

# IMPROVING THE NUMERICAL MODELING OF THE O I RESONANCE TRIPLET IN THE SOLAR SPECTRUM

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## ABSTRACT

We present a slight modification to an existing multilevel radiative transfer code that allows us to include the effects of frequency cross redistribution (XRD) between lines sharing the same upper level. With this improved code, we calculate theoretical profiles of the O I resonance triplet lines at 130 nm through a hydrostatic model of the average quiet Sun. The width of the calculated XRD profiles show good agreement with an observed, spatially averaged disk-center spectrum obtained with the high-resolution telescope spectrometer (HRTS) spectrograph. This is in stark contrast to profiles calculated with complete frequency redistribution (CRD) and ordinary partial frequency redistribution (PRD), which have Lorentzian wings that are too broad. We find deep central reversals, contrary to most observed profiles, but we note that this discrepancy is to a large degree the result of limited instrumental spectral resolution.

*Subject headings:* line: formation — methods: numerical — radiative transfer — Sun: chromosphere — Sun: UV radiation

## 1. INTRODUCTION

The nature of the solar chromosphere is still very much a mystery. Despite decades of observations and extensive modeling efforts, we cannot currently even agree whether it is present all the time or just intermittently (Kalkofen 2001; Carlsson & Stein 1995). To resolve this awkward disagreement, we clearly need to improve our diagnostic capabilities and to model the chromosphere realistically, so that we can derive physical quantities accurately and decisively. In this paper, we attempt to provide a small addition to the chromospheric diagnostic tool box by describing a more realistic way to model the O I triplet at 130 nm and interpret its observed shape.

Previous modeling efforts of the O I triplet have been presented by Skelton & Shine (1982) and Carlsson & Judge (1993), among others. Comparing their calculated O I profiles with observed spectra from the spectrometer on *OSO 8*, Skelton & Shine (1982) established that fluorescence by hydrogen Ly $\beta$  is a major factor in the formation of these lines. Ly $\beta$  pumps O I atoms from the  $^3P_2$  ground state to the  $^3D$  level, from which about 10% undergo a cascade to the  $^3S$  common upper level of the resonance triplet. They further found that their calculated line profiles had central absorption reversals that were too deep and Lorentzian wings that were too broad compared to the observations, which prompted them to suggest that the lines should be treated with partial frequency redistribution (PRD) instead of the approximation of complete redistribution (CRD). This was confirmed by Carlsson & Judge (1993), who mimicked PRD formation of the lines by employing Doppler instead of Voigt profiles, which indeed successfully elimi-

nated the broad wings of the lines but did not reproduce the relative emission strength of the three lines.

Observations with good spectral and spatial resolution taken with the S082-B spectrograph on board *Skylab* have been presented by Roussel-Dupre (1985). He notes that the lines show central absorption reversals at some locations on the disk, notably toward the limb, and that the actual reversals are probably deeper than those derived from observations with limited spectral resolution.

In this paper, we present calculations of O I line formation, including the effects of PRD. As we will show below, however, this does not adequately reduce the broadening of the calculated oxygen lines. To achieve the latter, we also need to include the effects of cross redistribution (hereafter XRD), which accounts for the coherency in scattering from one line into one of its subordinate lines through a common upper level (e.g., Hubený et al. 1983a, 1983b). By contrast, effects of XRD are not important in the solar Ca II lines because the infrared triplet lines are weaker and occur at much longer wavelengths than the H and K lines with which they share upper levels (Uitenbroek 1989a). For illustrative purposes, all our calculations were done through the average quiet-Sun model of Fontenla et al. (1993, their Model C, hereafter FAL-C). We employ the same atomic model for O I as Carlsson & Judge (1993), and account for Ly $\beta$  fluorescence by using the population numbers of the ground- and second-excited levels of hydrogen from the atmospheric model to calculate the radiation field in the  $^3P$ – $^3D$  transition of O I. This dependence of the oxygen triplet strength on Ly $\beta$  fluorescence may be one of the interesting applications of these lines, as it opens the possibility of diagnosing inhomogeneities through the pumping characteristic of the excitation.

