

COHERENT LINE FORMATION WITH DEPTH-DEPENDENT
PARAMETERS

by

T. R. Carson

*University Observatory
St. Andrews, U.K.*

ABSTRACT

A discrete ordinate method is developed for solving the equation of coherent line formation, for arbitrary given variations with depth in an atmosphere of the temperature (or Planck function, assuming local thermodynamic equilibrium) and the line absorption and scattering coefficients. The direct solution thus obtained can then be used as the starting point of an iterative procedure. Results obtained for an exactly soluble case indicate the utility of the method.

Key words: numerical methods, coherent line formation.

INTRODUCTION

The equation of coherent line formation can be solved exactly only in a number of special cases where certain restrictions are put upon the problem (see references). Such restrictions may include the imposition of simplifying boundary conditions and/or assuming particular variations with optical depth of parameters such as the temperature and the coefficient of absorption and scattering in the line. When these restrictions are invalid, or otherwise unacceptable, a rigorous solution may still be obtained by numerical iteration from an initially guessed

trial solution, but this method converges very slowly when the scattering coefficient is large compared with the absorption coefficient. In the method of the present paper none of the above mentioned simplifications is assumed. The equation of transfer is written in the form of an integral equation for the source function for which a solution is obtained directly by reduction of the integral equation to a set of simultaneous linear equations. Iteration from the direct solution then leads to more accurate results, as indicated by applying the method to a known soluble case.

THE EQUATION OF TRANSFER

The equation of radiative transfer, including line absorption, in plane parallel geometry may be written

$$\mu \frac{dI_{\nu}(x, \mu)}{\rho dx} = -(k_{\nu} + \ell_{\nu}) I_{\nu}(x, \mu) + (1-\epsilon) \ell_{\nu} J_{\nu}(x) + (k_{\nu} + \ell_{\nu}) B_{\nu}(T(x))$$

where ν is the frequency, x is the geometrical depth measured in the direction of the outward normal to the atmosphere, μ is the cosine of the angle between the direction of transfer and the outward normal, and ρ is the mass density. $I_{\nu}(x, \mu)$ is the specific intensity of radiation, $J_{\nu}(x)$ the mean intensity, $B_{\nu}(T)$ the Planck function for temperature T , k_{ν} and ℓ_{ν} are the continuous and line mass absorption coefficient and $(1-\epsilon)$ is the fraction of radiation absorbed which is scattered. Introducing an optical depth τ_{ν} defined in terms of some absorption coefficient k_{ν} by the relation

$$d\tau_{\nu} = -k_{\nu} \rho dx$$

the equation of transfer takes the form

$$\mu \frac{dI_v(\tau_v, \mu)}{d\tau_v} = \alpha_v(\tau_v)I_v(\tau_v, \mu) +$$

$$- \beta_v(\tau_v)J_v(\tau_v) - \gamma_v(\tau_v)B_v(\tau_v)$$

$$\alpha_v = \frac{k_v + \ell_v}{\kappa_v}$$

$$\beta_v = \frac{(1 - \epsilon)\ell_v}{\kappa_v}$$

$$\gamma_v = \frac{k_v + \ell_v}{\kappa_v}$$

Defining the source function

$$S_v(\tau_v) = \beta_v(\tau_v)J_v(\tau_v) + \gamma_v(\tau_v)B_v(\tau_v)$$

the equation of transfer becomes

$$\mu \frac{dI_v(\tau_v, \mu)}{d\tau_v} = \alpha_v(\tau_v)I_v(\tau_v, \mu) - S_v(\tau_v)$$

for which the solution may be formally written down

$$I_v(\tau_v, -\mu) = \int_0^{\tau_v} \exp \left\{ - \int_{\tau'_v}^{\tau_v} \alpha_v(\tau''_v) \frac{d\tau''_v}{\mu} \right\} S_v(\tau'_v) \frac{d\tau'_v}{\mu}$$

$$I_v(\tau_v, +\mu) = \int_{\tau_v}^{\infty} \exp \left\{ - \int_{\tau_v}^{\tau'_v} \alpha_v(\tau''_v) \frac{d\tau''_v}{\mu} \right\} S_v(\tau'_v) \frac{d\tau'_v}{\mu}$$

