

SIMPLIFIED DESCRIPTION OF THE LINE ABSORPTION COEFFICIENT IN BLANKETING EFFECT COMPUTATION

INTRODUCTORY REPORT

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Abstract—A brief review of some of the main models that have been utilized in the description of line absorption is given. It includes models for non-overlapping single lines, for single lines with correction for overlap and for overlapping lines with the distribution of lines being regular, random or a mixture of both.

1. INTRODUCTION

THE PROBLEM of the construction of a model atmosphere can be divided into two parts; the first part giving the march of temperature and pressure as a function of optical depth and the second part giving the emergent spectrum of the model. The physics used in these two parts should, in principle, be the same. In practice however, one can get away by using, among other things, a cruder representation of line absorption in the first part than in the second part. For example it is possible, with the aid of modern high speed electronic computers, like C.D.C.3600, I.B.M.7094, etc. to consider 150 000 or even more *individual* lines in one calculation, as has been accomplished by CHURCHILL, HAGSTROM, WEISNER and ARMSTRONG.⁽¹⁾ The maximum number of lines that can be treated individually can be easily increased with the availability of bigger and faster computers. In fact, it is possible to consider about one million lines individually at the moment.⁽²⁾ For certain applications, like computing the march of temperature and pressure in the model atmosphere, this enormous effort is, in general, not justified. Even for computing the emergent spectrum, certain moderation in the number of lines individually considered may be required, depending on the dispersion of the available experimental or observational spectra.

Alternatively, one can consider a certain number of strong or important lines individually, and treat the rest of the lines by "statistical models" in which various procedures may be followed to average over the fine structure of the spectra. In what follows, we will try to consider some of the methods that have been used to simplify the description of line absorption in blanketing effect computations.

2. NON-OVERLAPPING LINES MODELS

The "picket-fence" model

The "picket-fence" model of CHANDRASEKHAR⁽³⁾ is perhaps the earliest exhaustive

treatment of the effect of line blanketing in a stellar atmosphere. It has been generalized by MÜNCH⁽⁴⁾ to account for a slow dependence of the line probability on wavelength. These models, though very much idealized, are nevertheless useful for estimating the effect of lines on the model atmosphere with the least amount of numerical work.

The box approximation model

One need not consider these equal intensity rectangular line profiles to be spread uniformly throughout the spectrum. For example, if one is considering the vibration-rotation bands of H₂O, and if one approximates these bands by rectangular profiles, one needs to consider only bands centred at 6.3 μ , 2.7 μ , 1.9 μ , 1.4 μ and 1.1 μ , with different band widths and mean intensity of the bands. This "box approximation" can be refined by giving the bands a more realistic shape.

The single line model

This leads us to consider bands with non-overlapping spectral lines or rather single lines with various shapes. This implies that the lines are narrow and that there are large gaps between lines. If A_ν is the fractional absorption and k_ν the line absorption coefficient, at frequency ν , and a the amount of absorbing material, then the equivalent width of a line is given by:

$$W(a) = \int_{-\infty}^{\infty} A_\nu d\nu = \int_{-\infty}^{\infty} (1 - \exp[-k_\nu a]) d\nu \quad (1)$$

in the case of an absorption line with no re-emission. If the average spacing between the lines is d , the average absorption on the single line model is:

$$\bar{A} = (1/d) \int_{-\infty}^{\infty} (1 - \exp[-k_\nu a]) d\nu \quad (2)$$

This has been evaluated for various shapes of k_ν , some of which we will now consider.

(i) *Lorentz or dispersion shape.* Here

$$k_\nu = S\alpha/\pi(\nu^2 + \alpha^2), \quad (3)$$

where S and α are the line intensity and the damping constant, respectively. Note that the frequency is measured from the centre of the line. Then, if

$$x = \nu/d, \quad y = \alpha/d, \quad u = Sa/2\pi\alpha,$$

$$\bar{A} = \int_{-\infty}^{\infty} \{1 - \exp[-2uy^2/(x^2 + y^2)]\} dx \quad (4)$$

$$= 2\pi y e^{-u} \{J_0(iu) - iJ_1(iu)\} \equiv 2\pi y L(u). \quad (5)$$

Here J_0 and J_1 are Bessel functions of zero and first order with an imaginary argument and $L(u)$ is known as the LANDENBERG-REICHE⁽⁵⁾ function. A tabulation of $L(u)$ has been given by KAPLAN and EGGERS.^{(6),(7)} Asymptotic expansions are also available for $L(u)$.