This paper is organized as follows: We briefly discuss the radiative transfer with XRD in § 2. Results are presented in § 3, and conclusions are given in § 4.

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## 2. RADIATIVE TRANSFER METHOD WITH XRD

The O I resonance triplet is strong enough so that coherent scattering (excitation in the line followed by radiative de-excitation without disturbing the excited level) plays an important role in its formation. In addition, the lines are of comparable strength and obviously occur closely in wavelength. These conditions imply that we should also allow for coherent photon conversion: excitation in one of the lines followed by coherent de-excitation into one of the other triplet lines. To solve for radiative transfer in the O I atom, we employ the Multilevel Accelerated Lambda Iteration (MALI) code for PRD described by Uitenbroek (2001). Apart from a slight modification to the routine performing the evaluation of the scattering integral, which we describe below, this transfer code is already capable of dealing with XRD. The emission profile of a line, for which coherent scattering and coherent conversion from one line to the other is important, is evaluated in the following way.

Following the notation of Uitenbroek (2001), the laboratory frame redistribution function

$$R_{kji}(v, \mathbf{n}; v', \mathbf{n}') dv dv' \frac{d\Omega}{4\pi} \frac{d\Omega'}{4\pi} \quad (1)$$

describes the probability that a scattered photon is re-emitted in line  $(i, j)$  in a frequency range of  $(v, v + \delta v)$  and solid angle  $d\Omega$  around direction  $\mathbf{n}$ , when it is absorbed in line  $(k, j)$  at a frequency between  $(v', v' + \delta v')$  and from an angle  $d\Omega'$  around  $\mathbf{n}'$ . With the redistribution function  $R_{kji}$  (equation 1), we can formulate the ratio  $\rho_{ij}$  of the PRD to CRD emission profiles:

$$\rho_{ij}(v, \mathbf{n}) \equiv \frac{\psi_{ij}^{\text{PRD}}}{\phi_{ij}} = 1 + \frac{\gamma \sum_{k < j} n_k B_{kj}}{n_j P_j} \oint \frac{d\Omega'}{4\pi} \int dv' I(v', \mathbf{n}') \times \left[ \frac{R_{kji}^{II}(v, \mathbf{n}; v', \mathbf{n}')}{\phi_{ij}(v, \mathbf{n})} - \phi_{kj}(v', \mathbf{n}') \right], \quad (2)$$

where  $n_{k,j}$  are the population numbers for levels  $k, j$ ,  $B_{kj}$  is the Einstein coefficient for absorption, and  $P_j$  is the total (radiative plus collisional) transition rate out of upper level  $j$ . The coherency fraction

$$\gamma \equiv P_j / (P_j + Q^E), \quad (3)$$

with  $Q^E$  the total rate of elastic (coherency-destroying) collisions of the upper level, is the same for all the transitions originating from upper level  $j$ . It represents the fraction of scattering events that occur coherently. Thus, equation (2) describes how the PRD emission profile for the line  $(i, j)$  depends on the intensity in the line itself ( $k = i$ ), and in its subordinate lines ( $k \neq i$ ) through cross redistribution.

### 2.1. Integration of the Scattering Integral

The integration of intensity  $I$  and redistribution function  $R$  that appears in the definition of  $\rho$  (eq. [2]) can be evaluated efficiently using Uitenbroek's (1989b) modification for XRD of Gouttebroze's (1986) approximation of the normalized angle-averaged redistribution function  $g^{II}(x, x') \equiv R^{II}(x, x')/\phi(x)$  ( $x$  is reduced frequency in Doppler units), and the integration method described by Uitenbroek (2001). The latter scheme takes advantage of the limited intervals for each emission frequency,  $x$ , over which  $g^{II}(x, x')$  differs appreciably from zero as a function of absorption

