BANDWIDTH REQUIREMENTS IN SPECTRAL LINE TRANSFER CALCULATIONS

by

R. Grant Athay

High Altitude Observatory
National Center for Atmospheric Research
Boulder, Colorado

ABSTRACT

Accurate evaluation of a line source function, S, requires that the frequency bandwidth be sufficiently large to include properly transfer effects in the line wings. The bandwidth required to achieve a given level of accuracy in the evaluation of S can be specified, in units of the Doppler width, in terms of three parameters: the ratio of continuum to line opacity, r_0, the probability for collisional de-excitation, ε, and the Voigt wing parameter $\underline{a}$. Bandwidths required to give S to an accuracy of 2 percent are given for values of ε and r_0 from 10^{-2} to 10^{-8} and for values of $\underline{a}$ from 10^{-2} to 10^{-5}.

Key words: line source function, bandwidth requirements.

I. INTRODUCTION

In computing a line source function, S, by numerical techniques, it is generally necessary to discretize the frequency variable and to limit the frequency range to some finite band centered on the line. The accuracy with which S can be evaluated depends upon both the nesting of the frequency points and the total bandwidth considered.

The bandwidth required to achieve a given level of accuracy in S depends upon the extent of the line wings and, in addition, upon departures from local thermodynamic equilibrium, LTE. In LTE one frequency

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can be treated independently of any other frequency and the required bandwidth reduces to zero. In non-LTE S depends upon radiation transfer effects over a band of frequencies that, for some lines, may be very broad. Generally, if a line has negligible wings the bandwidth can safely be restricted to the Doppler core and the bandwidth is sufficiently narrow that it presents no particular difficulties. When, however, the line wings are strongly developed the problem of properly treating the entire bandwidth of the line with a set of discrete frequency points may lead to serious difficulties. It is essential to know, therefore, how far into the line wings the bandwidth must extend in order to give an accurate evaluation of S.

The strength and extent of line wings are determined by two parameters: the Voigt parameter $\underline{a}$ and the ratio of continuum to line opacity, $r_o = d\tau_c/d\tau_o$. If we define the shape factor for the line absorption coefficient to be ϕ_y, where y is a dimensionless frequency measured in units of the Doppler width, i.e., $y = \Delta\nu/\Delta\nu_D$, we may approximate ϕ_y for a Voigt profile by

$$\phi_y = e^{-y^2} \qquad y \leq 1$$

$$\phi_y = e^{-y^2} + \frac{a}{\sqrt{\pi}\, y^2} \qquad y > 1 \tag{1}$$

An element of opacity at frequency y is then given by

$$d\tau_y = \phi_y \, d\tau_o + d\tau_c$$

$$= (\phi_y + r_o)\, d\tau_o$$

For constant r_o, $\tau_y(\text{line}) = \tau_c$ for a value of y such that $\phi_y = r_o$ and $\tau_y(\text{line}) = 10^{-n}\,\tau_c$ for $\phi_y = 10^{-n}\, r_o$. One may reasonably argue that the effects of the wings are adequately included if $\tau_y(\text{line}) = 10^{-2}\,\tau_c$. Equation (1) gives for this case a limiting y of

$$y_1 = 7.5\,(a/r_o)^{1/2} \tag{2}$$

In extreme cases such as the H and K lines of Ca II or Lyman-α in the solar spectrum $(a/r_o)^{1/2} \approx 10^4$. Hence, we find $y_1 \approx 10^5$.

To properly treat such large values of y is both difficult and time consuming. Furthermore, it is totally unnecessary in cases where the wings are formed in LTE.

The purpose of the calculations presented here is to evaluate the bandwidth requirements for a range of the relevant parameters. We treat the simple case of a two-level atom, which requires only one parameter in addition to $\underline{a}$ and r_o. The added parameter is the ratio of collisional to radiative de-excitation rates, which we define as $\varepsilon = C_{21}/A_{21}$ where the subscripts designate the upper and lower levels respectively. For a given set of ε, $\underline{a}$ and r_o, we evaluate the minimum value of y for which S is accurate to 2 percent at each depth. The parameters ε, $\underline{a}$ and r_o together with the temperature and Doppler width are held constant with depth.

