

# An operator splitting method for line radiation with partial redistribution in atmospheres with shocks

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Received 27 October 1993 / Accepted 5 March 1994

**Abstract.** An operator splitting method for the calculation of spectral line radiation assuming partial redistribution is discussed which is suitable for atmospheres with shock discontinuities.

**Key words:** methods: numerical – lines: profiles – shock waves – stars: chromosphere – lines: formation

## 1. Introduction

The numerical treatment of radiation transport in spectral lines when shocks are present and when partial frequency redistribution is assumed is difficult and needs an efficient method of solution. Available methods (e.g. Uitenbroek 1990) do not allow for grid spacings with zero optical distances as occurs when shocks are treated as discontinuities. In the present work an operator splitting method is presented which allows the efficient computation of source functions and line profiles. This method uses a diagonal operator after Olson & Kunacz (1987) and is outlined in Sect. 2. Section 3, discusses the convergence properties of the method. The conclusions are presented in Sect. 4.

## 2. Method

### 2.1. Radiative transfer in the observers frame

The situation for which the present method to compute spectral lines is envisioned is a plane parallel atmosphere permeated by vertically propagating acoustic shock waves of moderate amplitude. Here moderate means that the velocity amplitude is at most of the order of the sound speed. The wave causes temperature  $T$ , density  $\rho$  and velocity  $u$  fluctuations which at the shocks jump over an infinitesimally small distance from a front shock state to a back shock state. A typical situation for which we envision the method is shown in Fig. 1 which is taken from an acoustic wave calculation in the solar atmosphere by Ramacher & Ulmschneider (1992). Here the velocity jumps are from about -4 km/s in front of the shock to roughly +4 km/s behind the shock. The temperature jump at the shocks is about

5000 K. Because of the occurrence of these jumps the radiative transfer is considered in the observers frame.

For a spectral line with background continuum the transfer equation may be written

$$\mu \frac{\partial I_{\nu\mu}(\tau)}{\partial \tau} = [\varphi_{\nu\mu}(\tau) + r(\tau)] [I_{\nu\mu}(\tau) - S_{\nu\mu}(\tau)] \quad , \quad (1)$$

where

$$\tau(z) = \int_z^\infty \chi_L(z') dz' \quad , \quad (2)$$

is the reference (line center) optical depth and

$$r(z) = \frac{\chi_C(z)}{\chi_L(z)} \quad , \quad (3)$$

is the ratio of background to line center opacities.  $z$  is the geometrical height and  $I_{\nu\mu}$  the specific monochromatic intensity of a beam of radiation inclined by an angle  $\vartheta$  with respect to the outwardly directed  $z$ -axis.  $\mu = \cos \vartheta$  and  $\nu$  is the frequency.  $\chi_L$  and  $\chi_C$  are frequency-independent line and continuum opacities.  $\varphi_{\nu\mu}$  is the absorption profile, given by

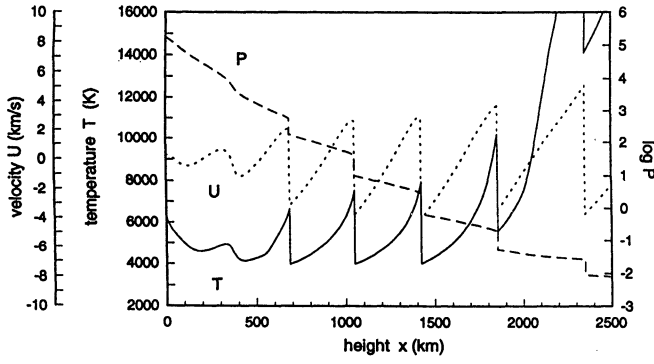
$$\varphi_{\nu\mu} = \frac{H(a, \nu)}{\sqrt{\pi} \Delta\nu_D} \quad , \quad (4)$$

with

$$a = \frac{\Gamma}{4\pi \Delta\nu_D} \quad , \quad (5)$$

$$\nu = \frac{\nu - \nu_0 (1 - \mu u(z)/c_L)}{\Delta\nu_D} \quad . \quad (6)$$

$\Gamma$  is the damping constant,  $\Delta\nu_D$  the thermal Doppler width,  $u$  the gas velocity and  $c_L$  the light velocity. The absorption profile satisfies the normalisation condition



**Fig. 1.** Acoustic wave with period  $P = 45$  s and initial energy flux  $F_M = 2 \cdot 10^8 \text{ erg cm}^{-2} \text{ s}^{-1}$  after Rammacher & Ulmschneider (1992). Temperature  $T$  (K), velocity  $u$  (km/s), pressure  $\log p$  (dyn/cm<sup>2</sup>) are shown as function of Euler height  $x$  (km)

$$\int_{-1}^1 \int_{-\infty}^{\infty} \varphi_{\nu\mu} d\nu = 1. \quad (7)$$

The total source function is given by

$$S_{\nu\mu}(\tau) = \frac{\varphi_{\nu\mu}(\tau) S_{\nu\mu}^L(\tau) + r(\tau) B(\tau)}{\varphi_{\nu\mu}(\tau) + r(\tau)}, \quad (8)$$

where  $B$  is the Planck function and  $S_L$  the line source function given by (Cheng 1992)