For $u < 1$ (i.e. the weak line approximation):

$$L(u) = u \left[1 - \sum_{n=1}^{\infty} (-1)^{n+1} \frac{(2n-1)(2n-3)\dots 5 \cdot 3 \cdot 1}{n!(n+1)!} u^n \right]. \quad (6)$$

For $u > 1$ (i.e. the strong line approximation):

$$L(u) = \left(\frac{2u}{\pi} \right)^{1/2} \left[1 - \sum_{n=1}^{\infty} \frac{(2n-1)^2(2n-3)^2(2n-5)^2 \dots 3^2 \cdot 1^2}{n!(8u)^n} \right]. \quad (7)$$

The limit for $L(u)$ as $u \rightarrow \infty$ is $(2u/\pi)^{1/2}$, which is reached, for all practical purposes, for $u > 3$.

It can be shown that for $u \ll 1$, independent of line contour,

$$\bar{A} = 2\pi y u. \quad (8)$$

(ii) *Doppler shape.* For a Doppler broadened profile,

$$k_\nu = \frac{S}{\Delta\nu_D(\pi)^{1/2}} \exp(-\nu^2/\Delta\nu_D^2), \quad (9)$$

where

$$\Delta\nu_D = (2kT/mc^2)^{1/2} \nu_0. \quad (10)$$

If $x = \nu/\Delta\nu_D$ and $w = Sa/\Delta\nu_D(\pi)^{1/2}$, the mean absorption is⁽⁸⁾

$$\bar{A} = (\Delta\nu_D/d) \int_{-\infty}^{\infty} (1 - \exp[-we^{-x^2}]) dx, \quad (11)$$

or

$$\bar{A} = [(\pi)^{1/2} w \Delta\nu_D/d] \left\{ 1 + \sum_{n=1}^{\infty} (-1)^n \frac{w^n}{(n+1)!(n+1)^{1/2}} \right\}. \quad (12)$$

The series in the above expression converges very slowly for large values of w .

However, for large values of w , one has the following asymptotic expansion:⁽⁸⁾

$$\bar{A} = (2\Delta\nu_D/d) \{ (\ln w)^{1/2} + 0.2886 (\ln w)^{-1/2} - 0.1335 (\ln w)^{-3/2} + 0.0070 (\ln w)^{-5/2} + \dots \}. \quad (13)$$

(iii) *Doppler and dispersion profile.* It is not possible to give a general analytic solution for the combined Doppler and dispersion broadened line. Tables have been given by VAN DER HELD⁽⁹⁾ for this case. A special case of vibration-rotation bands of diatomic molecules has been treated by THOMSON^{(10),(11)} and the needed tables given. An asymptotic expansion for the strong lines ($u \gg 1$) has been given by PLASS and FIVEL.⁽¹²⁾

3. SINGLE LINE MODELS AND OVERLAP

The various methods described in the last section are not valid for overlapping lines. Several procedures have been utilized in the literature to modify single line models to incorporate overlapping. Among them is the doublet model. REICHE⁽¹³⁾ has considered the problem of two equal overlapping lines. The more general case of two overlapping lines with arbitrary half-width and strength has been treated by SAKAI and STAUFFER.⁽¹⁴⁾

They have essentially expressed the combined equivalent width of the two lines as the sum of the separate equivalent widths minus a correction factor. The evaluation of this correction factor is rather complicated and they have given, for the case of dispersion profile, an approximate solution with a maximum error of less than 5 per cent. PLASS⁽¹⁵⁾ has tried for this case, to give more exact and simple expressions, which gave excellent results in a few specific cases. SAKAI⁽¹⁶⁾ has given, however, a unified solution applicable to all cases with errors of less than 1.5 per cent.

The doublet model has been generalized by MATOSSI, MEYER and RUSCHER⁽¹⁷⁾ in order to increase indefinitely the number of overlapping Lorentz lines, with the LADENBURG and REICHE solution, equation (5), as a boundary condition. This model is rather cumbersome to use. Hence, it has been hardly exploited even though it is a very general model.