II. CALCULATIONS AND RESULTS

The line source function is computed using the flux divergence method of Athay and Skumanich (1967). In their formulation for a two-level atom with non-coherent scattering, the frequency independent source function is given by

$$S = B + \frac{2N}{\varepsilon+\delta} \int_0^\infty \frac{\phi_y}{\phi_y + r_o} \frac{dH_y}{d\tau_o} dy \quad , \tag{2}$$

where B is the Planck function, H_y is the monochromatic net flux,

$$N = (2 \int_0^\infty \phi_y \, dy)^{-1} \approx \pi^{-1/2} \quad , \tag{3}$$

and

$$\delta = 2\pi^{-1/2} r_o \int_0^\infty \frac{\phi_y}{\phi_y + r_o} dy. \tag{4}$$

We note from the form of equation (3) that two general conclusions can be stated about the required bandwidth as follows:

(1) If $\delta > \varepsilon$, y_1 must be sufficiently large to give an accurate value of

$$\frac{1}{\delta} \int_0^{y_1} \frac{\phi_y}{\phi_y + r_o} \frac{dH_y}{d\tau_o} \, dy .$$

This quantity would be independent of y_1 if $dH_y/d\tau_o$ were constant with y, which is true in LTE but not in the general case. In non-LTE the quantity $dH_y/d\tau_o$ is relatively large near line center and decreases to a relatively small, constant value at some point in the line wings.

At the surface $\tau_o = 0$, $S/B \propto \delta^{1/2}$. Thus, if we considered that only δ depended upon y_1 we would require 4 percent accuracy in δ to attain 2 percent accuracy in S.

Also, we note that in the case, $\delta \gg \varepsilon$, the required bandwidth is independent of ε.

(2) If $\varepsilon \gg \delta$, the bandwidth will depend upon ε. For large ε, the non-LTE effects will be limited to the Doppler core and $y = 3$ will suffice. For small ε, the required bandwidth will extend into the wings, but not so far as in case 1 for a value of δ equal to the ε of case 2.

It is clear from case 1 that an extreme limit on y_1 for 2 percent accuracy in S is given by the condition that δ be accurate to 4 percent. Thus, if we write

$$\delta = 2\pi^{-1/2} r_o \int_0^{y_1} \frac{1}{1 + \frac{\sqrt{\pi} r_o}{a} y^2} \, dy$$

$$= 2\pi^{-3/4} (a\, r_o)^{1/2} \tan^{-1} y_1 (\sqrt{\pi} r_o/a)^{1/2} \qquad (5)$$

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$$= \pi^{1/4} (a\ r_o)^{1/2} \quad y_1 = \infty ,$$

the 4 percent criterion for δ gives

$$y_1 = 11.5\ (a/r_o)^{1/2} \quad , \tag{6}$$

which is about a factor 1.5 greater than the value given by equation (2). The limit on y_1 set by equation (2) corresponds to approximately 6 percent accuracy in δ, or 3 percent accuracy in S if $\delta >> \varepsilon$.

To evaluate y_1 more explicitly for a given combination of ε, r_o and a, we solve equation (3) for a set of values of y_1. We increase y_1, step-wise, until an increase in y_1 by a factor of ten changes S by less than 2 percent at each optical depth point. We assume that S has converged to a correct solution when this condition is met.