$$S_{\nu\mu}^L(\tau) = [1 - \epsilon(\tau)] \frac{1}{\varphi_{\nu\mu}(\tau)} \int_{-\infty}^{+\infty} \int_{-1}^1 R(\nu, \mu, \nu', \mu', \tau) I_{\nu'\mu'}^+(\tau) d\mu' d\nu' + \epsilon(\tau) B(\tau). \quad (9)$$

$$\epsilon(\tau) = \frac{\epsilon'}{1 + \epsilon'} \quad \text{where} \quad \epsilon'(\tau) = \frac{n_e \Omega_{21}}{A_{21}} \left(1 - e^{-h\nu/kT}\right), \quad (10)$$

is the photon destruction probability and  $R$  is the redistribution function. For  $\epsilon$  and  $R$  see Mihalas (1978) Chap. 11 and 13. For  $R$  we take either the redistribution function  $R_{II}$  if we consider PRD or  $\varphi_{\nu\mu}\varphi_{\nu'\mu'}$  when CRD is considered (see e.g. Mihalas 1978, Eq. 13-73). Note that in the CRD case the source function  $S_{\nu\mu}^L$  becomes independent of  $\nu$  and  $\mu$ .

We now restrict ourselves to two beams along the ray  $\mu = \cos \vartheta$ , where we have ingoing  $I_{\nu\mu}^-(\tau)$  and outgoing  $I_{\nu\mu}^+(\tau)$  photons, and where from now on  $\mu = |\mu|$ . For an extension of the present method to an arbitrary number of beams see Buchholz and Ulmschneider (1994, in preparation). In the two-beam approximation Eq. (1) can be written

$$\mu \frac{\partial I_{\nu\mu}^+(\tau)}{\partial \tau} = [\varphi_{\nu\mu}^+(\tau) + r(\tau)] [I_{\nu\mu}^+(\tau) - S_{\nu}^+(\tau)], \quad (11)$$

$$-\mu \frac{\partial I_{\nu\mu}^-(\tau)}{\partial \tau} = [\varphi_{\nu\mu}^-(\tau) + r(\tau)] [I_{\nu\mu}^-(\tau) - S_{\nu}^-(\tau)], \quad (12)$$

where  $\tau$  after Eq. (2) does not depend on direction. The total source functions are then given by

$$S_{\nu}^+(\tau) = \frac{\varphi_{\nu\mu}^+(\tau) S_{\nu\mu}^L(\tau) + r(\tau) B(\tau)}{\varphi_{\nu\mu}^+(\tau) + r(\tau)}, \quad (13)$$

$$S_{\nu}^-(\tau) = \frac{\varphi_{\nu\mu}^-(\tau) S_{\nu\mu}^L(\tau) + r(\tau) B(\tau)}{\varphi_{\nu\mu}^-(\tau) + r(\tau)}. \quad (14)$$

Defining

$$G(\nu, \mu, \nu', \mu', \tau) \equiv \frac{R(\nu, \mu, \nu', \mu', \tau)}{\varphi_{\nu\mu}(\tau)}, \quad (15)$$

the line source functions are written

$$S_{\nu\mu}^L(\tau) = [1 - \epsilon(\tau)] \int_{-\infty}^{+\infty} G(\nu, \mu, \nu', \mu', \tau) I_{\nu'\mu'}^+(\tau) d\nu' +$$

$$[1 - \epsilon(\tau)] \int_{-\infty}^{+\infty} G(\nu, \mu, \nu', -\mu', \tau) I_{\nu'\mu'}^-(\tau) d\nu' + \epsilon(\tau) B(\tau), \quad (16)$$

$$S_{\nu\mu}^L(\tau) = [1 - \epsilon(\tau)] \int_{-\infty}^{+\infty} G(\nu, -\mu, \nu', \mu', \tau) I_{\nu'\mu'}^+(\tau) d\nu' +$$

$$[1 - \epsilon(\tau)] \int_{-\infty}^{+\infty} G(\nu, -\mu, \nu', -\mu', \tau) I_{\nu'\mu'}^-(\tau) d\nu' + \epsilon(\tau) B(\tau). \quad (17)$$

As the number of photons must be conserved during the scattering process we must require that

$$\int_{-\infty}^{+\infty} G(\nu, \mu, \nu', \mu', \tau) d\nu' + \int_{-\infty}^{+\infty} G(\nu, -\mu, \nu', \mu', \tau) d\nu' = 1, \quad (18)$$

$$\int_{-\infty}^{+\infty} G(\nu, \mu, \nu', -\mu', \tau) d\nu' + \int_{-\infty}^{+\infty} G(\nu, -\mu, \nu', -\mu', \tau) d\nu' = 1. \quad (19)$$

We now assume that the redistribution functions  $G$  are not strongly  $\mu$ -dependent and that the  $\mu$ -dependence enters the problem only, because it Doppler shifts frequencies due to the thermal motion of the gas particles and of the macroscopic fluid motion. In Eqs. (11), (12) and (16), (17), photons with  $\nu', \mu'$  enter a gas element, are scattered and emerge with  $\nu, \mu$ . Here