4. OVERLAPPING LINES MODELS

The Elsasser or regular model

The absorption due to the overlapping of neighbouring lines has been treated by ELSASSER⁽¹⁸⁾ in an idealized way. This model consists of an infinite number of lines of equal intensity and distributed at equal intervals. It is difficult to find such a distribution of lines in nature and one may have to resort to using more than one ELSASSER band to represent the observed spectra satisfactorily. For dispersion line contour, the only case for which the ELSASSER model has been solved, the absorption coefficient at frequency displacement ν from the centre of one particular line is:

$$k_\nu = \sum_{-\infty}^{\infty} \frac{S}{\pi} \frac{\alpha}{(\nu - nd)^2 + \alpha^2}. \quad (14)$$

Here we see that line centres are located at $0, \pm d, \pm 2d, \dots$. Using the notation of equation (4), one obtains, after the summation of the infinite series:

$$ak_x = 2\pi uy \frac{\sinh 2\pi y}{\cosh 2\pi y - \cos 2\pi x}. \quad (15)$$

From this, the average fractional absorption is obtained, as before, with the result that

$$\begin{aligned} \bar{A} &= 1 - \int_{-1/2}^{1/2} \exp\left(-2\pi uy \frac{\sinh 2\pi y}{\cosh 2\pi y - \cos 2\pi x}\right) dx, \\ &\equiv 1 - E(y, u). \end{aligned} \quad (16)$$

This result has been expressed in somewhat different forms as well. Since the line pattern is assumed to be repetitive, the above result also applies to a frequency interval that is an arbitrary integral multiple of d . This integral has been solved numerically by GOODY,⁽¹⁷⁾ KAPLAN⁽¹⁹⁾ and by WARK and WOLK.⁽²⁰⁾ KAPLAN's series representation diverges beyond $2\pi y = 1.76$. PLASS⁽²¹⁾ has considered various approximating functions for this integral and the regions of their validity. An analytic solution of ELSASSER integral has been found by SEITZ and LUNDHOLM⁽²²⁾ and it is:

$$\bar{A} = \sinh 2\pi y \sum_{n=0}^{\infty} a_{2n}/(n!)^2 2^{2n}. \quad (17)$$

SEITZ and LUNDHOLM have given the first few values of a_{2n} as well as the recursion relation between the coefficients.

A few special cases of equation (16) can be considered. For example, when $y \rightarrow \infty$,

$$\bar{A} \rightarrow 1 - \exp(-2\pi y u). \quad (18)$$

In this limit the lines overlap and there is no fine structure; for weak lines, equation (8) is obtained. On the other hand, for strong lines when $u \gg 1$,

$$\bar{A} \rightarrow 1 - \operatorname{erf}\{\pi y(2u)^{1/2}\}, \quad (19)$$

where erf denotes the error function.

The Mayer-Goody model or random model

MAYER⁽²³⁾ and GOODY^{(7),(24)} have considered the average absorption at the centre of an infinite array with random separation and intensity. If n is the number of absorption lines, d the mean line spacing, $N(v_1, v_2 \dots v_n) dv_1 dv_2 \dots dv_n$ the probability that lines occur in the frequency range $(v_1, v_1 + dv_1), \dots (v_n, v_n + dv_n)$, $P(S) dS$, the probability that one line has an intensity in the range $(S, S + dS)$, k_r the absorption coefficient at a distance v_r from the line centre and a is the amount of absorbing material, then the mean absorption due to n lines in all possible arrangements is:

$$\bar{A} = 1 - \frac{\int_{-nd/2}^{+nd/2} \dots \int_{-nd/2}^{+nd/2} N(v_1 \dots v_n) dv_1 \dots dv_n \int_0^\infty \dots \int_0^\infty \prod_1^n P(S_r) e^{-k_r a} dS_r}{\int_{-nd/2}^{+nd/2} \dots \int_{-nd/2}^{+nd/2} N(v_1 \dots v_n) dv_1 \dots dv_n \int_0^\infty \dots \int_0^\infty \prod_1^n P(S_r) dS_r}. \quad (20)$$

If all arrangements of line positions are equally possible, then N is simply a constant and may be cancelled out. All the frequency and all the intensity integrations are now the same and with slight rearrangement, equation (20) can be written, in the limit of $n \rightarrow \infty$, as

$$\bar{A} = 1 - \exp\left[-\frac{1}{d} \int_{-\infty}^{+\infty} \int_0^\infty P(S)(1 - e^{-k\alpha}) dS dv \Big/ \int_0^\infty P(S) dS\right]. \quad (21)$$

