Astron. Astrophys. 297, 771–778 (1995)

ASTRONOMY AND ASTROPHYSICS

A new approximate operator method for partial frequency redistribution problems

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Received 25 August 1994 / Accepted 20 October 1994

Abstract. Methods for the solution of non–LTE partial frequency redistribution (PRD) radiative transfer problems are presented. By explicitly treating the partial frequency coherence, convergence difficulties caused by using a Complete Redistribution Approximation are completely overcome. A new core–wing treatment of the redistribution both avoids the explicit solution of the frequency coupled system, and permits the use of simple Approximate Operator Iteration to solve PRD problems extremely efficiently.

Key words: radiative transfer – methods: numerical – stars: atmospheres – lines: formation

1. Introduction

Partially coherent scattering can have important effects on the formation of strong resonance lines in stellar atmospheres. Detailed studies of the mechanisms for photon emission and absorption leading to the frequency redistribution functions can be found in the works of Hummer (1962) or, more recently, Omont et al. (1972).

The effects of frequency redistribution can strongly modify computed line profiles. Inclusion of a correct representation of scattering processes in numerical radiative transfer computations began with Hummer (1969). This work showed the importance of partial frequency redistribution (PRD) in the modelling of resonance lines, especially far from the Doppler core where photons scattering is almost coherent. Rapid development of computing resources in the 70's allowed the application of radiative transfer including PRD to the explanation of the observed profiles of strong solar resonance lines. Among other studies (for a review, see Linsky 1985), we can mention the work of Shine et al. (1975), who demonstrated that PRD is needed to reproduce the limb–darkening (at all wavelengths) of the chromospheric Ca II K line profiles. PRD likewise plays a crucial role in the modelling of resonance lines formed in quiescent prominences (e.g. H I Lyα), where the scattering of chromospheric radiation is the main source of emission in these structures (Heinzel et al. 1987; Paletou et al. 1993). Partial frequency redistribution effects should also be included in other astrophysical models, for instance, quasi–stellar objects H I Lyα emission, as pointed out by Avrett & Loeser (1988), the modelling of Fe II and Mg II resonance lines in active galactic nuclei (Collin–Souffrin & Dumont 1986), and the H I Lyα albedo of giant planet's atmosphere like Jupiter (Ben Jaffel et al. 1988).

In the present article, we introduce new approximate operator techniques which permit the efficient solution of PRD problems. These new methods are presented, in Sects. 4 and 5, in the context of the two–level atom problem. Our purpose is to overcome the limitations of Scharmer's approach (1983). That numerical procedure, while providing a fast and easy way to treat some PRD problems, is known to fail at large frequencies (more than, say, 100 Doppler widths from line center) in PRD–R_{II} (coherent scattering in the atom's frame, see Hummer 1962), if the slab remains optically thick at these frequencies. This is due to the fact that outside the Doppler core the scattering becomes quasi–coherent, which is obviously very far from the physical assumption of non–coherence underlying the complete redistribution (CRD) approximation. The approach advocated by Cannon et al. (1975) and Scharmer (1983) which uses the CRD approximation over the entire line is poor in the wings, and, indeed, does not converge in the extreme line wings. In Sect. 4, we show that this difficulty is completely overcome by explicitly treating the local partial coherence of the scattering process. In Sect. 5, we present a faster, but equally robust method which uses the CRD approximation in the line core and, coherent scattering for wing frequencies. This later method, which is based on approximate operators for both the frequency redistribution and the radiation transport completely avoids the solution of large systems of simultaneous equations and is the

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** The National Center for Atmospheric Research is sponsored by the National Science Foundation.

clear "method-of-choice" for the solution of transfer problems involving PRD.

2. PRD scattering by a two–level atom

We treat here the case of a two–level atom with a background continuum, and partial frequency redistribution. For notational simplicity we shall not write the optical depth dependence of the quantities explicitly.

The monochromatic source function S_x can be expressed as

$$S_x = \frac{\phi_x}{\phi_x + r} S_{lx} + \frac{r}{\phi_x + r} B \tag{1}$$

where x is the frequency measured from line center in Doppler units ($x = \Delta\nu/\Delta\nu_D$), ϕ_x is the absorption profile (we shall use a Voigt profile for all computations refered hereafter), B the Planck function and r the ratio of continuum to line opacity. The two–level atom line source function S_{lx} is given by

$$S_{lx} = (1-\epsilon)\bar{J}_x + \epsilon B \tag{2}$$

where ϵ is the collisional destruction probability and $\bar{J}_x$ the PRD scattering integral. This formalism is equivalent to the CRD case except that, in PRD, the scattering integral is *frequency dependent*.