The values of y_1 tested are 3, 4 10^k, 3 × 10^k, and 10^{k+1} for $k > 1$. The spacings of the y points for $y < 10$ are as follows:

$0 \le y \le 3$	$3 \le y \le 4$	$4 \le y \le 10$
0.25	0.5	3

For $y \ge 10^k$, $k \ge 1$, four points in y are used per decade. These are spaced at 1.5 × 10^k, 3 × 10^k, 6.5 × 10^k and 10^{k+1}. As an example, if $y_1 = 10^3$ the number of points used is:

$0 \le y \le 3$	$3 \le y \le 4$	$4 \le y \le 10$
13	2	2

$10 \le y \le 100$	$100 \le y \le 1000$
4	4

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After y_1 is carried far enough to show convergence a minimum value of y_1 is determined that gives S accurate to 2 percent. These minimum values are obtained by interpolation between the tested values of y_1. They should be accurate to at least a factor of two.

It is possible, of course, that our convergence criterion is not strict enough. When both ε and r_O are small and when a is large the convergence is very slow. For example, with $\varepsilon = r_O = 10^{-8}$ and $a = 10^{-2}$ the 2 percent criterion gives $y_1 \gtrsim 2 \times 10^4$ whereas a 10 percent criterion gives $y_1 \gtrsim 500$. We note, however, that $y_1 = 2 \times 10^4$ is about a factor of two greater than the value given by equation (6). Hence, we conclude that our convergence test is valid in this case, which is the case of slowest convergence treated here. In all other cases, y_1 is less than or equal to the value given by equation (2) and the convergence is reasonably fast.

The greatest likelihood of error in determining y_1 by the method described is in underestimating y_1. Thus, it is more likely that the value of y_1 given for a particular set of values of ε, r_O and a is too low, rather than too high.

The convergence of S to its correct solution as y_1 increases occurs differently in different parts of the atmosphere and for different values of the various parameters. The most notable effects are related to the wing parameter a. For $\tau_O << a^{-1}$, the convergence is from below, i.e., if y_1 is too small S is too small. For $\tau_O >> a^{-1}$, however, the convergence is from above. Also, if $(\varepsilon + r_O) < a \lesssim 10 (\varepsilon + r_O)$ the convergence of S is much more rapid for $\tau_O >> a^{-1}$. These two effects are illustrated in Figure 1.

Values of y_1 for the 2 percent criterion are shown in Figure 2 for different combinations of values of r_O and ε between 10^{-2} and 10^{-8} and for values of a between 10^{-2} and 10^{-5}. Computations were made each two decades in ε and r_O (10^{-2}, 10^{-4}, 10^{-6} and 10^{-8}) and each decade in a (10^{-2}, 10^{-3}, 10^{-4} and 10^{-5}). The curves shown, therefore, are drawn through four points in each case. We emphasize again that the absolute errors in y_1 may be as large as a factor of two. On the other hand, the curves drawn through the points show a large measure of continuity from one curve to another. Thus, the errors do not appear to be so large as to obscure the nature of the curves.

There are threshold effects around $y_1 = 3$ for $a \leq 10^{-3}$ and $y_1 = 15$ for $a = 10^{-2}$ that strongly