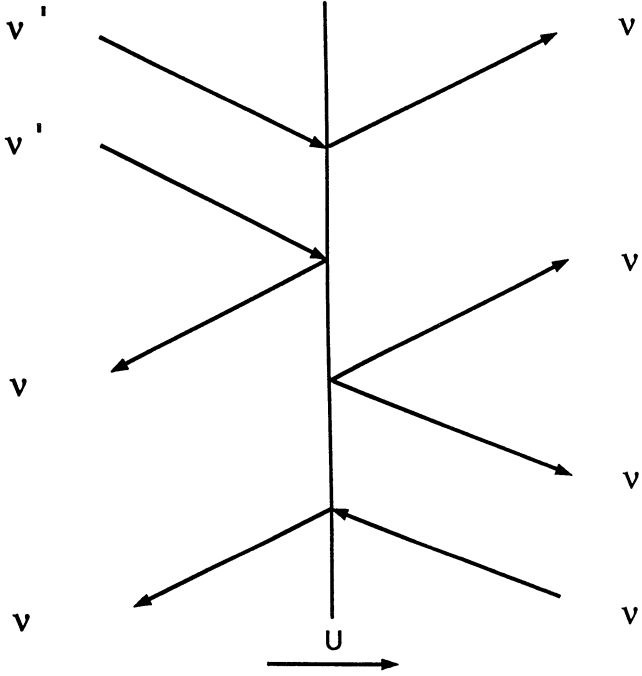


Fig. 2. Scattering cases in a two-beam approximation

$\mu$  either remains unchanged or photons are scattered into  $-\mu$ . This allows to drop the  $\mu$ -dependence in the  $G$ -functions except where it influences the frequencies  $\nu$ .

Consider the scattering process in a gas element moving with the velocity  $u$  in  $+z$ -direction. Figure 2 shows the possible scattering processes. From Fig. 2, following a photon from the laboratory frame into the comoving frame of the gas element where it suffers a scattering event and reemerges Doppler shifted back in the laboratory frame, we have the four cases

$$\begin{aligned} G^{++}(\nu, \nu', \tau) &= G(\nu - \nu_0 - \nu_0 \frac{u\mu}{c_L}, \nu' - \nu_0 - \nu_0 \frac{u\mu}{c_L}, \tau) \\ G^{+-}(\nu, \nu', \tau) &= G(\nu - \nu_0 + \nu_0 \frac{u\mu}{c_L}, \nu' - \nu_0 - \nu_0 \frac{u\mu}{c_L}, \tau) \\ G^{-+}(\nu, \nu', \tau) &= G(\nu - \nu_0 - \nu_0 \frac{u\mu}{c_L}, \nu' - \nu_0 + \nu_0 \frac{u\mu}{c_L}, \tau) \\ G^{--}(\nu, \nu', \tau) &= G(\nu - \nu_0 + \nu_0 \frac{u\mu}{c_L}, \nu' - \nu_0 + \nu_0 \frac{u\mu}{c_L}, \tau) \end{aligned} \quad (20)$$

With these redistribution functions the source functions (16), (17) are greatly simplified.

Integrating Eqs. (11), (12) one has the formal solution

$$\begin{aligned} I_{\nu}^{+}(\tau) &= \int_{\tau}^{\tau_N} \left[ \varphi \left( \tau', \nu - \nu_0 \frac{u(\tau')\mu}{c_L} \right) + r(\tau') \right] S_{\nu}^{+}(\tau') \cdot \\ &\exp \left\{ - \int_{\tau}^{\tau'} \left[ \varphi \left( \tau'', \nu - \nu_0 \frac{u(\tau'')\mu}{c_L} \right) + r(\tau'') \right] \frac{d\tau''}{\mu} \right\} \frac{d\tau'}{\mu} \\ &+ I_{\nu}^{+}(\tau_N) \exp \left\{ - \int_{\tau}^{\tau_N} \left[ \varphi \left( \tau'', \nu - \nu_0 \frac{u(\tau'')\mu}{c_L} \right) \right. \right. \end{aligned}$$

$$\left. + r(\tau'') \right] \frac{d\tau''}{\mu} \left. \right\} \quad (21)$$

$$\begin{aligned} I_{\nu}^{-}(\tau) &= - \int_0^{\tau} \left[ \varphi \left( \tau', \nu + \nu_0 \frac{u(\tau')\mu}{c_L} \right) + r(\tau') \right] S_{\nu}^{-}(\tau') \cdot \\ &\exp \left\{ \int_{\tau'}^{\tau} \left[ \varphi \left( \tau'', \nu + \nu_0 \frac{u(\tau'')\mu}{c_L} \right) + r(\tau'') \right] \frac{d\tau''}{\mu} \right\} \frac{d\tau'}{\mu} \\ &+ I_{\nu}^{-}(\tau_1) \exp \left\{ \int_0^{\tau} \left[ \varphi \left( \tau'', \nu + \nu_0 \frac{u(\tau'')\mu}{c_L} \right) \right. \right. \\ &\left. \left. + r(\tau'') \right] \frac{d\tau''}{\mu} \right\} . \end{aligned} \quad (22)$$

Here  $I_{\nu\mu}(\tau_1)$ ,  $I_{\nu\mu}(\tau_N)$  are boundary intensities which can be set equal to zero if one has no incident radiation at the surface  $\tau_1$  and if the optical depth at the bottom  $\tau_N$  is very large. The profile function  $\varphi_{\nu\mu}$  has been written explicitly.