Following the Jefferies' notation (1968) and assuming isotropic scattering, let us define $g_{xx'} = R_{xx'}/\phi_x$ where $R_{xx'}$ is the angle–averaged redistribution function and ϕ_x the line absorption profile. The mean PRD intensity is

$$\bar{J}_x = \int g_{xx'} J_{x'} dx' \tag{3}$$

with

$$J_x = \frac{1}{2} \int I_{x\mu} d\mu \tag{4}$$

being the angle–average of the specific intensity $I_{x\mu}$ (μ is the cosine of the angle from the slab normal). The formal solution of the radiative transfer equation can be stated as

$$J_x = \Lambda_x[S_x] \tag{5}$$

We seek to find a numerical scheme such that, given an estimate at iteration (n) of quantity X, $X^{(n)}$, the solution of the non–LTE radiation transfer problem for a two–level atom in PRD will be given by $X^{(n+1)} = X^{(n)} + \delta X^{(n)}$ when $\delta X^{(n)}/X^{(n)} \to 0$. The source function perturbation and approximate monochromatic Λ^*_x operator follow from

$$\begin{cases} S_x^{(n+1)} = S_x^{(n)} + \delta S_x^{(n)} \\ \Lambda_x[\,] = \Lambda^*_x[\,] + \delta\Lambda_x[\,] \end{cases} \tag{6}$$

where the superscript (n) refers to the estimate at step n of the iterative scheme. Hence, the effect of the perturbation on the intensity is, to first order,

$$J_x^{(n+1)} = J_x^{(n)} + \Lambda^*_x[\delta S_x^{(n)}] \tag{7}$$

and the perturbation of the scattering integral is

$$\bar{J}_x^{(n+1)} = \bar{J}_x^{(n)} + \int g_{xx'} \Lambda^*_{x'}[\delta S_{x'}^{(n)}] dx' \tag{8}$$

Our goal is to solve Eq. (2) iteratively for $\delta S_{lx}^{(n)}$,

$$S_{lx}^{(n)} + \delta S_{lx}^{(n)} = (1-\epsilon)\bar{J}_x^{(n+1)} + \epsilon B \tag{9}$$

Explicitly expressing the change in the mean PRD intensity in terms of source function perturbations, we obtain the equations for δS_{lx}

$$\delta S_{lx}^{(n)} - (1-\epsilon) \int g_{xx'} \Lambda^*_{x'}[p_{x'} \delta S_{lx'}^{(n)}] dx' = r_x \tag{10}$$

where the probability that a photon is absorbed in the line appears as

$$p_x = \frac{\phi_x}{\phi_x + r} \tag{11}$$

and the frequency dependent residual

$$r_x = (1-\epsilon)\bar{J}_x^{(n)} + \epsilon B - S_{lx}^{(n)} \tag{12}$$

The above equations have been derived for a general approximate Λ^* operator; however, the problem is greatly simplified by using the local approximate operator of Olson et al. (1986; hereafter OAB). Instead of a general operator, the perturbation in the monochromatic radiation field is then estimated by simple multiplication

$$\delta J_x \approx \Lambda^*_x \, \delta S_x \tag{13}$$

Using this local, i.e. diagonal, monochromatic approximate Λ–operator, the Λ^*_x appearing in the frequency–dependent integral is simply a scalar variable, and the line source function corrections δS_{lx} are found from the system of linear equations

$$\delta S_{lx}^{(n)} - (1-\epsilon) \sum_{x'} \tilde{g}_{xx'} p_{x'} \Lambda^*_{x'} \delta S_{lx'}^{(n)} = r_x \tag{14}$$

where the $\tilde{g}_{xx'}$ are the elements of the redistribution matrix as well as the weights used in the numerical evaluation of the PRD scattering integral (Eq. (3)). The new PRD algorithm can be described as:

(0) given an initial source function, S_x,
(1) compute $\bar{J}_x$ from Eqs. (3) and (5),
(2) at each depth, solve the δS_{lx} equations (14),
(3) then update S_{lx} and S_x (Eq. (1)),
(4) test for convergence and return to (1) if not.

Scharmer's approach (1983), hereafter CRDA, to the treatment of PRD problems differs from this in that he used $\phi_{x'}$ instead of $g_{xx'}$, i.e. assumed CRD, in the correction equation (14). The schemes being presented here avoid the CRDA approximation, and solve directly for the frequency dependent source function corrections. They explicitly treat the correlation in the

frequency dependent source function caused by PRD. In the first, the frequency–by–frequency or FBF method, the true $g_{xx'}$ matrix is used. This requires the solution of systems of $N_{\rm freq}$ linear equations *at each depth in the atmosphere*, but overcomes the convergence problems of CRDA. A method similar to this has been independently derived by Ulmschneider (1994). In the second, a Core–Wing approximation to the true redistribution is used in place of $g_{xx'}$. The idea of using coherent scattering in the line wings instead of complete redistribution goes back to Jefferies & White (1960). It has been widely used to avoid solving coupled PRD problems, improved by Kneer (1975) and extended by Hubený (1985). We shall demonstrate that it can be the basis of an extremely efficient *iterative* approximation for the true PRD operator. This new method (CRDCS) method is as computationally efficient as CRDA, but like FBF converges even for the most difficult cases.