frequency  $x'$ . According to Gouttebroze (1986), the scattering integral is to be calculated in three different regions: the core region  $|x| < 2$ , the wing region  $|x| > 4$ , and the intermediate region  $2 \leq |x| \leq 4$ . In the wing region, the function  $g^{II}(x, x')$  for ordinary redistribution is symmetric around  $x' = x$ . In the generalized case of XRD, however,  $g$  is symmetric around reduced frequency  $x' = \alpha x$  in the wing region, where  $\alpha$  is the wavelength ratio of the line into which the photon is emitted over that of the line into which it was absorbed (Uitenbroek 1989b). The factor  $\alpha$  is introduced because coherent scattering by definition occurs in each line at a given distance in energy  $h(\nu - \nu_0)$  away from line center. Thus, for XRD the integration limits specified in Uitenbroek (2001, eq. [32]) have to be adjusted in the wing and intermediate regions:

$$\begin{aligned} \alpha(x - 5) &\leq x' \leq 4, & \text{for } -4 \leq x \leq -2, \\ -4 &\leq x' \leq \alpha(x + 5), & \text{for } 2 \leq x \leq 4, \\ \alpha(x - 5) &\leq x' \leq \alpha(x + 5), & \text{for } |x| > 4. \end{aligned} \quad (4)$$

The limits remain unchanged in the core region.

## 3. RESULTS

We compare our calculated line profiles with a photographic long-slit spectrum obtained during the HRTS I rocket flight (Bartoe et al. 1978). This spectrum covers a substantial cross section of the solar disk, but we selected a quiet region near disk center for our comparison.

Figure 1 shows the computed disk-center profiles of the O I resonance triplet through the FAL-C model for CRD and ordinary PRD compared with the disk-center HRTS spectrum. While the PRD line profiles show an improvement over the CRD profiles for the 130.2 line, it is clear that the former still result in the wings of this line and the 130.5 nm line being too wide. The reason for this is that ordinary PRD does not allow for the full amount of coherent scattering in the triplet as it only accounts for this coherency when a photon absorbed in one line is re-emitted into the same line. For a given line, all excitations in the two other triplet lines are then counted as incoherent excitations of the upper level followed by de-excitation distributed in frequency according to complete redistribution. Looking at equation (2) for the profile coefficient ratio  $\rho_{ij}$ , we can see that only one out of the possible three (similar) terms in the sum over  $k$  is accounted for in that case, reducing the effect on the emission profile.

The form of equation (2) suggests that PRD effects will be enhanced if we account for coherent scattering from other lines in addition to the line itself. It also presents a simple way of testing this proposition before we even do the full XRD calculation; namely, by eliminating two of the triplet lines in the transfer equations and accounting for regular PRD in the one remaining line. This simple approximation reduces the rate  $P_j$  in the denominator of equation (2), thereby increasing the coherent scattering contribution to  $\rho$  to a level comparable to that expected under XRD. In effect, we increase the fraction of coherent excitations in the remaining line by reducing the incoherent excitations while keeping the coherent ones.

Plotting the single PRD profile for the 130.2 nm line along with the observed HRTS line profiles (Fig. 2), we see that this simulation of XRD has indeed resulted in a line that does not broaden excessively in the wings. However,