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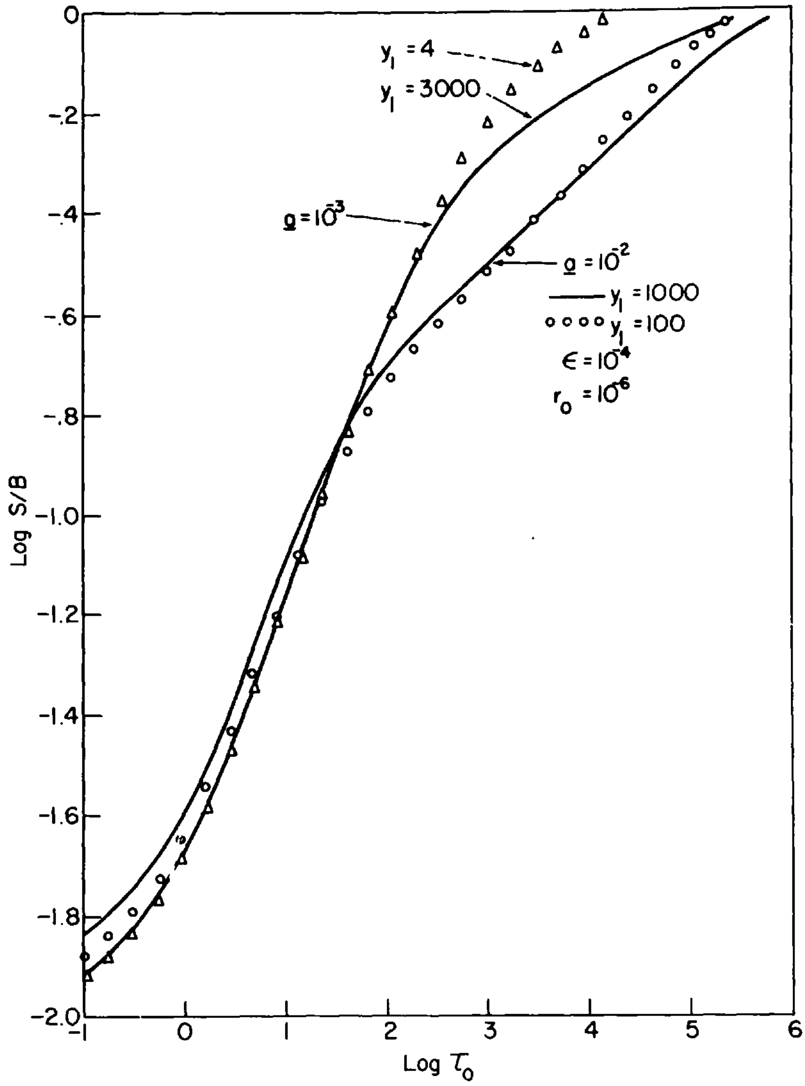

Figure 1. Illustration of approach to proper solution as y_1 is increased for two cases $\underline{a} = 10^{-3}$ and $\underline{a} = 10^{-2}$

influence the shapes of the curves for small values of y_1. However, certain systematic effects are evident in the curves whenever y_1 is large or when either ε or r_O is small.

In the plot of log y_1 versus log δ in Figure 2, it is evident that for $\delta \gg \varepsilon$ $y_1 \propto \delta^{-1}$. Within the range of δ and $\underline{a}$ where this is evident, viz., $\delta \leq 10^{-3}$ and $\underline{a} \geq 10^{-3}$ line wings are well developed. Equation (5) shows that, for this case, $\delta \propto r_O^{1/2}$. Thus, we find a region where $y_1 \propto r_O^{-1/2}$ as predicted by equations (2) and (6). The plots of log y_1 versus log r_O exhibit the $r_O^{-1/2}$ dependence for $r_O = 10^{-6}$ and 10^{-8}. Also, when $\delta \ll \varepsilon$ the results in Figure 2 show y_1 to be independent of δ. The same effect is again evident in the plot of log y_1 versus log r_O for $\varepsilon = 10^{-2}$.