3. Construction of the local monochromatic Λ^*_x operator

In order to evaluate the Λ^*_x operators, we use a diagonal approximate operator scheme as developed in OAB. The 1D short characteristics method with monotonic parabolic interpolation is described in Auer & Paletou (1994). The Λ^*_x operators are simply the diagonal of the full monochromatic Λ_x operator. Formally, $\Lambda^*_{x,dd} = \Lambda_{x,dd'}[\delta_{dd'}]$ where $\delta_{dd'}$ is the Dirac function. From the integral equations corresponding to a discretizaton of $S(\tau)$, after angular integration, we, thus, obtain at each depth the diagonal elements of Λ^*_x. For both the formal solution of the transfer equation and the computation of the diagonal Λ^*_x operators the 1D short characteristics method is used.

3.1. Approximation at small optical depths

The formal radiative transfer equation is solved using piecewise quadratic expansions of the source functions. This requires the evaluation of the weights w_i corresponding to polynomial terms τ^i. These weights can be generated by recursion and appear in Auer & Paletou (1994; Eq. (10)) as

$$\begin{cases} w_0 = 1 - e^{-\Delta\tau} \\ w_1 = w_0 - \Delta\tau e^{-\Delta\tau} \\ w_2 = 2w_1 - \Delta\tau^2 e^{-\Delta\tau} \end{cases} \tag{15}$$

However, we have noticed that care must be used to avoid unrealistic and/or negative values of the specific intensities $I_{\mu xd}$ when dealing with very small optical depths. These numerical artifacts (round–off) can simply be avoided by using expansions of the integral formal solution weights at low optical depths.To avoid round–off problems, for $\Delta\tau < 10^{-2}$ we recommend to use the following power series expansions:

$$w_{(n=0,1,2)} = \Delta\tau^{(n+1)}\left[\frac{1}{n+1} - \frac{\Delta\tau}{n+2} + \frac{\Delta\tau^2}{2(n+3)} - \frac{\Delta\tau^3}{6(n+4)} + \frac{\Delta\tau^4}{24(n+5)}\right] \tag{16}$$

This guarantees positiveness of the computed specific intensities especially at large frequencies where an oversampling of the optical depth scale occurs in the range $0 < \tau_x < 10^{-2}$.

4. Frequency–by–frequency method

The system of linear equations in Eq. (14) can be summarized by the formal expression

$$\boldsymbol{M} \cdot \boldsymbol{\delta S} = \boldsymbol{r} \tag{17}$$

where $\boldsymbol{r}$ is the right–hand side of Eq. (14). The elements of $\boldsymbol{M}$ are of the form

$$M_{ij} = \delta_{ij} - (1-\epsilon)\tilde{g}_{ij}\Lambda^*_j p_j \;\; ; \;\; i,j = 1,...,N_{\rm freq} \tag{18}$$

where δ_{ij} is the Kronecker's symbol and the indexes i and j refer respectively to the discretized values of x and x'.

The solution of the system requires the inversion of a $(N_{\rm freq} \times N_{\rm freq})$ matrix *at each depth in the atmosphere* but this computational cost may be significantly reduced. During the iterations for the frequency dependent source function, the $\boldsymbol{M}$ matrices do not change, although the $\boldsymbol{r}$ do vary from one iteration to another. This system of linear equations can be solved using the LU decomposition scheme (cf. Press et al. 1986). For this method the decomposition of the $\boldsymbol{M}$ matrices is the major computational cost. The reduced matrices may be stored and then reused to find the later corrections at very little computational effort. That is, in the first iteration, one computes $\boldsymbol{M}$ and its LU decomposition, at each depth. Then, we store the matrix in its factored form. In subsequent iterations, we simply (1) read the LU matrices from the storage file and (2) perform the resolution of the system for the new right–hand side $\boldsymbol{r}$. The time for the solution with a new right–hand side is only a small fraction of the "once only" LU factorization.

4.1. Properties of the FBF method

We shall concentrate here on $R_{\rm II}$ redistribution which describes the case of coherent scattering in the atom's frame (Hummer 1962). For realistic cases of resonance line transfer, we should use the general expression (Omont et al. 1972)

$$R(x,x') = \gamma R_{\rm II}(x,x') + (1-\gamma)R_{\rm III}(x,x') \tag{19}$$

but for the following illustrative examples, we shall restrict ourselves to cases involving pure $R_{\rm II}$ redistribution, i.e. we set the branching ratio $\gamma = 1$. In this case, the CRDA method is known to converge properly *as long as the slab is optically thin at frequencies where the scattering is nearly coherent* (see Auer & Paletou 1994). Our frequency–by–frequency (FBF) method overcomes the limitation of the CRDA approximation as demonstrated here.

