ABSORPTION BAND

The empirical band absorption function mentioned in section 3.2.3 may be integrated to give a function for flux as follows:

$$\begin{aligned}
 W_f(m) &= 2 \int A + B \log(\mu m) \frac{d\mu}{\mu^3} \\
 &= A + B \log(m) + 2 B \int \log(\mu) \frac{d\mu}{\mu^3} \\
 &= A + B \log(m) + B/2 \\
 &= A + B \log(e^{1/2} m) \\
 &= W(e^{1/2} m), \quad e^{1/2} \approx 1.649
 \end{aligned} \tag{5.5}$$

#### 5.4 DIFFUSIVITY FACTOR

We note that several of the above forms give

$$T_f(m) = T(\beta m), \text{ or } W_f(m) = W(\beta m). \quad (5.6)$$

We should also include the weak limit, for which  $\beta = 2$ . Elsasser found that empirically the Elsasser model could be well approximated by the same expression with  $\beta = 1.66$ , and in general this diffusivity factor is a good approximation for a wide range of band models, with an accuracy of 1 - 2 percent. A useful survey of the diffusivity factor is given by Armstrong (1968b).

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