THE POLARIZATION-FREE APPROXIMATION APPLIED TO MULTI-LEVEL NON-LTE RADIATIVE TRANSFER

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Abstract. The polarization-free (POF) approximation (Trujillo Bueno and Landi Degl’Innocenti, 1996) is capable of accounting for the approximate influence of the magnetic field on the statistical equilibrium, without actually solving the full Stokes vector radiative transfer equation. The method introduces the Zeeman splitting or broadening of the line absorption profile $\phi_I$ in the scalar radiative transfer equation, but the coupling between Stokes $I$ and the other Stokes parameters is neglected. The expected influence of the magnetic field is largest for strongly-split strong lines and the effect is greatly enhanced by gradients in the magnetic field strength. Formally the interaction with the other Stokes parameters may not be neglected for strongly-split strong lines, but it turns out that the error in Stokes $I$ obtained through the POF approximation to a large extent cancels the neglect of interaction with the other Stokes parameters, so that the resulting line source functions and line opacities are more accurate than those obtained with the field-free approach. Although its merits have so far only been tested for a two-level atom, we apply the POF approximation to multi-level non-LTE radiative transfer problems on the premise that there is no essential difference between these two cases. Final verification of its validity in multi-level cases still awaits the completion of a non-LTE Stokes vector transfer code.

For two realistic multi-level cases (CaII and MgI in the solar atmosphere) it is demonstrated that the POF method leads to small changes, with respect to the field-free method, in the line source functions and emergent Stokes vector profiles (much smaller than for a two-level atom). Real atoms are dominated by strong ultraviolet lines (only weakly split) and continua, and most lines with large magnetic splitting (in the red and the infrared) are at higher excitation energies, i.e. they are relatively weak and unable to produce significant changes in the statistical equilibrium. We find that it is generally unpredictable by how much the POF results will differ from the field-free results, so that it is nearly always necessary to confirm predictions by actual computations.

The POF approximation provides more reliable results than the field-free approximation without significantly complicating the radiative transfer problem, i.e. without solving any extra equations and without excessive computational resource requirements, so that it is to be preferred over the field-free approximation.

Key words: Line formation – Magnetic fields – Polarization – Radiative transfer – Sun: atmosphere – Sun: magnetic fields

1. Introduction

In the framework of multi-level non-LTE radiative transfer in a magnetized atmosphere the field-free approximation (Rees, 1969) is often invoked to avoid having to deal with the possible influence of the magnetic field on the statistical equilibrium of a multi-level atom. Contrary to general belief, this approximation is not well-founded; to our knowledge its accuracy has only been assessed for one particular case, namely the CaII H & K resonance lines.
(Auer et al., 1977). And even in that case only homogeneous magnetic fields were considered.

Computations for a two-level atom (Trujillo Bueno and Landi Degl’Innocenti, 1996) have shown that the magnetic field can have a non-negligible influence on the statistical equilibrium, especially in the presence of magnetic field gradients. The magnetic field most sensitively affects the statistical equilibrium through a strongly-split strong line.

Determining the exact impact of a magnetic field requires consistent solution of the multi-level non-LTE polarized radiative transfer and statistical equilibrium equations, which is a difficult problem. Although this type of problems can be solved via the application of recently-developed very efficient iterative schemes (Trujillo Bueno and Fabiani Bendicho, 1995), it remains a difficult problem.

As an intermediate step towards this consistent solution Trujillo Bueno and Landi Degl’Innocenti (1996) proposed the polarization-free (POF) approximation, which takes into account in an approximate manner the influence of the magnetic field on the statistical equilibrium without solving the full Stokes vector transfer equation. This is done by incorporating into the conventional scalar radiative transfer equation the magnetic splitting of the line absorption profile $\phi_I$, while still neglecting the interaction of Stokes $I$ with the other Stokes parameters $(Q, U, V)$.

Relying on its proven accuracy for a two-level atom, this paper discusses the implementation of the POF approximation in Carlsson’s (1986) radiative transfer code MULTI and subsequent application to realistic multi-level radiative transfer problems. It is set up as follows: Section 2 outlines the principles of the POF method, Section 3 discusses the essentials of its implementation in MULTI, Section 4 shows a few examples of applications and Section 5 summarizes the results and discusses the usefulness of the method.

2. Principles of the POF approximation

The formulation of the polarization-free approximation starts from the $I$-component of the Stokes vector radiative transfer equation (see Rees et al., 1989, for the notation):

$$\frac{dI}{dz} = (\kappa_c S_c + \kappa_0 S_L \phi_I) - (\kappa_c + \kappa_0 \phi_I)I - \kappa_0 (\phi_Q Q + \phi_U U + \phi_V V). \quad (1)$$

For many cases, in particular for weakly-split lines and for not too strong lines in general, Stokes $Q, U$ and $V$ are one or two orders of magnitude smaller than $I$ and the absorption coefficients $\phi_X$ ($X = \{Q, U, V\}$) are at most of the same order as $\phi_I$, so that we may safely neglect the last term in this equation. Neglecting that term, but still preserving the magnetic field...
dependence of $\phi_I$ leads to the polarization-free equation of transfer (Trujillo Bueno and Landi Degl’Innocenti, 1996). That equation only involves the $I$-component of the Stokes vector, it takes into account the magnetic splitting pattern of the line absorption profile $\phi_I$, and it reduces to the standard non-magnetic radiative transfer equation in case of zero fields. It reads:

$$\frac{dI_{\text{PF}}}{dz} = (\kappa_C S_C + \kappa_0 S_L \phi_I) - (\kappa_C + \kappa_0 \phi_I) I_{\text{PF}},$$

with the total line absorption profile

$$\phi_I = \frac{1}{2} \phi_p \sin^2 \gamma + \frac{1}{4}(\phi_b + \phi_r)(1 + \cos^2 \gamma).$$

In the latter formula, $\phi_p$, $\phi_b$ and $\phi_r$ signify the generalized absorption profiles for the different polarization states and $\gamma$ is the angle between the magnetic field vector and the ray under consideration.