For illustrative purposes, consider one dimensional constant–property slabs with optical depths at line center τ_0 varying from 10^6 to 10^{12}. The Planck function B is constant and set to unity within the slab and the continuum absorption coefficient was set to 0. The Voigt parameter a is set to 10^{-3} and the collisional destruction probability $\epsilon = 10^{-4}$. The frequency grid extends up to 1000 Doppler widths from line center. A resolution of 0.25 Doppler width is used in the core, for $0 < x < 4$, and the grid is logarithmically spaced for wing frequencies. For

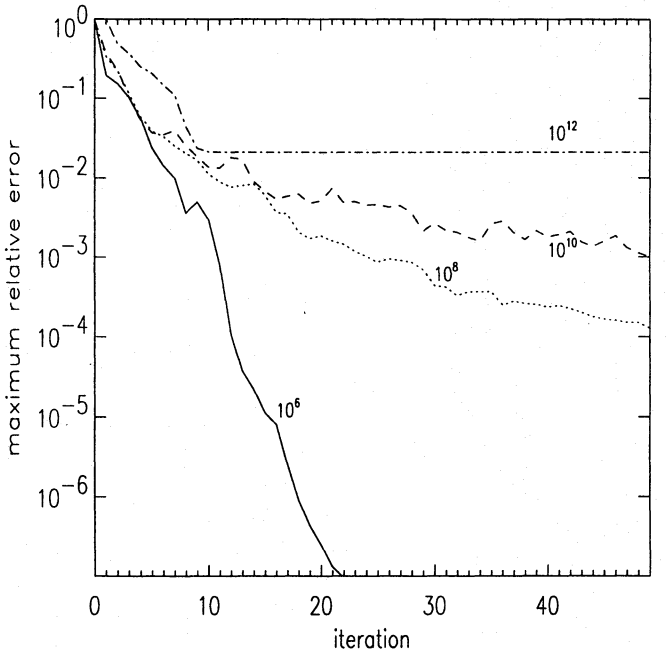

Fig. 1. Convergence of the relative error in the line source functions, using CRDA, obtained for various line center opacity values, $\tau_0 = 10^6, 10^8, 10^{10}, 10^{12}$. The CRDA scheme fails to converge for large values of τ_0

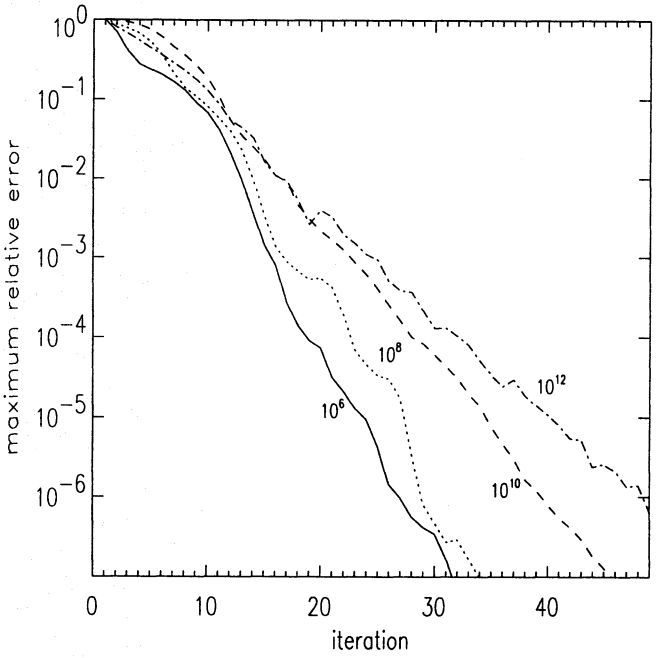

Fig. 2. Same as Fig. 1 but with the FBF scheme. With the new method, we have convergence for all the cases treated here. The most important to feature is that convergence can be obtained even for cases for which the CRDA scheme fails

R_{II}, which is evaluated following Gouttebroze (1986), the diagonal of the redistribution matrix goes to the limit of coherent scattering at large frequencies (i.e. diag[g] $\rightarrow$ 1). We have accelerated the convergence of the PRD schemes using the ORTHDX procedure described in Auer (1991).

For $\tau_0 = 10^6$, as shown in Fig. 1, the CRDA method is very efficient since the slab thickness at the largest frequency considered is only about 10^{-4}. Although the FBF method (Fig. 2) shows good convergence, more iterations (10) are needed to achieve an accuracy of $10^{-3} \times \epsilon$ in the line source functions. On the other hand, the complete failure of the CRDA method is obvious in Fig. 1 when τ_0 is large. The convergence slows progressively and finally "breaks down" for τ_0 larger than 10^{10}. On the contrary, the new method is still convergent even for very large line center optical depths (for $\tau_0 = 10^{12}$, $\tau_{x=1000} > 100$). As long as the CRDA scheme converges properly, both methods yield identical solutions, but the performance of the CRDA approximation dramatically worsens as the optical depth is increased. When $\tau_{x_{max}} > 1$ and $g_{x_{max}x_{max}} \approx 1$ the CRDA scheme simply fails to converge.

5. Core–Wing method

While the FBF approach rectifies the failings of the CRDA scheme, it has several major drawbacks. It requires a large amount of both memory and computing time for realistic radiative transfer problems especially in 2D geometry. In order to overcome this, we recommend finding the corrections to the source function by approximating not only the Λ–operator but also the frequency redistribution function, $g_{xx'}$. Our new method blends the two "limits": (1) CRD approximation and (2) coherent scattering, and is as robust as FBF but computationally much more efficient.