With  $N_{\tau}$  depth and  $N_{\nu}$  frequency points Eqs. (16), (17) can be written as matrix equations, where the number of subscripts indicates the size of the matrices

$$\mathbf{S}_{\nu\tau}^{+} = \mathbf{R}_{\nu\nu'\tau}^{++} \mathbf{I}_{\nu'\tau}^{+} + \mathbf{R}_{\nu\nu'\tau}^{+-} \mathbf{I}_{\nu'\tau}^{-} + \epsilon_{\tau} \mathbf{B}_{\nu\tau} \quad , \quad (23)$$

$$\mathbf{S}_{\nu\tau}^{-} = \mathbf{R}_{\nu\nu'\tau}^{-+} \mathbf{I}_{\nu'\tau}^{+} + \mathbf{R}_{\nu\nu'\tau}^{--} \mathbf{I}_{\nu'\tau}^{-} + \epsilon_{\tau} \mathbf{B}_{\nu\tau} \quad , \quad (24)$$

where for every depth point  $\tau$ ,  $\epsilon_{\tau}$  is a scalar function and the  $\mathbf{B}$ 's are vectors of size  $N_{\nu}$  with the identical values of the Planck function at line center ( $\nu = \nu_0$ ) as components. Here

$$\begin{aligned} \mathbf{R}_{\nu\nu'\tau}^{++} &\equiv (1 - \epsilon_{\tau}) \mathbf{W} \mathbf{G}_{\nu\nu'\tau}^{++} \\ \mathbf{R}_{\nu\nu'\tau}^{+-} &\equiv (1 - \epsilon_{\tau}) \mathbf{W} \mathbf{G}_{\nu\nu'\tau}^{+-} \\ \mathbf{R}_{\nu\nu'\tau}^{-+} &\equiv (1 - \epsilon_{\tau}) \mathbf{W} \mathbf{G}_{\nu\nu'\tau}^{-+} \\ \mathbf{R}_{\nu\nu'\tau}^{--} &\equiv (1 - \epsilon_{\tau}) \mathbf{W} \mathbf{G}_{\nu\nu'\tau}^{--} \end{aligned} \quad (25)$$

where  $\mathbf{W}$  is a diagonal matrix of size  $N_{\nu} \times N_{\nu}$  which contains the frequency integration weights. For every depth point  $\tau$ , the  $\mathbf{I}$ 's and  $\mathbf{S}$ 's are vectors of length  $N_{\nu}$  and the  $\mathbf{R}$ 's matrices of size  $N_{\nu} \times N_{\nu}$ . For the formal solution one similarly finds

$$\mathbf{I}_{\nu'\tau}^{+} = \Lambda_{\nu'\tau\tau'}^{+} \mathbf{S}_{\nu'\tau'}^{+} \quad , \quad (26)$$

$$\mathbf{I}_{\nu'\tau}^{-} = \Lambda_{\nu'\tau\tau'}^{-} \mathbf{S}_{\nu'\tau'}^{-} \quad , \quad (27)$$

where the  $\Lambda$ -operator is a matrix of size  $N_{\tau} \times N_{\tau}$  for every frequency point  $\nu'$ . In principle Eqs. (23) to (27) can be solved by direct matrix manipulations. This however involves inversions of large matrices and is very time consuming. It is therefore advantageous to use an operator splitting method.

## 2.2. The operator splitting method

The operator splitting method supposes that a simplified operator,  $\Lambda^*$ , in our case a diagonal operator (given in the appendix), can be found which leads to an approximate solution and which in a series of perturbation iterations lets the approximate solution converge to the true solution. The speed of the method derives from the greatly simplified matrix inversion. Assume that

$$\Lambda^+ = \Lambda^{*+} + (\Lambda^+ - \Lambda^{*+}) \quad , \quad \Lambda^- = \Lambda^{*-} + (\Lambda^- - \Lambda^{*-}) \quad , \quad (28)$$

where  $\Lambda^{*+}$ ,  $\Lambda^{*-}$  are two in  $\tau\tau'$  diagonal operators. Then by inserting Eqs. (26), (27) in (23), (24) one has

$$\begin{aligned} S_{\nu\tau}^+ &= \mathbf{R}_{\nu\nu'\tau}^{++} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau}^+ + \mathbf{R}_{\nu\nu'\tau}^{++} (\Lambda^+ - \Lambda^{*+})_{\nu'\tau\tau'} S_{\nu'\tau'}^+ \\ &+ \mathbf{R}_{\nu\nu'\tau}^{+-} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau}^- + \mathbf{R}_{\nu\nu'\tau}^{+-} (\Lambda^- - \Lambda^{*-})_{\nu'\tau\tau'} S_{\nu'\tau'}^- + \epsilon_\tau \mathbf{B}_{\nu\tau}, \end{aligned} \quad (29)$$

$$\begin{aligned} S_{\nu\tau}^- &= \mathbf{R}_{\nu\nu'\tau}^{-+} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau}^+ + \mathbf{R}_{\nu\nu'\tau}^{-+} (\Lambda^+ - \Lambda^{*+})_{\nu'\tau\tau'} S_{\nu'\tau'}^+ \\ &+ \mathbf{R}_{\nu\nu'\tau}^{--} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau}^- + \mathbf{R}_{\nu\nu'\tau}^{--} (\Lambda^- - \Lambda^{*-})_{\nu'\tau\tau'} S_{\nu'\tau'}^- + \epsilon_\tau \mathbf{B}_{\nu\tau}. \end{aligned} \quad (30)$$