Using the relations

$$\begin{aligned}
 J_{\nu}(\tau_{\nu}) &= \frac{1}{2} \int_{-1}^{+1} I_{\nu}(\tau_{\nu}, \mu) d\mu \\
 &= \frac{1}{2} \int_0^{\infty} S_{\nu}(\tau'_{\nu}) E_1 \left\{ \left| \int_{\tau'_{\nu}}^{\tau_{\nu}} \alpha_{\nu}(\tau''_{\nu}) d\tau''_{\nu} \right| \right\} d\tau'_{\nu} ,
 \end{aligned}$$

where $E_n(x)$ is the exponential integral of index n definedⁿ by

$$E_n(x) = \int_1^{\infty} e^{-xt} t^{-n} dt = \int_0^1 e^{-xs} s^{n-2} ds$$

the source function $S_{\nu}(\tau_{\nu})$ then satisfies the integral equation

$$\begin{aligned}
 S_{\nu}(\tau_{\nu}) &= \frac{\beta_{\nu}(\tau_{\nu})}{2} \left[\int_0^{\infty} S_{\nu}(\tau'_{\nu}) E_1 \left\{ \left| \int_{\tau'_{\nu}}^{\tau_{\nu}} \alpha_{\nu}(\tau''_{\nu}) d\tau''_{\nu} \right| \right\} d\tau'_{\nu} \right] + \\
 &+ \gamma_{\nu}(\tau_{\nu}) B_{\nu}(\tau_{\nu})
 \end{aligned}$$

SOLUTION FOR THE SOURCE FUNCTION

Suppressing the indicated frequency dependence of all quantities, the integral equation for the source function may be written

$$S(\tau) = \frac{\beta}{2} \left[\int_0^{\infty} S(\tau') E_1 \{ f(\tau, \tau') \} d\tau' \right] + \gamma B(\tau)$$

where

$$f(\tau, \tau') = \left| \int_{\tau}^{\tau'} \alpha(\tau'') d\tau'' \right|$$

Choosing a set of points of subdivision τ_i with appropriate weights a_i , the integral over τ' may be replaced by a summation, thus transforming the integral equation into a set of simultaneous linear equations

$$S_i = \frac{\beta_i}{2} \left[\sum_j a_j E_1 \{ f_{ij} \} S_j \right] + \gamma_i B_i$$

where the indices i, j denote that the quantities are evaluated for τ_i, τ_j . The calculation of the coefficient matrix elements is straightforward as long as the range of integration does not include an interval or subdivision one end of which corresponds to $j = i$. For $j = i$, f_{ij} vanishes and hence $E_1 \{ f_{ij} \}$ is infinite. We must therefore find an alternative expression for the integral over those ranges of integration that include the singularity viz.,

$$\int_{\tau_{i-1}}^{\tau_i} E_1 \left\{ f(\tau_i, \tau') \right\} S(\tau') d\tau'$$

and

$$\int_{\tau_i}^{\tau_{i+1}} E_1 \left\{ f(\tau_i, \tau') \right\} S(\tau') d\tau'$$

Since as $f \rightarrow 0$

$$E_1(f) \rightarrow -\gamma - \sum_1^{\infty} \frac{(-1)^n f^n}{n \cdot n!} - \ln f = E_1'(f) - \ln f$$

where $\gamma = 0.577215665\dots$ we may isolate the singularity in the $\ln f$ term and write

$$\int E_1 \left\{ f(\tau') \right\} S(\tau') d\tau' = \int E_1 \left\{ f(\tau') \right\} S(\tau') d\tau' +$$

$$- \int \ln f(\tau') S(\tau') d\tau'$$

integrand of the first term on the right-hand is now everywhere finite and so the integral is represented by a quadrature formula in the way, as a weighted sum of the values of the integrand at the points of subdivision. The second integral may also be so represented provided we make some assumptions about the variation of the integrand. Thus expanding $\phi(\tau'')$ about $\tau'' = \tau_i$