The scheme has a strong physical basis. The origin of the frequency redistribution when a photon is scattered coherently in the atomic frame, i.e. R_{II}, is the fact that the Doppler shift for the incoming and outgoing direction are not the same because of the change in direction. Very roughly, $x_{out} = x_{in} \pm O(1$ Doppler width). For $x_{in} \simeq 0$ this corresponds to redistribution across the line core. For $x_{in} \gg 1$ the Doppler shift is nearly negligible so $x_{out} \simeq x_{in}$ in the wings. This suggests that one may approximate the redistribution function as Complete Redistribution over the core and Coherent Scattering in the wings (or CRDCS). We are lead graphically to the same idea if we plot $g_{xx'}$ as in Fig. 3.

We accordingly divide the frequency domain into a core region ($x \leq x_c$) and a wing region, for larger x. Instead of the true redistribution function, we use $g_{xx'} \approx \phi_{x'}$ for $x, x' \leq x_c$, and $g_{xx'} \approx \delta(x - x')$, for $x' > x_c$. This leads to an approximate redistribution function which has complete redistribution for core frequencies and coherent scattering for wing frequencies:

$$\int g_{xx'} J_{x'} dx' \approx (1 - \alpha_x) \int_{core} \phi_{x'} J_{x'} dx' + \alpha_x \int_{wing} \delta(x - x') J_{x'} dx' \qquad (20)$$

We have introduced the splitting coefficient, α_x, in order to switch smoothly between the two different scattering regimes.

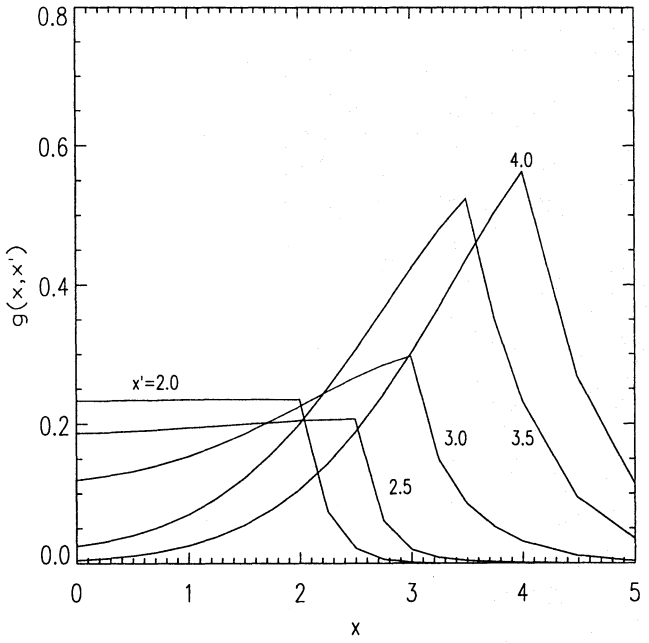

Fig. 3. Behaviour of $g_{xx'}$ as a function of x for different values of x' ($a = 10^{-3}$). It illustrates the transition between the two regimes: CRD–like for core frequencies, small x', and $g_{xx'}$ is centered on $x = 0$; quasi–coherence for wing frequencies, $g_{xx'}$ is peaked at $x = x'$

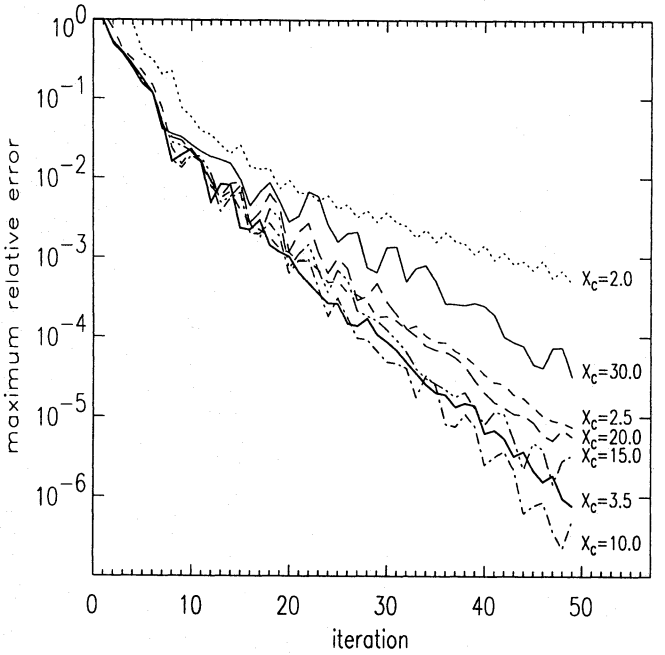

Fig. 4. Convergence of the maximum relative error in the line source functions obtained with the CRDCS scheme, for different values of the Core–Wing separation frequency. This numerical experimentation demonstrates that $x_c = 3.5$ is a reasonable choice