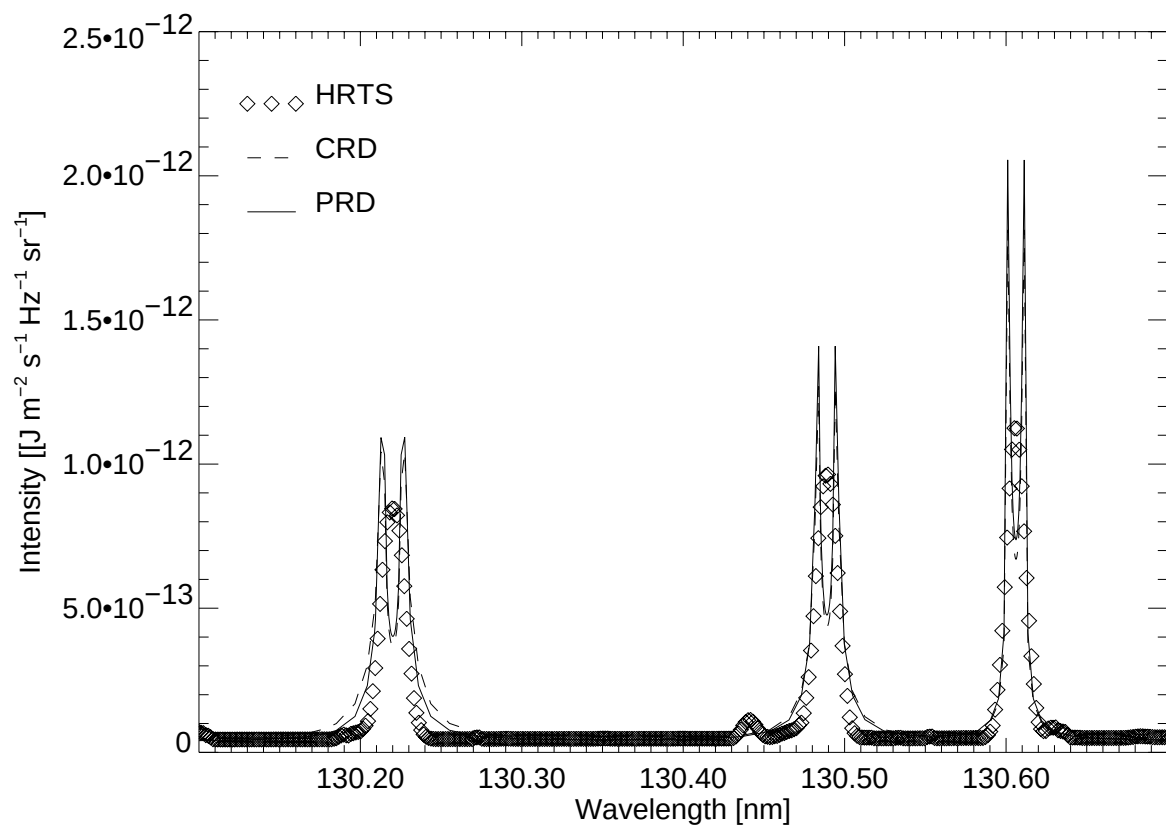


FIG. 1.—Computed CRD (*dashed curve*) and ordinary PRD (*solid curve*) profiles compared with the disk-center HRTS profile (*diamonds*)