$$\alpha(\tau'') = \alpha_i + \alpha'_i(\tau'' - \tau_i) + \dots$$

where $\alpha'_i = (d\alpha(\tau'')/d\tau'')_{\tau_i}$ we have up to the terms

$$\alpha_i(\tau_i - \tau') - \frac{\alpha'_i}{2}(\tau' - \tau_i)^2, \quad \tau' \leq \tau_i$$

$$=$$

$$\alpha_i(\tau' - \tau_i) + \frac{\alpha'_i}{2}(\tau' - \tau_i)^2, \quad \tau' \geq \tau_i$$

$$+ \ln(\tau_i - \tau') + \ln \left\{ 1 - \frac{\alpha'_i}{2\alpha_i}(\tau_i - \tau') \right\}, \quad \tau' \leq \tau_i$$

) =

$$+ \ln(\tau' - \tau_i) + \ln \left\{ 1 + \frac{\alpha'_i}{2\alpha_i}(\tau' - \tau_i) \right\}, \quad \tau' \geq \tau_i.$$

Since $S(\tau') = S(\tau_i) = S_i$ and taking it outside the integral sign we have

$$\int_{\tau_{i-1}}^{\tau_i} \ln f(\tau') S(\tau') d\tau' = S_i \left[(\ln \alpha_i) \tau + \dots \right]$$

$$+ F_1(t) + F_2(t, -b) \Big], \quad t = \tau_i - \tau_{i-1}$$

$$\int_{\tau_i}^{\tau_{i+1}} \ln f(\tau') S(\tau') d\tau' = S_i \left[(\ln \alpha_i) t + \right.$$

$$\left. + F_1(t) + F_2(t, +b) \right], \quad t = \tau_{i+1} - \tau_i$$

where $b = \alpha'_i / 2\alpha_i$ and

$$F_1(t) = \int_0^t \ln x dx = \left[x(\ln x - 1) \right]_0^t = t(\ln t - 1)$$

$$\begin{aligned} F_2(t, b) &= \int_0^t \ln(1+bx) dx = \left[\frac{1}{b}(1+bx) \left\{ \ln(1+bx) - 1 \right\} \right]_0^t = \\ &= \frac{1}{b} \left[(1+bt) \left\{ \ln(1+bt) - 1 \right\} - 1 \right]. \end{aligned}$$

Now replacing the derivative α'_i by the divided differences

$$\alpha'_i = (\alpha_i - \alpha_{i-1}) / (\tau_i - \tau_{i-1}), \quad \tau_{i-1} < \tau' < \tau_i$$

$$\alpha'_i = (\alpha_{i+1} - \alpha_i) / (\tau_{i+1} - \tau_i), \quad \tau_i < \tau' < \tau_{i+1}$$

we obtain an expression for the integral through the singularity at τ_i in terms of S_i , thus completing the reduction of the integral equation to a set of simultaneous linear equations.

THE EMERGENT INTENSITY

Given the source function, the specific intensity at any depth and in any direction may then be

obtained. To facilitate the quadrature we write

$$f(\tau') = f_i + f'(\tau' - \tau_i)$$

$$S(\tau') = S_i + S'(\tau' - \tau_i)$$

where f is as defined, $f_i = f(\tau_i)$, $S_i = S(\tau_i)$ and the primes denote derivatives. The contribution to I_ν due to the source function in any interval (τ_1, τ_2) is then

$$\begin{aligned} \Delta_{12} I_\nu &= \frac{1}{\mu} \int_{\tau_1}^{\tau_2} \exp \left[- \left\{ f(\tau') \right\} / \mu \right] S(\tau') d\tau' \\ &= \frac{1}{\mu} e^{-a} \left[\left(\frac{1}{b} S_1 + \frac{1}{b^2} S'_{12} \right) (1 - e^{-bt}) - \frac{1}{b} S'_{12} t e^{-bt} \right], \end{aligned}$$

where $t = \tau_2 - \tau_1$, $a = f_1/\mu$, $b = f'_{12}/\mu$, $f'_{12} = (f_2 - f_1)/t$, $S'_{12} = (S_2 - S_1)/t$. The intensity emergent from the atmosphere in the direction corresponding to μ is simply $I_\nu(o, \mu)$ from which the equivalent width of a line in wavelength units is given by