Physically a reasonable choice for the separation frequency x_c is 3.5 Doppler widths. Numerical experimentation, Fig. 4, has both validated this choice and demonstrated the relative insensitivity of the method to values $2 \leq x_c \leq 10$. Further, for the core frequencies, we can set the α_x coefficient to 0. This makes the core δS_{lx} independent of the corrections in the wings which greatly simplifies the solution of the system, as we show below. At larger frequencies, $g_{xx'}$ begins to show the quasi–coherent nature of the R_{II} frequency redistribution, since the function becomes peaked at $x = x'$. To avoid complete decoupling of the core and wing frequency domains, and to insure a progressive switch between the CRD and coherent scattering approximations, for large frequencies (larger than x_c), we use $\alpha_x = g_{xx}$, i.e. the diagonal value of the redistribution matrix at frequency x (see Fig. 5). As shown further in Figs. 6-7, this α_x and $x_c = 3.5$ yield a robustly convergent method, which is easily solved.

The approximate redistribution operator, Eq. (20), when coupled with the OAB approximation, Eq. (13), yields an estimate of the change in $\bar{J}_x$ in terms of the change in S_{lx}:

$$\delta\bar{J}_x \approx (1-\alpha_x)\delta\bar{J}_c + \alpha_x p_x \Lambda^*_x \delta S_{lx} \tag{21}$$

with

$$\delta\bar{J}_c = \int_{-x_c}^{+x_c} \phi_{x'} p_{x'} \Lambda^*_{x'} \delta S_{lx'} dx' \tag{22}$$

The equation for δS_{lx} is obtained by substituting the approximation Eq. (21) into Eq. (10)

$$\delta S^{(n)}_{lx} - (1-\alpha_x)(1-\epsilon)\int_{core} \phi_{x'} p_{x'} \Lambda^*_{x'} \delta S^{(n)}_{lx'} dx' -$$

$$\alpha_x(1-\epsilon)\sum_{wing} p_{x'} \Lambda^*_{x'} \delta S^{(n)}_{lx'} \delta(x-x') = r_x \tag{23}$$

The critical feature of this equation is the simplicity of the coupling between different frequencies: wing frequencies drop out for $x \leq x_c$, and in the wings, core frequencies appear only as a single integral. It is accordingly possible to find all the δS_{lx} from simple scalar equations, completely avoiding the solution of any systems of equations no matter how large the frequency grid is.

5.1. Core frequencies

We solve first for the core corrections. As we just noted, because $\alpha_x = 0$ for $x \leq x_c$, the solution for the core is independent of the wings. The core integral is frequency independent, so following Scharmer (1983) we can define

$$\Delta T = (1-\epsilon)\int_{core} \phi_{x'} p_{x'} \Lambda^*_{x'} \delta S^{(n)}_{lx'} dx' \tag{24}$$

which implies

$$\delta S^{(n)}_{lx} - \Delta T = r_x \tag{25}$$

Integrating over the core, $(1-\epsilon)\int_{core} \phi_{x'} p_{x'} \Lambda^*_{x'}[\ ]dx'$, we can write a scalar equation for ΔT, using the facts that ΔT is frequency independent and Λ^*_x is a local value not a spatial operator.

$$\left(1-(1-\epsilon)\int_{core} \phi_{x'} \Lambda^*_{x'} p_{x'} dx'\right)\Delta T = \bar{r} \tag{26}$$

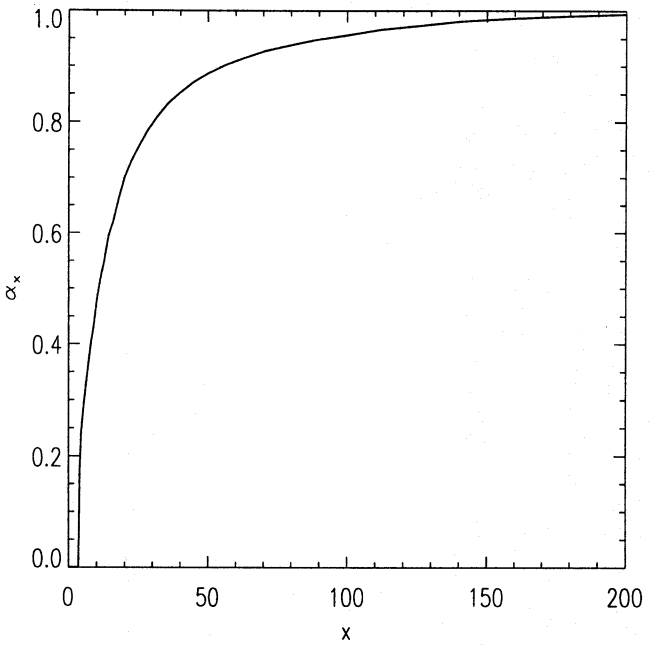

Fig. 5. The set of α_x values we adopted is displayed in this figure, as a function of x the reduced frequency from line center. The diagonal value of the redistribution matrix permits to shift smoothly towards coherent scattering in the far wings