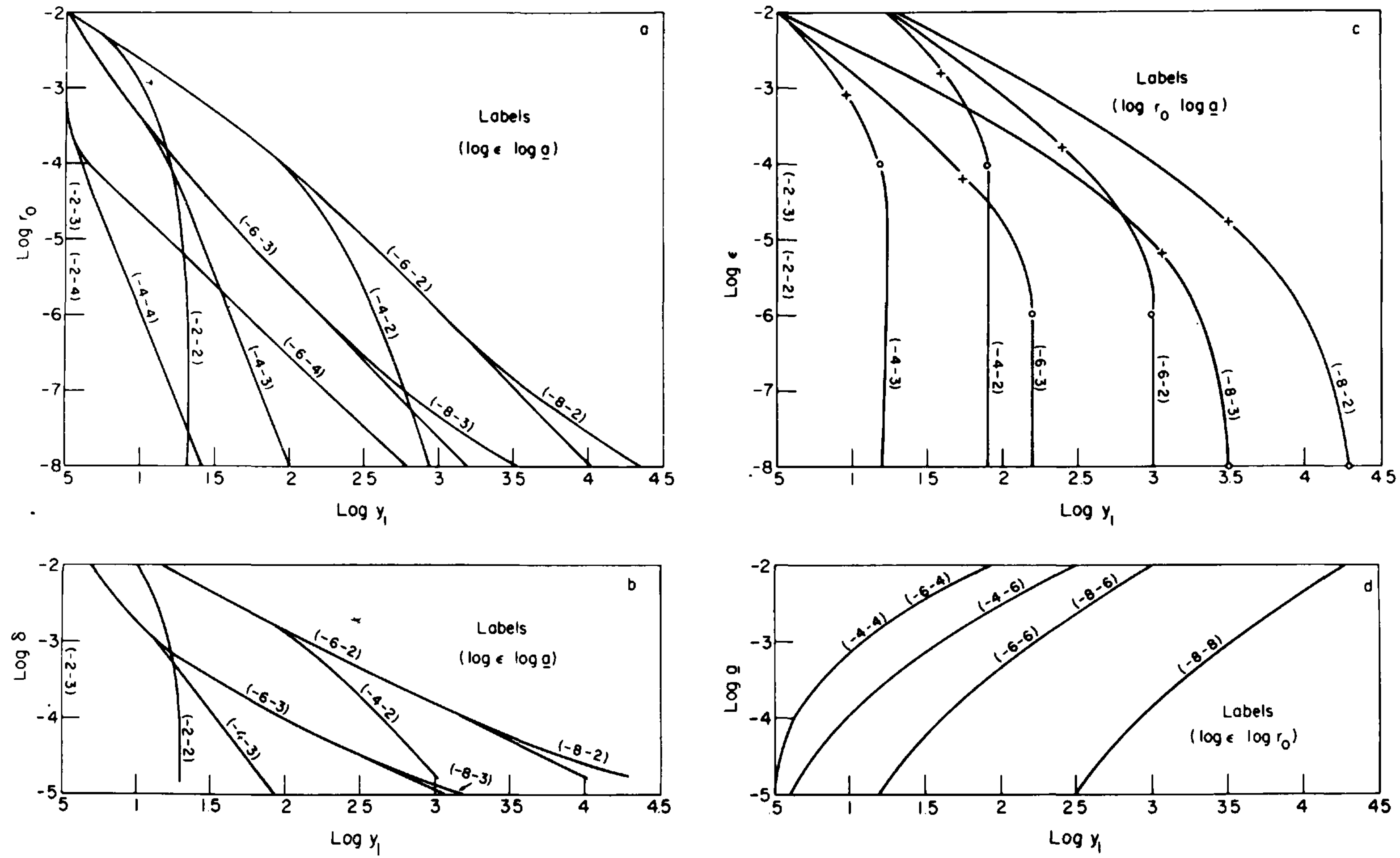

Figure 2. Dependence of y_1 upon a - r_O, b - δ, c - ε and d - a. Note saturation effects for δ << ε in figure b and for ε << δ in figure c.

Similarly, in the plot of log y_1 versus log $\underline{a}$ we find that when $\underline{a} \lesssim 10^{-3}$ and y_1 is well away from its threshold values $y_1 \propto \underline{a}^{1/2}$ as expected. There is a tendency in all four curves of log y_1 versus log $\underline{a}$ to have more nearly $y_1 \propto \underline{a}$ for $\underline{a} > 10^{-3}$. To preserve the $\underline{a}^{1/2}$ dependence it would be necessary to reduce all of the y_1 values for $\underline{a} = 10^{-2}$ by about a factor of two. While this is permissable for individual points it seems unlikely that all of the values of y_1 for $\underline{a} = 10^{-2}$ would be overestimated by the same amount.