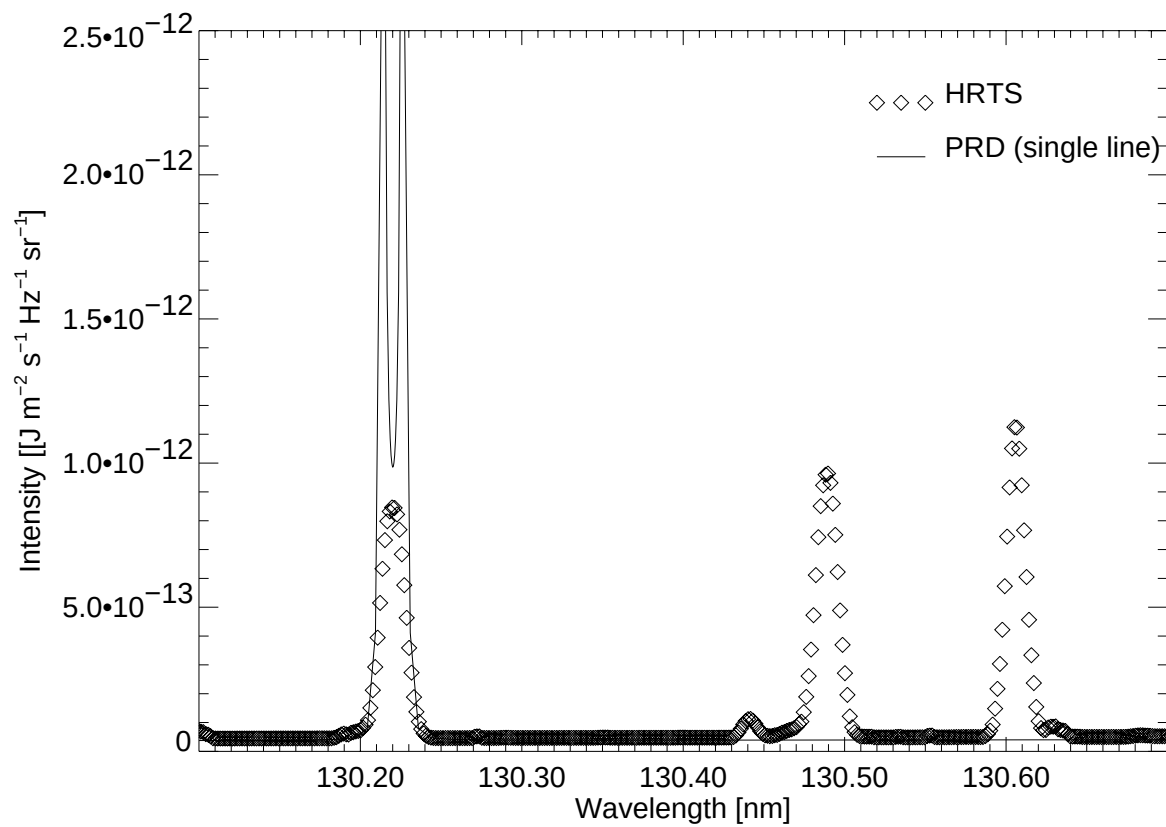


FIG. 2.—Computed PRD profile for the 130.2 nm line as a single line compared with the disk-center HRTS profile (*diamonds*)

the line is much too bright because all the collisional excitations from the triplet ground level can now only de-excite radiatively through the single 130.2 nm line.

Finally, with the changes to the radiative transfer code described in the previous section, we can now model the full triplet using XRD. Figure 3 shows the calculated XRD profiles through model FAL-C of the quiet Sun compared to the HRTS spectrum. As expected from our models of the single line profiles, the XRD profiles are not overly broadened in the line wings and fit the width of the observed profiles almost perfectly. We still calculate the lines with central line reversals where none are observed at disk center in the HRTS I spectrum. This may be explained in part by the fact that the modeled lines do not account for the limited spectral resolution of the HRTS instrument, noise introduced by the use of film, or any macroscopic motions in the solar atmosphere. For comparison, therefore, we also plot the theoretical line curves smeared with a 0.006 nm FWHM Gaussian broadening, which corresponds to the instrumental spectral resolution. We see that this reduces the central absorption troughs by a considerable amount while it does not affect the width of the lines too much. In addition, the relative strength of the three lines is now closely matched with the observations.

#### 4. CONCLUSION

We successfully added the capability to perform cross redistribution calculations to our multilevel radiative transfer code (Uitenbroek 2001). This addition conserves the

favorable convergence properties of the code; the same number of iterations was needed to achieve convergence with XRD with the employed O I atomic model as were needed for ordinary PRD. Our calculations have shown that ordinary PRD slightly improves the fit of the O I resonance triplet lines to observed line profiles over CRD but does not adequately reduce the width of their wings. Only when the emission profile of each of the triplet lines accounts for coherent excitations in the other two lines (in addition to those in the line itself) can we reproduce the observed line widths. We also show that a simple approximation for the shape of each individual triplet line can be achieved by eliminating the other two triplet lines from the transfer equations, thereby effectively increasing the fraction of coherent scattering in that line, and mimicking the amount of coherency that would be appropriate for the full XRD solution. The obvious drawback of this approximation is that it overestimates emission, because the  $^3S$  upper level can only de-excite radiatively through the one remaining line. Through the addition of instrumental broadening, the calculated central line reversals are substantially diminished and show better agreement with observed profiles, which mostly lack such reversals.