Assume that the source functions can be written as a series with successive terms of decreasing magnitude  $S_{\nu\tau}^+ \equiv S_{\nu\tau}^{+0} + S_{\nu\tau}^{+1} + \dots$ ,  $S_{\nu\tau}^- \equiv S_{\nu\tau}^{-0} + S_{\nu\tau}^{-1} + \dots$ . Inserting these expansions and collecting terms of the same order, noting that the terms with  $\Lambda - \Lambda^*$  are of lower order, one finds for the zeroth order

$$S_{\nu\tau}^{+0} = \mathbf{R}_{\nu\nu'\tau}^{++} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau}^{+0} + \mathbf{R}_{\nu\nu'\tau}^{+-} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau}^{-0} + \epsilon_\tau \mathbf{B}_{\nu\tau} \quad , \quad (31)$$

$$S_{\nu\tau}^{-0} = \mathbf{R}_{\nu\nu'\tau}^{-+} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau}^{+0} + \mathbf{R}_{\nu\nu'\tau}^{--} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau}^{-0} + \epsilon_\tau \mathbf{B}_{\nu\tau} \quad , \quad (32)$$

for the first order

$$\begin{aligned} S_{\nu\tau}^{+1} &= \mathbf{R}_{\nu\nu'\tau}^{++} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau}^{+1} + \mathbf{R}_{\nu\nu'\tau}^{++} (\Lambda^+ - \Lambda^{*+})_{\nu'\tau\tau'} S_{\nu'\tau'}^{+0} \\ &+ \mathbf{R}_{\nu\nu'\tau}^{+-} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau}^{-1} + \mathbf{R}_{\nu\nu'\tau}^{+-} (\Lambda^- - \Lambda^{*-})_{\nu'\tau\tau'} S_{\nu'\tau'}^{-0} \quad , \end{aligned} \quad (33)$$

$$\begin{aligned} S_{\nu\tau}^{-1} &= \mathbf{R}_{\nu\nu'\tau}^{-+} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau}^{+1} + \mathbf{R}_{\nu\nu'\tau}^{-+} (\Lambda^+ - \Lambda^{*+})_{\nu'\tau\tau'} S_{\nu'\tau'}^{+0} \\ &+ \mathbf{R}_{\nu\nu'\tau}^{--} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau}^{-1} + \mathbf{R}_{\nu\nu'\tau}^{--} (\Lambda^- - \Lambda^{*-})_{\nu'\tau\tau'} S_{\nu'\tau'}^{-0} \quad , \end{aligned} \quad (34)$$

and for the  $k$ -th order

$$\begin{aligned} S_{\nu\tau}^{+k} &= \mathbf{R}_{\nu\nu'\tau}^{++} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau}^{+k} + \mathbf{R}_{\nu\nu'\tau}^{++} (\Lambda^+ - \Lambda^{*+})_{\nu'\tau\tau'} S_{\nu'\tau'}^{+,k-1} \\ &+ \mathbf{R}_{\nu\nu'\tau}^{+-} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau}^{-k} + \mathbf{R}_{\nu\nu'\tau}^{+-} (\Lambda^- - \Lambda^{*-})_{\nu'\tau\tau'} S_{\nu'\tau'}^{-,k-1} \quad , \end{aligned} \quad (35)$$

$$\begin{aligned} S_{\nu\tau}^{-k} &= \mathbf{R}_{\nu\nu'\tau}^{-+} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau}^{+k} + \mathbf{R}_{\nu\nu'\tau}^{-+} (\Lambda^+ - \Lambda^{*+})_{\nu'\tau\tau'} S_{\nu'\tau'}^{+,k-1} \\ &+ \mathbf{R}_{\nu\nu'\tau}^{--} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau}^{-k} + \mathbf{R}_{\nu\nu'\tau}^{--} (\Lambda^- - \Lambda^{*-})_{\nu'\tau\tau'} S_{\nu'\tau'}^{-,k-1} \quad . \end{aligned} \quad (36)$$

Adding Eqs. (31), (33), (35) as well as (32), (34), (36) up to  $k$  and defining successive approximations of the source functions by

$$S_{\nu\tau k}^+ \equiv \sum_{j=0}^k S_{\nu\tau}^{+j} \quad ; \quad S_{\nu\tau k}^- \equiv \sum_{j=0}^k S_{\nu\tau}^{-j} \quad , \quad (37)$$

one finally finds

$$\begin{aligned} &(1 - \mathbf{R}_{\nu\nu'\tau}^{++} \Lambda_{\nu'\tau}^{*+}) S_{\nu\tau k}^+ \\ &= +\mathbf{R}_{\nu\nu'\tau}^{+-} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau k}^- + \epsilon_\tau \mathbf{B}_{\nu\tau} + \mathbf{R}_{\nu\nu'\tau}^{++} \mathbf{I}_{\nu'\tau, k-1}^+ \\ &- \mathbf{R}_{\nu\nu'\tau}^{+-} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau, k-1}^+ + \mathbf{R}_{\nu\nu'\tau}^{+-} \mathbf{I}_{\nu'\tau, k-1}^- - \mathbf{R}_{\nu\nu'\tau}^{--} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau, k-1}^- \quad , \end{aligned} \quad (38)$$