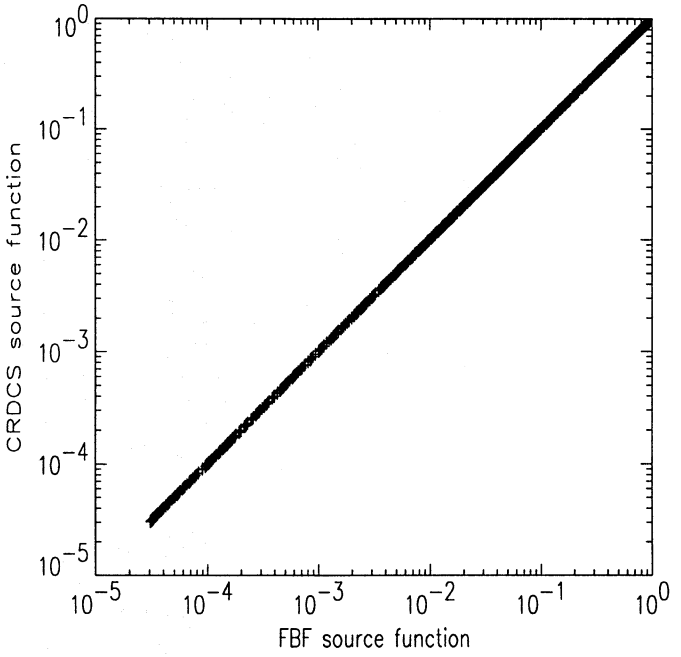

Fig. 6. The agreement between the FBF and the CRDCS scheme is excellent as we obtain a nearly perfect 45° slope line when plotting the values of the source functions computed using the two methods against each other

where $\bar{r} = (1-\epsilon)\int_{core}\phi_{x'}\Lambda^*_{x'}p_{x'}r_{x'}dx'$. ΔT is found by a single division at each point in the grid. Once the ΔT have been evaluated, the source function corrections for core frequencies are merely the sum of a frequency independent term plus a frequency dependent one, the residual r_x (cf. Eq. (25)).

5.2. *Wing frequencies*

The coherent scattering approximation used for wing frequencies makes the evaluation of the related source function corrections also very simple and fast. Using the monochromatic diagonal operator Λ^*_x and, assuming that ΔT has been previously determined for core frequencies, at a given depth the corrections for $x > x_c$ are

$$\delta S^{(n)}_{lx} = \frac{r_x + (1-\alpha_x)\Delta T}{1-\alpha_x(1-\epsilon)\Lambda^*_x p_x} \qquad (27)$$

which is equivalent to solving a *diagonal system* of equations.

5.3. *Properties of the CRDCS method*

After all the δS_{lx} have been determined from Eqs. (25–27), the source functions are corrected, a formal solution for the radiation field is made and r_x is reevaluated. The system is iterated to convergence. As in Auer & Paletou (1994) the corrections converge rapidly. We may check the relative precision of the CRDCS method against the FBF one. To this end, we choose a pathologically numerically difficult case, with a line center opacity $\tau_0 = 10^{15}$, a frequency grid ranging 1000 Doppler widths from line center and $\epsilon = 10^{-8}$. Convergence is reached with 50 iterations for the FBF scheme and 80 iterations for the CRDCS scheme with a relative accuracy of 1% (in the source functions) between each method's solution. In Fig. 6, we have plotted $S_{\rm CRDCS}$ against $S_{\rm FBF}$. Although there is a 10^4 range in the source function, we have a 45° slope line, demonstrating the excellent agreement between the two solutions.

Table 1. As a function of the number of spatial grid points, N, we obtain the following time ratios for one FBF iteration against one CRDCS iteration: $t_1^{\rm fact}$ when the LU factorization is performed at each iteration and $t_1^{\rm oo}$ when it is performed "once only"

N	$t_1^{\rm fact}$	$t_1^{\rm oo}$
40	8.75	1.23
70	9.86	1.32

Despite the fact that the new CRDCS converges for cases where CRDA completely fails, the new method requires *no more computational effort* per iteration.

5.3.1. Rate of convergence

In order to compare the convergence properties of the CRDCS method with the others, we have plotted, in Fig. 7, the maximum relative error in the line source functions for the same cases as in Sect. 4.

If the slab is thin at wing frequencies ($\tau_0 = 10^6$), the rate of convergence is almost the same as the one obtained with the CRDA method. For such slabs then, the CRDCS scheme appears to converge in fewer iterations than the FBF one. For more dif-