In order to integrate this expression, $P(S)$ must be known. One of the forms for $P(S)$ that has often been used is:

$$P(S) = (1/\sigma) e^{-S/\sigma}, \quad (22)$$

where σ is a constant. Then,

$$\bar{A} = 1 - \exp\left[-\frac{1}{d} \int_{-\infty}^{+\infty} \frac{a\sigma f(v, \alpha)}{1 + a\sigma f(v, \alpha)} dv\right]. \quad (23)$$

Here we have assumed that $k = Sf(v, \alpha)$ with $f(v, \alpha)$ giving the shape of a single line. Thus

we see that the problem of a complicated absorption band is reduced to an integral involving the shape of a single line. This leads to immense simplification.

If we assume dispersion profile for the lines, then:

$$f(\nu, \alpha) = (\alpha/\pi)/(\nu^2 + \alpha^2) \quad (24)$$

and

$$\bar{A} = 1 - \exp\left[-\frac{a\sigma\alpha}{d(\alpha^2 + a\sigma\alpha/\pi)^{1/2}}\right]. \quad (25)$$

If

$$P(S) = K/S, \quad S \leq S', \quad (26)$$

where K and S' are adjustable constants, then for the dispersion profile:

$$\bar{A} = 1 - \exp\left[-\frac{2\pi K\alpha}{d}\{e^{-u}J_0(iu) + 2ue^{-u}[J_0(iu) + J_1(iu)]\} - 1\right], \quad (27)$$

where $u = S'a/2\pi\alpha$, and J_0 and J_1 are the Bessel functions of zero and first order.

Similar cases have been considered for the Doppler profile and for the combined Doppler and dispersion profile.

Arbitrary line variance model

Whereas the ELSASSER model is characterized by complete regularity, randomness is the hallmark of the MAYER-GOODY model. It is rather unlikely that these two special cases will include all kinds of line spacing. In fact, a very good possibility exists that the line spacing is a mixture of order and disorder. Such a general case have recently been considered by KING.⁽²⁵⁾

If one represents the character of the line spacing by the variance of the line array defined as the ratio of the average of the square of the line separation to the square of the mean spacing less unity then

$$\text{variance} \equiv (\bar{\delta}^2/d^2) - 1. \quad (28)$$

Note that for the ELSASSER model the variance vanishes, whereas for the MAYER-GOODY model it is unity.

For clustering of lines with superposition, the variance tends to infinity. Between the values of 0 and 1 of variance, the model shows a mixture of order and disorder.

$$\text{If the probability density} \equiv dN/d\nu \propto \nu^{1/n-1} \quad (29)$$

where N is the number of lines and ν the frequency, then $n > 1$ denotes clustering, while for $n < 1$ increasing line order occurs. For such a probability distribution,

$$\text{variance} = [(2n)!/(n!)^2] - 1. \quad (30)$$

Then for a dispersion profile and for opaque line centre approximation ($Su/2\pi\alpha \gg 1$), the mean fractional absorption is given by:

$$\bar{A} = 1 - \Gamma(n, [n!A_{n0}]^{1/n})/\Gamma(n), \quad (31)$$

where $A_{no} = (4 Su_a/d^2)^{1/2}$, and the incomplete gamma function is defined by:

$$\Gamma(a, z) = \int_z^{\infty} e^{-t} t^{a-1} dt. \quad (32)$$

The ELSASSER and MAYER-GOODY models are special cases of equation (31) with $n = \frac{1}{2}$ and 1, respectively.

The modulated band-absorption model.

Experimental spectroscopists have frequently represented the absorption properties of a variety of molecules by simple empirical formulas. They have found that for moderate to strong absorption, band absorption follows a logarithmic law. However, none of the band models discussed above exhibit such a behaviour. This is perhaps due to neglect of some effects in the formulation of the problem. This missing link has been found by KING⁽²⁶⁾ to be the finite width of the bands. All the theoretical models, discussed above, assume infinite band width. KING has derived band models, which comprise an infinite array of the ELSASSER or MAYER-GOODY type, modulated by a band envelope whose intensity falls off exponentially from the band centre (to make the band width finite). This modulated band absorption model does exhibit logarithmic band absorption.