$$\begin{aligned} &(1 - \mathbf{R}_{\nu\nu'\tau}^{--} \Lambda_{\nu'\tau}^{*-}) S_{\nu\tau k}^- \\ &= +\mathbf{R}_{\nu\nu'\tau}^{-+} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau k}^+ + \epsilon_\tau \mathbf{B}_{\nu\tau} + \mathbf{R}_{\nu\nu'\tau}^{-+} \mathbf{I}_{\nu'\tau, k-1}^+ \\ &- \mathbf{R}_{\nu\nu'\tau}^{--} \Lambda_{\nu'\tau}^{*+} S_{\nu'\tau, k-1}^+ + \mathbf{R}_{\nu\nu'\tau}^{--} \mathbf{I}_{\nu'\tau, k-1}^- - \mathbf{R}_{\nu\nu'\tau}^{--} \Lambda_{\nu'\tau}^{*-} S_{\nu'\tau, k-1}^- \quad , \end{aligned} \quad (39)$$

where for the  $k-1$ -st approximation of the source function the formal solution

$$\begin{aligned} \mathbf{I}_{\nu'\tau, k-1}^+ &= \Lambda_{\nu'\tau\tau'}^+ S_{\nu'\tau', k-1}^+ \\ \mathbf{I}_{\nu'\tau, k-1}^- &= \Lambda_{\nu'\tau\tau'}^- S_{\nu'\tau', k-1}^- \quad , \end{aligned} \quad (40)$$

has been used. Equations (38), (39) constitute a system of equations for the  $k$ -th approximation of the source functions given in terms of the  $k-1$ -st approximation. The advantage this system is, that it involves only quantities of a fixed depth  $\tau$  and that the matrices need only be of the  $N_\nu \times N_\nu$  size while the full dependence enters when the formal solution is computed.

To solve this system of equations we define eight auxiliary matrices

$$\begin{aligned} \mathbf{A}_{\nu\nu'\tau}^{++} &\equiv \mathbf{R}_{\nu\nu'\tau}^{++} \Lambda_{\nu'\tau}^{*+} \quad , \quad \mathbf{A}_{\nu\nu'\tau}^{+-} \equiv \mathbf{R}_{\nu\nu'\tau}^{+-} \Lambda_{\nu'\tau}^{*+} \\ \mathbf{A}_{\nu\nu'\tau}^{+ -} &\equiv \mathbf{R}_{\nu\nu'\tau}^{+-} \Lambda_{\nu'\tau}^{*-} \quad , \quad \mathbf{A}_{\nu\nu'\tau}^{--} \equiv \mathbf{R}_{\nu\nu'\tau}^{--} \Lambda_{\nu'\tau}^{*-} \quad , \end{aligned} \quad (41)$$

$$\mathbf{D}_{\nu\nu'\tau} \equiv (1 - \mathbf{A}_{\nu\nu'\tau}^{--})^{-1} \quad , \quad (42)$$

$$\mathbf{F}_{\nu\nu'\tau} \equiv (1 - \mathbf{A}_{\nu\nu'\tau}^{++} - \mathbf{A}_{\nu\nu'\tau}^{+-} \mathbf{D}_{\nu\nu'\tau} \mathbf{A}_{\nu\nu'\tau}^{+ -})^{-1} \quad , \quad (43)$$

$$\mathbf{G}_{\nu\nu'\tau} \equiv \mathbf{D}_{\nu\nu'\tau} \mathbf{A}_{\nu\nu'\tau}^{+ -} \quad , \quad (44)$$

$$\mathbf{H}_{\nu\nu'\tau} \equiv \mathbf{F}_{\nu\nu'\tau} \mathbf{A}_{\nu\nu'\tau}^{+-} \mathbf{D}_{\nu\nu'\tau} \quad , \quad (45)$$

and two error vectors

$$\mathbf{E}_{\nu\tau, k-1}^+ \equiv \mathbf{R}_{\nu\nu'\tau}^{++} \mathbf{I}_{\nu'\tau, k-1}^+ + \mathbf{R}_{\nu\nu'\tau}^{+-} \mathbf{I}_{\nu'\tau, k-1}^- + \epsilon_\tau \mathbf{B}_{\nu\tau} - S_{\nu\tau, k-1}^+ \quad , \quad (46)$$

$$\mathbf{E}_{\nu\tau,k-1}^- \equiv \mathbf{R}_{\nu\nu'\tau}^+ \mathbf{I}_{\nu'\tau,k-1}^+ + \mathbf{R}_{\nu\nu'\tau}^- \mathbf{I}_{\nu'\tau,k-1}^- + \epsilon_\tau \mathbf{B}_{\nu\tau} - \mathbf{S}_{\nu'\tau,k-1}^- . \quad (47)$$