$$W_\lambda(\mu) = \int \left\{ 1 - R_\lambda(o, \mu) \right\} d\lambda,$$

where the residual intensity

$$R_\lambda(o, \mu) = \frac{I_\lambda(o, \mu)}{I_\lambda^c(o, \mu)}$$

and $I_\lambda^c(o, \mu)$ is the background or continuous emergent intensity in the absence of line absorption. When the integrated width, and not the variation with the angle of emergence, is required we have instead

$$W_\lambda = \int \left\{ 1 - R_\lambda(o) \right\} d\lambda$$

with

$$R_{\lambda}(o) = \frac{\int_0^1 \mu I_{\lambda}(o, \mu) d\mu}{\int_0^1 \mu I_{\lambda}^C(o, \mu) d\mu}$$

NUMERICAL CALCULATIONS

To test the feasibility of our method we apply it to a situation where the solution is already accurately known. For $\kappa_{\nu} = k_{\nu}$ (so that τ_{ν} is now the optical depth in the continuum) and with $\eta = \ell_{\nu}/k_{\nu}$ constant with depth, $\varepsilon = 0$ and a temperature distribution such that $B_{\nu}(\tau_{\nu}) = B_0(1 + 3/2 \tau_{\nu})$ the exact solution has been given by Chandrasekhar (1947) in the form

$$R(o, \mu) = H(\mu) \left[\frac{2}{3} + \mu\delta + \frac{1}{2} \delta^{1/2} (1-\delta) \alpha_1 \right] \delta^{1/2} / \left(\mu + \frac{2}{3} \right)$$

$$R(o) = 3 \left[\frac{1}{2} \delta \alpha_2 + \frac{1}{3} \alpha_1 + \frac{1}{4} \delta^{1/2} (1-\delta) \alpha_1^{1/2} \right] \delta^{1/2}$$

where $\delta = 1/(1+\eta)$ and

$$\alpha_n = \int_0^1 \mu^n H(\mu) d\mu$$

$H(\mu)$ being the solution of the integral equation

$$H(\mu) = 1 + \frac{1}{2} (1-\delta) \mu H(\mu) \int_0^1 \frac{H(\mu') d\mu'}{\mu + \mu'}$$

In applying the method of solution developed in the present paper, the number and distribution of the points of subdivision in optical depth have to be specified. It seemed desirable to have a distribution with zero optical depth as one end point and for which the points of subdivision were closer together at small optical depth than at large optical

depth. The points of subdivision were therefore chosen according to the formula

$$\tau_n = A(n-1)^2, \quad n = 1, \dots, N$$

with A and N as variable parameters. Because of the unequal intervals the trapezoidal rule was used in performing the relevant quadratures.

Calculations were carried out for $N = 25$ and with A taking the values 0.01, 0.02 and 0.04. The results for $R_\lambda(o)$ for various values of $1/(1+\eta)$ obtained from both the direct and iterated solutions, are shown in Table 1 together with the exact results. It may be seen that the direct solution is very good for small η but can be considerably in error for large η . However iteration of the solution leads to a very marked improvement, but for any value of η the best direct solution does not necessarily lead to the best iterated solution. Thus while $A = 0.02$ gives the best iterated solution for small η , that for large η is obtained with $A = 0.01$, indicating that small optical depths are more important for strong lines than for weak lines. The results have also been used to calculate the equivalent width W_λ of a line, for various values of the Voigt profile parameter a which is the ratio of the Lorentz width to the Gaussian width and for various values of η_0 , the value of η at the line centre. Table 2 gives the values of $\log(W_\lambda/\lambda)$. It will be observed that both the direct and iterated solutions give good agreement with the exact results. In particular the iterated solution for $A = 0.02$ gives results which are indistinguishable from the exact results for all values of the parameters considered. This convergence of the calculated values of the equivalent width must be due to the fact that the important contributions come from regions of the line where η is small, for which values both the direct and iterated solutions are most accurate.