Now that we have gained a better understanding of the narrowness of the O I triplet lines as being due to coherent scattering, including the effects of coherent conversion from one triplet line to the other, these lines present a more reliable diagnostic tool to analyze chromospheric observations. By comparing calculated profiles of these lines through

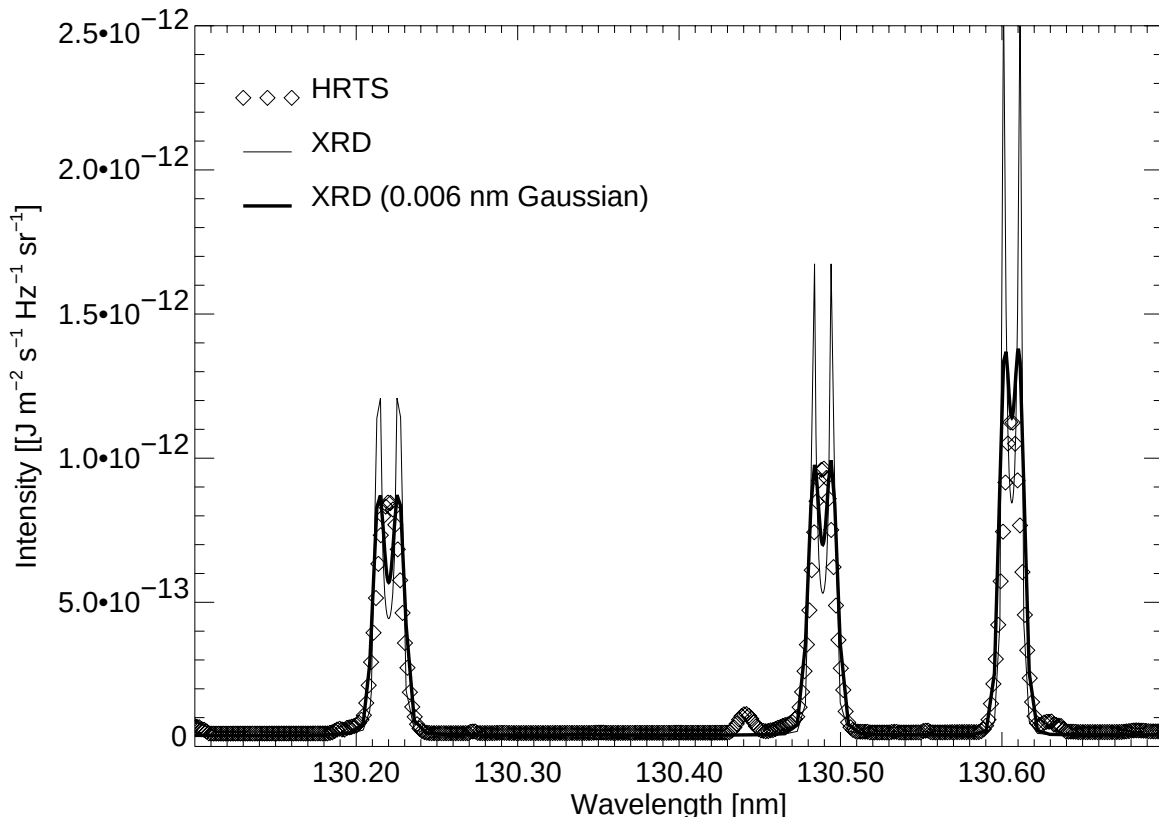


FIG. 3.—Computed XRD profile (*thin solid*) for the O I triplet compared with the disk-center HRTS profile (*diamonds*). Also plotted are the XRD profiles broadened by the 0.006 nm instrumental resolution (*thick solid curve*).

hydrostatic as well as dynamic models of the solar atmosphere with spatially and temporally resolved profiles from instruments like the HRTS and SUMER spectrographs, we should then be able to draw firmer conclusions about the nature of the solar chromosphere and the permanence of its existence.

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