Adding and subtracting  $\mathbf{S}_{\nu\tau,k-1}^+$ ,  $\mathbf{S}_{\nu'\tau,k-1}^+$  in Eqs. (38) and (39) the system can be written

$$\begin{aligned} (1 - \mathbf{A}_{\nu\nu'\tau}^{++})(\mathbf{S}_{\nu\tau,k}^+ - \mathbf{S}_{\nu\tau,k-1}^+) \\ = \mathbf{A}_{\nu\nu'\tau}^{+-}(\mathbf{S}_{\nu\tau,k}^- - \mathbf{S}_{\nu\tau,k-1}^-) + \mathbf{E}_{\nu\tau,k-1}^+ , \end{aligned} \quad (48)$$

$$\begin{aligned} (1 - \mathbf{A}_{\nu\nu'\tau}^{--})(\mathbf{S}_{\nu\tau,k}^- - \mathbf{S}_{\nu\tau,k-1}^-) \\ = \mathbf{A}_{\nu\nu'\tau}^{-+}(\mathbf{S}_{\nu\tau,k}^+ - \mathbf{S}_{\nu\tau,k-1}^+) + \mathbf{E}_{\nu\tau,k-1}^- , \end{aligned} \quad (49)$$

and eventually

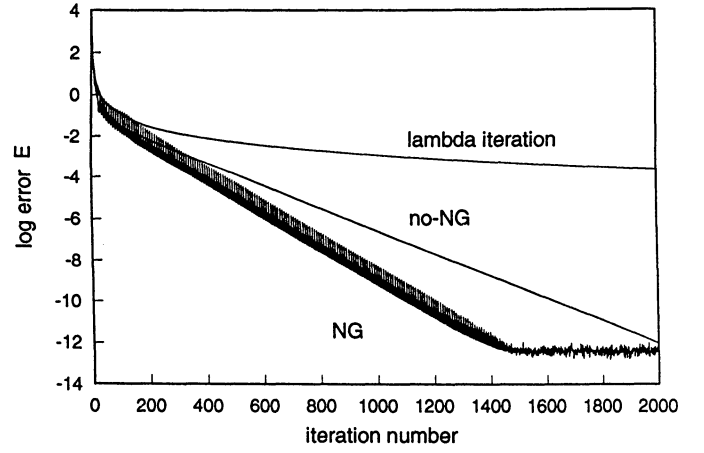
$$(\mathbf{S}_{\nu\tau,k}^- - \mathbf{S}_{\nu\tau,k-1}^-) = \mathbf{G}_{\nu\nu'\tau}(\mathbf{S}_{\nu\tau,k}^+ - \mathbf{S}_{\nu\tau,k-1}^+) + \mathbf{D}_{\nu\nu'\tau} \mathbf{E}_{\nu\tau,k-1}^+ , \quad (50)$$

$$(\mathbf{S}_{\nu\tau,k}^+ - \mathbf{S}_{\nu\tau,k-1}^+) = \mathbf{H}_{\nu\nu'\tau} \mathbf{E}_{\nu\tau,k-1}^- + \mathbf{F}_{\nu\nu'\tau} \mathbf{E}_{\nu\tau,k-1}^+ . \quad (51)$$

The procedure to solve the system (38), (39) is as follows. On basis of the information about the line, the atmosphere model and the frequency, angle and depth grids the redistribution matrices and the auxiliary matrices can be computed. These matrices need to be calculated only once, at the start of the iteration. For the redistribution matrices  $G$  the redistribution function  $R_{II}$  is used either alone or in the form of Eq. (13-73) by Mihalas (1978, p. 435). For  $R_{II}$  the approximation of Gouttebroze (1986) was used. The simplified diagonal operator,  $\Lambda^*$ , constructed using the method of Kalkofen & Ulmschneider (1984) is given in the appendix. The solution is obtained by the following iteration steps. With the  $k-1$ -st estimate of the source functions  $\mathbf{S}_{\nu\tau,k-1}^+$ ,  $\mathbf{S}_{\nu\tau,k-1}^-$ , the formal solution is computed via Eqs. (40), using the linear method of Kalkofen & Ulmschneider (1984). The error vectors  $\mathbf{E}_{\nu\tau,k-1}^+$ ,  $\mathbf{E}_{\nu\tau,k-1}^-$ , are evaluated from Eqs. (46), (47). By using Eq. (51) and subsequently (50), the  $k$ -th estimate of the source functions are found etc.

### 3. The convergence properties of the method

In his discussion of the acceleration of the iterative convergence in methods of radiative transfer, Auer (1987, 1991) uses an exact solution to test his complete redistribution method. In our case of partial redistribution an exact solution is not known to us. To assess the convergence properties of our method we therefore generated an “exact” solution by slightly modifying the source



**Fig. 3.** Maximum error versus iteration number for our method with and without NG-acceleration, and using the lambda- iteration

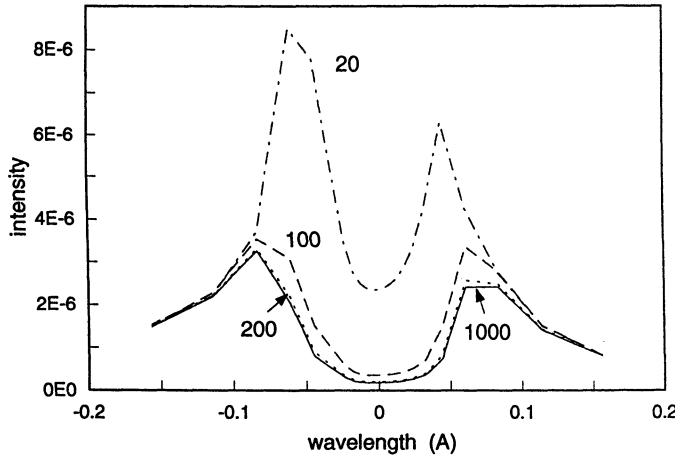
term. To improve the convergence in our iteration scheme we follow Auer and employ the NG-acceleration in the following way. For every frequency and angle point, we retain the source functions as function of depth of four subsequent iterations. Similarly as discussed in Auer (1987) we then extrapolate to an improved source function vector at the given frequency and angle in such a way as to make the least squares sum of the source function changes  $\delta S$  a minimum.