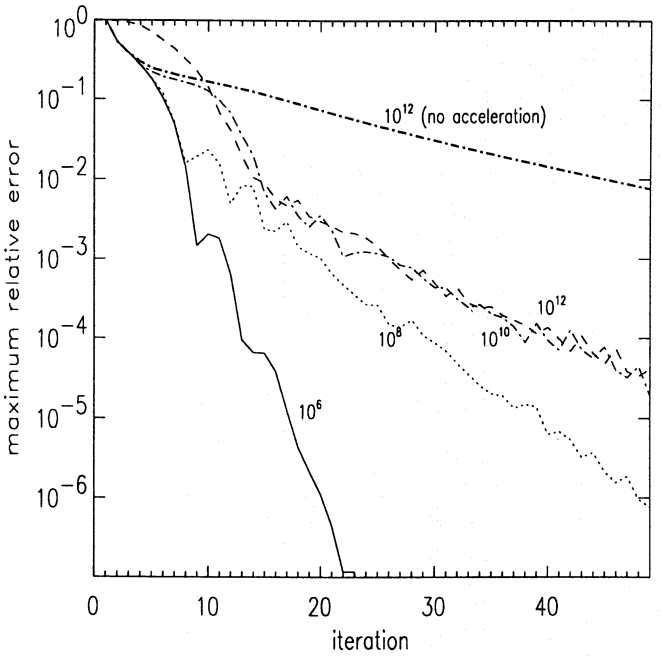

Fig. 7. Same as Fig. 1 but with the CRDCS scheme ($x_c = 3.5$). For low τ_0 slabs, the rate of convergence is almost the same as for the CRDA method. When τ_0 increases, the favorable convergence property of the CRDCS is preserved. The importance of acceleration of convergence is also shown on the $\tau_0 = 10^{12}$ case

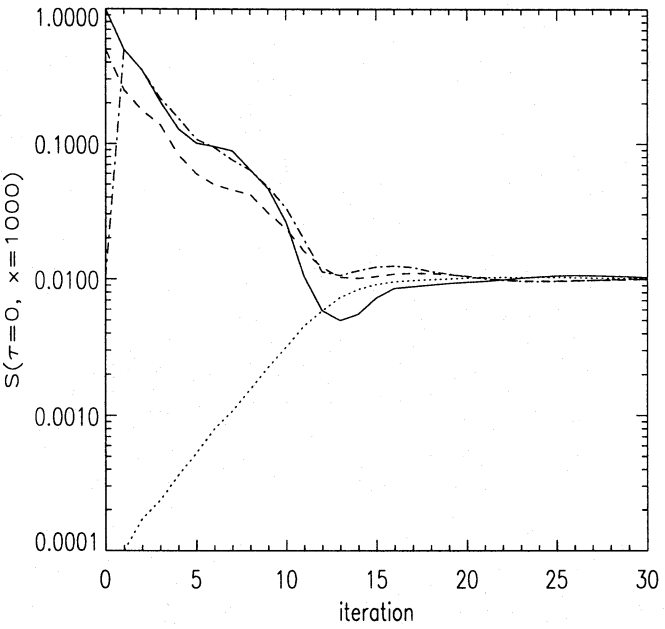

Fig. 8. Evolution of the surface source function at $x = 1000$ obtained with the CRDCS scheme and for various initial values ($S_{\rm CRD}$, 0, $\frac{1}{2}B$ and B)

ficult cases, with very large optical depths, the CRDCS scheme shows a good rate of convergence but, as expected, it is less rapidly than the FBF one. Note that one CRDCS iteration can be a factor of ten faster than one FBF iteration so that despite the increase in the number of iterations, there is a dramatic decrease in the computational cost (see Table 1). In addition the memory storage for the CRDCS is dramatically less. The most critical point, however, is that even for difficult cases, the CRDCS scheme *always converges* while the CRDA one *does not*.

5.3.2. Non–sensitivity of the iterative scheme to the initial guess

A check of convergence, especially at high frequencies, is provided by investigating the effect of different initial values for the source function on the iterative scheme. In Fig. 8 we plot the line source function values for each iteration at the surface of the slab and at the larger grid frequency (1000 Doppler widths away from line center). We use four different initial values, ranging from the CRD solution, 0, $\frac{1}{2}B$ and B. As one can see in Fig. 8, whatever the initial value of the line source function, a unique solution is reached after 30 iterations of the CRDCS scheme. Equivalent behavior is found at larger depths in the atmosphere as well as for other frequencies, showing the good convergence of the scheme.

6. Conclusion

We have developed new methods for the numerical solution of radiative transfer problems including the effects of PRD. These schemes are based on approximation of both the frequency redistribution and radiative operators. Convergence is obtained for a wider class of problems than is possible using Scharmer's approach (1983), including thick slabs with $R_{\rm II}$ redistribution very far from line center. While we have found that simultaneous solution for the frequency dependent source function ensures convergence, a simple Core–Wing approximation to the redistribution leads to a scheme which is equally robust and dramatically more efficient with respect to both computing time and memory requirements. Further, the new CRDCS is as computationally efficient as the earlier CRDA approach, converges as rapidly as CRDA for the cases in which that method works and, most importantly, converges rapidly for all cases. Finally, we should note that although our presentation has used the OAB approximation, the Core–Wing correction method can be used with any other Approximate Lambda Operators to achieve even higher rates of convergence.

Acknowledgements. Frédéric Paletou thanks the High Altitude Observatory for supporting a post–doctoral stay which made this work possible and Phil Judge for a careful reading of the manuscript. This work has also been supported by the Los Alamos National Laboratory which is operated by the University of California for the U.S. Department of Energy.

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