5. THEORETICAL MODELS AND OBSERVATIONS

One needs some simple analysis to determine the right model for a given observed absorption spectrum. One way is to compare the empirical representation with the weak and strong line approximations of KING.⁽²⁶⁾ He has considered the bands of H₂O and CO₂ in this way. A somewhat different procedure has been suggested by OPPENHEIM and BEN-ARYEH,⁽²⁷⁾ who have applied the method to certain bands of N₂O, CO and H₂O.

6. A FEW MISCELLANEOUS APPROXIMATIONS

In this section, we have tried to give a few miscellaneous approximations that may be found useful in the representation of line blanketing.

Relation between "local" Planck and Rosseland mean

If a frequency interval contains a large number of lines but is still narrow enough to assume Planck function, continuous absorption coefficient, etc. as constant, then it is possible to give expressions relating the "local" Planck and Rosseland means. STEWART and PYATT^{(28),(29)} has given such relations for the ELSASSER band model and for the MAYER-GOODY band model. These relations are rather useful, because most of the calculations and measurements of molecular absorption coefficients give essentially the Planck mean only. For example, if $\bar{\kappa}_R$ and $\bar{\kappa}_P$ represent the Rosseland and Planck mean, respectively, and if we use the notation of equation (4), then, for

$$y \gg 1, \quad (33)$$

$$\bar{\kappa}_R = \bar{\kappa}_P$$

For $y \ll 1$,

$$\bar{\kappa}_R = \text{continuous absorption} \equiv \kappa_0 \quad (34)$$

i.e. the lines do not contribute to $\bar{\kappa}_R$.

For the ELSASSER model, if there is no continuum, then,

$$\bar{\kappa}_R = \bar{\kappa}_p / \coth 2\pi y. \quad (35)$$

Voigt profile

Several detailed computations of the combined Doppler and collision broadened profile or the Voigt profile have become recently available.^{(30),(31),(32)} However, for our purpose, approximate methods of folding the profile are needed. One way of accomplishing this is to use the least number of terms consistent with the accuracy desired in the expansion as given by HUMMER and others. An approximate procedure has also been considered recently by HANSEN,⁽³³⁾ who has also considered the combined Stark and Doppler profile. The method of HANSEN, however, may not be very efficient as it involves arctangents.

Band width

For the vibration-rotation bands of a diatomic molecule, one can easily determine the band widths of the fundamental and higher overtones. This has been done by PENNER.⁽¹¹⁾ As the principal factor determining the relative intensities of the rotational lines is $J \exp[-E(v, J)/kT]$, where v and J are the vibrational and rotational quantum numbers, k the Boltzman constant and T the absolute temperature, one can find the value of $J = J^*$ where the intensity is maximum. Then by limiting the minimum intensity relative to the maximum as 10^{-2} or 10^{-3} one can obtain the band width.

Asymmetric top molecules

The expression for the rotational energy levels for asymmetric top molecules for a given vibrational state is rather complicated.⁽³⁴⁾ It depends not only on J , the rotational quantum number but on τ or κ also, which defines the sublevels of the J -level. However, one can average all the levels with a given J and thus obtain an expression similar to that for diatomic molecules by⁽³⁵⁾ assuming

$$(A + B + C)/3 \equiv B_{\text{eff}},$$

where A , B and C are the three moments of inertias, and replacing B by B_{eff} in the rotational energy expression for a diatomic molecule.

7. CONCLUDING REMARKS

The main purpose of this report has been to acquaint the astrophysicists with the work done mainly by non-astrophysicists, especially meteorologists and physicists dealing with the properties of air. Some of the results mentioned above cannot be used directly in astrophysical applications. It is hoped, however, that some of these procedures will be found useful in developing astrophysical analogue for a simplified description of line-blanketing.

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DISCUSSION

T. R. CARSON: The work of Harris Mayer (Los Alamos Report LA-647) was entitled "Methods of Opacity Calculations". One of the reasons for the introduction of the statistical treatment of lines is that, although their positions are determined by the

equations of quantum mechanics, these equations are too difficult to solve. However, this method is no longer used in modern opacity calculations. Instead, one attempts to calculate, to the best of one's ability, the position and profile of each line or line component, and thereby construct a detailed absorption spectrum.