Employing 29 frequency, 2 angle and 170 depth points we iterate  $IT = 4000$  times until the relative deviations  $\delta S/S$  are less than a few times  $10^{-13}$ . In this situations the error vectors  $\delta S : \mathbf{E}_{\nu\tau,k-1}^+$ ,  $\mathbf{E}_{\nu\tau,k-1}^-$  have elements which are everywhere smaller than about  $5 \cdot 10^{-18}$ . Comparing this in Eqs. (46), (47) with the source term  $\epsilon \mathbf{B}$  we see that the error terms are everywhere at least  $3 \cdot 10^{-4}$  times smaller than the smallest value of  $\epsilon \mathbf{B}$  of  $1.8 \cdot 10^{-14}$ , which occurs at the front shock point near 1400 km (see Fig. 2 of Rammacher & Ulmschneider 1992). By adding the error vectors to the vector  $\epsilon \mathbf{B}$  we slightly modify our problem in that we now seek a solution for this combined source term. For this source term the source functions of the last iteration (at  $IT=4000$ ) are an exact solution to machine accuracy. This we henceforth call “exact” solution,  $S_{exact}$ , although it is only the exact solution to a slightly modified problem.

Using the thus found source functions as exact solution, we are able to investigate the convergence properties of our method. In Fig. 3 we give the maximum error  $E = |S - S_{exact}|/S_{exact}$  over all frequency, angle and depth points of a given iteration as function of the iteration number  $IT$ . It is seen that with the NG-acceleration, after about 1400 iterations, the source function has converged to machine accuracy. Without NG- acceleration, the convergence is noticeably slowed, while for the pure lambda-iteration the convergence is very slow as expected.

With about 200 iterations and using the NG-acceleration, a reasonable accuracy of about  $E = 0.1\%$  is reached. This is what one demands in practical applications. That  $IT = 200$  gives a reasonable accuracy is also seen from Fig. 4, which shows the emerging line intensity as function of iteration number  $IT$ .





**Fig. 4.** Emerging line intensity as function of iteration number using our method. Convergence is found after about 200 iterations

It remains to discuss why the convergence is an order of magnitude slower than that discussed by Auer (1987, 1991). First, our problem couples the source functions over the frequency integral which should lead to a much more difficult convergence behaviour. Second, we use the diagonal Olson+Kunasz operator which is known to lead to much slower convergence compared to a three or pentagonal operator or to the full Scharmer operator (Carlsson 1986). That this is so, has been tested by looking into the convergence property of the method in the CRD case, replacing  $R_{II}$  by  $\varphi_{\nu\mu}\varphi_{\nu'\mu'}$ . The error  $E = 5 \cdot 10^{-13}$  in this case was reached after about 300 iterations, using NG acceleration, which is much slower than the 55 iterations found for the same case using a three diagonal operator (Buchholz et al. 1994). The convergence of the method in the PRD case is thus as one expects from a diagonal operator. Finally note that the computer code including test output can be obtained from the author upon request.

#### 4. Conclusions

We have developed an operator splitting method for the calculation of spectral line radiation assuming partial redistribution. This method is able to treat shock discontinuities and leads to a reasonable accuracy in about 200 iterations. Machine accuracy is reached at about 1400 iterations.

**Acknowledgements.** The author thanks Larry Auer for helpful comments on the manuscript.

#### Appendix

This appendix gives the simplified diagonal operator,  $\Lambda^*$ , constructed on basis of the linear integration method of Kalkofen and Ulmschneider (1984). Assuming depth points  $k = 1, \dots, K$  counted downwards into the star and frequency points  $n = 1, \dots, N$  one computes for the outgoing beam the optical depths  $\tau_{n,k}^+$  and for the ingoing beam the optical depths  $\tau_{n,k}^-$ . One then has with  $\delta \equiv \tau_{n,k+1}^+ - \tau_{n,k}^+$

$$\Lambda_{n,k}^{*+} = \begin{cases} \frac{\delta}{2+\delta} & \delta \leq 1 \\ \frac{2\delta-1}{1+2\delta} & \delta > 1 \end{cases}, \quad (52)$$

for  $k = 1, \dots, K-1$ ,

$$\Lambda_{n,K}^{*+} = 1, \quad (53)$$

and with  $\delta \equiv \tau_{n,k}^- - \tau_{n,k-1}^-$

$$\Lambda_{n,k}^{*-} = \begin{cases} \frac{\delta}{2+\delta} & \delta \leq 1 \\ \frac{2\delta-1}{1+2\delta} & \delta > 1 \end{cases}, \quad (54)$$

for  $k = 2, \dots, K$ ,

$$\Lambda_{n,1}^{*-} = 0. \quad (55)$$

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