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TABLE 1.
 $R_\lambda(0)$

$\frac{1}{1+\eta}$	Exact	$\tau_n = 0.01(n-1)^2$		$\tau_n = 0.02(n-1)^2$		$\tau_n = 0.04(n-1)^2$	
		Direct	Iterated	Direct	Iterated	Direct	Iterated
1.000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.900	0.9481	0.9609	0.9500	0.9491	0.9481	0.9593	0.9476
0.800	0.8939	0.9207	0.8965	0.9185	0.8939	0.9180	0.8938
0.700	0.8369	0.8798	0.8397	0.8771	0.8367	0.8760	0.8362
0.600	0.7762	0.8381	0.7791	0.8352	0.7759	0.8329	0.7752
0.500	0.7109	0.7962	0.7128	0.7928	0.7101	0.7882	0.7084
0.400	0.6391	0.7548	0.6418	0.7496	0.6381	0.7400	0.6356
0.300	0.5580	0.7156	0.5585	0.7045	0.5557	0.6797	0.5522
0.200	0.4616	0.6819	0.4619	0.6442	0.4558	0.5674	0.4408
0.150	0.4036	0.6625	0.4014	0.5809	0.3921	0.4496	0.3857
0.100	0.3340	0.6009	0.3250	0.4309	0.2994	0.2679	0.3084
0.075	0.2919	0.5017	0.2724	0.2991	0.2268	0.1627	0.2586
0.050	0.2412	0.3056	0.1898	0.1517	0.2123	0.0678	0.1969
0.025	0.1735	0.0820	0.1444	0.0335	0.1302	0.0165	0.1144
0.000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

TABLE 2.

 $\text{Log}(W_\lambda/\lambda)$

log a	log η_0	Exact	$\tau_n = 0.01(n-1)^2$		$\tau_n = 0.02(n-1)^2$		$\tau_n = 0.04(n-1)^2$	
			Direct	Iterated	Direct	Iterated	Direct	Iterated
-2	-2	-7.255	-7.378	-7.271	-7.264	-7.255	-7.361	-7.251
	-1	-6.282	-6.405	-6.298	-6.290	-6.282	-6.387	-6.278
	0	-5.470	-5.593	-5.486	-5.478	-5.470	-5.575	-5.466
	1	-5.048	-5.171	-5.064	-5.056	-5.048	-5.154	-5.044
	2	-4.859	-4.982	-4.875	-4.867	-4.859	-4.964	-4.854
-1	-2	-7.248	-7.371	-7.264	-7.256	-7.248	-7.353	-7.243
	-1	-6.273	-6.396	-6.289	-6.282	-6.273	-6.379	-6.269
	0	-5.456	-5.579	-5.473	-5.465	-5.456	-5.562	-5.452
	1	-4.997	-5.120	-5.013	-5.006	-4.997	-5.103	-4.993
	2	-4.509	-4.632	-4.525	-4.517	-4.509	-4.614	-4.505
0	-2	-7.167	-7.290	-7.184	-7.176	-7.167	-7.273	-7.162
	-1	-6.189	-6.132	-6.205	-6.197	-6.189	-6.294	-6.185
	0	-5.338	-5.461	-5.355	-5.347	-5.338	-5.444	-5.334
	1	-4.760	-4.883	-4.776	-4.769	-4.760	-4.866	-4.756
	2	-4.303	-4.426	-4.319	-4.311	-4.303	-4.409	-4.299
1	-2	-7.103	-7.226	-7.119	-7.111	-7.103	-7.209	-7.099
	-1	-6.122	-6.245	-6.138	-6.130	-6.122	-6.227	-6.118
	0	-5.255	-5.378	-5.271	-5.263	-5.255	-5.360	-5.250
	1	-4.635	-4.758	-4.651	-4.643	-4.635	-4.740	-4.631
	2	-4.139	-4.262	-4.155	-4.147	-4.139	-4.244	-4.135

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DISCUSSION

Kalkofen to Grant: Can you apply your method to semi-infinite media?

Grant: We did not try that, but it may be possible to handle these cases.

Pecker: As we conclude today's session I would like to remind you once more that many phenomena that can be observed very clearly on the solar disk are practically invisible in stellar spectra or can be found only in the far UV. This means that many of the important phenomena that occur in extended atmospheres give only very small observable effects.