On the plots of log y_1 versus log ε in Figure 2 the plus signs indicate the points $\varepsilon = \delta$ and the open circles indicate the points $\varepsilon = r_O$. It is clear that the dependence of y_1 on ε weakens at about the point $\varepsilon = \delta$ and that y_1 becomes essentially independent of ε for $\varepsilon < 10^{-1}\delta$. For $\varepsilon > \delta$ and y_1 well away from its threshold values (i.e., on the curves $r_O = 10^{-8}$) it appears that $y_1 \propto \varepsilon^{-1}$.

To an accuracy of about a factor of two and for $y_1 \gtrsim 10$, the results in Figure 2 may be approximated by:

$$y_1 \approx \frac{a^{1/2}}{\varepsilon}, \qquad \varepsilon >> \delta$$

$$y_1 \approx \frac{1}{3}\frac{a^{1/2}}{\varepsilon}, \qquad \varepsilon \approx \delta \tag{7}$$

and

$$y_1 \approx 10(a/r_O)^{1/2} \approx 13\,\frac{a}{\delta}, \qquad \delta >> \varepsilon .$$

The first of these limits on y_1 corresponds to $\tau_y \approx \varepsilon^2 \tau_O$, or to $\tau_y = 1$ at $\tau_O = \varepsilon^{-2}$, the thermalization length for the pure dispersion case.

It should be remembered that the above values of y_1 are valid for the 2 percent criterion on the accuracy of S. When line wings are well developed and when $\delta >> \varepsilon$ the required values of y_1 for a given accuracy in δ can be estimated from equation (5). For 20 percent accuracy in δ, equation (5) gives values of y_1 a factor of five below those required for 4 percent accuracy and for 2 percent accuracy in δ a factor of two increase in y_1 is required. However, accuracy in δ is not the only criterion for accuracy in S.

Estimates of y_1 for 10 percent accuracy in S were made along with the estimates for 2 percent accuracy. A few checks were made on y_1 for 1 percent accuracy in S. In almost all cases where $\delta >> \varepsilon$ the changes in y_1 indicated in the preceding paragraph give an accuracy in S equal to twice the accuracy in δ, i.e., 20 percent accuracy in δ corresponds to 10 percent accuracy in S. In a few cases much larger changes in y_1 are indicated. For example, with $\underline{a} = 10^{-2}$ and $\varepsilon = r_O = 10^{-8}$ the estimated values of y_1 are 500, 2×10^4 and $> 10^5$ for accuracies in S of 10, 2 and 1 percent, respectively.

In the case of $\varepsilon >> \delta$, 10 percent accuracy in S requires values of y_1 about a factor of five below those given in Figure 2 and 1 percent accuracy in S requires values of y_1 about a factor of two larger than those given in Figure 2.

A few additional calculations were made in which both B and $\Delta\nu_D$ varied with depth. The depth variation of B mimicked the solar atmosphere and $\Delta\nu_D$ was equated to the thermal Doppler width. This did not produce any substantial change in y_1. However, rapid depth variations in any one of the parameters influencing S, viz., B, $\Delta\nu_D$, ε, r_O and $\underline{a}$ may very well lead to significant changes in y_1. It is perhaps wise in using the results in Figure 2 and equation (7) to use the minimum values of ε and r_O and maximum values of $\underline{a}$ for a particular problem.

Although calculations have not been made for multilevel atoms, I see no particular reason why the inclusion of added levels should increase the values of y_1. However, if the added levels increase the effective value of ε the required values of y_1 may be substantially reduced. It would seem entirely safe, therefore, to use the results found here for multilevel problems.

REFERENCE

Athay, R. G., and Skumanich, A. 1967, *Ann. d'Ap.*, 30, 669.

DISCUSSION

Underhill: Have you investigated what happens if you encounter a neighbouring line in your necessary bandwidth y_1 (100 Doppler-widths) for the frequency integration?

Athay: No, I don't know what happens to y_1 in that case.