For strongly-split strong lines, however, the POF approximation seems equally inappropriate as the field-free approach, since then the interaction of Stokes $I$ with the other Stokes parameters should be strong and the last term of Equation (1) becomes significant. Fortunately, as shown by comparison with the exact solution for a two-level atom (Trujillo Bueno and Landi Degl’Innocenti, 1996), inclusion of the magnetic splitting of the line absorption profile (in the scalar radiative transfer equation) introduces an error in $I$ that largely cancels the missing interaction with Stokes $Q$, $U$ and $V$, so that the final result for the line source function and line opacity is significantly better than with the field-free approach.

3. Implementation in a multi-level radiative transfer code

We have implemented the modified expression for the line absorption profile of the POF approximation in version 2.1 of Carlsson’s (1986) radiative transfer code MULT1. Relatively few modifications to the existing code were necessary and only minor amounts of additional code needed to be written:

- The input routine ATOM now needs to read the level Landé factors $g$ and orbital quantum numbers $S$, $L$ and $J$ (with an option to compute $g$ assuming LS-coupling).
- A new routine (RDFIELD) was introduced to read the magnetic field configuration and interpolate it to the appropriate depth grid.
- The line absorption profile, variable PHI, instead of being a single Voigt profile now consists of the sum of several Voigt functions each with their own weight and wavelength shift. This sum is computed by means of a slightly modified version of the generalized Voigt function routines of the
Stokes Profile and Synthesis Routine (SPSR) of Murphy and Rees (1990). This change affects routines PROFIL and TAUNYQ.

In MULTI the frequency quadrature points are close and equidistant in frequency in the first few Doppler widths from the line core (input parameter Q0) and beyond that they are equidistant in the logarithm of the frequency. This assures that the integrals in the rate equations (Scharmer and Carlsson, 1985, Equation (3.20)) are computed fairly accurately (but see Stift and Moser (1993) on the use of adaptive frequency grids). Due to magnetic splitting the line profile widths increase and one has to modify the frequency grid accordingly to obtain accurate representation of all absorption components. Without resorting to adaptive frequency grids one generally requires an increase of Q0 that depends on the splitting characteristics and wavelength of the line and on the maximum expected value of the magnetic field strength. An increase of the number of frequency points (NQ) may then be needed in order to avoid too large spacing of the grid points.

The CPU-time per iteration is dominated by the time required to update the radiation field and the rate matrix. This time scales linearly with the total number of angle-frequency points in all transitions, so that occasional large increases of NQ (for long-wavelength lines) do not excessively burden the computations. A magnetic field makes the line absorption profiles direction-dependent (just as a macroscopic velocity does), but it also requires the sum of a number of Voigt profiles to be computed. The initialization of the profiles therefore becomes considerably more time-consuming, but it remains only a small fraction of the total CPU-time. The direction-dependence of the line profiles and the associated additional read operations do not markedly increase the CPU-time per iteration.

The current implementation of the POF approximation in MULTI is valid for vertical magnetic fields, for which case the line absorption profile only depends on the inclination of the line of sight, i.e. the μ value of the angle-quadrature points. For inclined fields the line absorption profile also depends on the azimuth angle of the line of sight. A future paper will deal with the details of how to treat inclined fields. In any case, it can be shown (e.g. Trujillo Bueno, 1995; in preparation) that the field strength plays a much more important role than the inclination, so that the use of vertical fields is not a significant limitation here.

Computations for a simplified model atmosphere and a two-level atom served to test the implementation of the method. The results can be summarized as follows (see Trujillo Bueno and Landi Degl’Innocenti (1996) for more details). A depth-independent magnetic field has only very limited influence on the line source function $S_{1}$: it starts to drop below the Planck function $B_{\nu}$ slightly deeper in the atmosphere than without magnetic field.
Once the field is strong enough to completely split the line into its Zeeman components, further increase of $B$ has no effect on $S_L$: the components of the line behave as if they were completely independent lines of comparable strength and the net effect is simply a small inward shift of their formation; the line profiles are only slightly affected. Gradients in $B$, in particular the ones that cause significant changes of the line splitting within the line formation region (e.g. unsplit at one end and completely split at the other end), produce significantly larger line source function and line profile changes: in this case there is a competition between increased line photon losses due to decreased line opacity (line split into several components) and trapping of continuum photons due to the depth-dependence of the wavelength shifts of the individual line components. Provided the gradients occur in the line formation region, strong outward decrease of $B$ causes $S_L$ to drop below its field-free value and strong outward increase produces an enhancement of $S_L$. Mixed or even completely opposite behavior may occur if the regions of line formation and large field strength gradients only partially coincide.

4. Applications

Below we briefly show application of the POF approximation to two realistic multi-level atoms. One should bear in mind that the findings for a two-level atom need not always hold for multi-level cases: interlocking line systems may even produce opposite behavior for some lines. In such cases a strong gradient in the field strength may cause a source function decrease in one line and an increase in another. Additionally, ultraviolet lines, which nearly always dominate the overall excitation equilibrium, are relatively insensitive to magnetic splitting, so that the influence of the magnetic field on the level populations is expected to be much smaller than for a two-level atom.

Although not explicitly shown here, the strength of the field is much more important than its inclination (Domke and Staude, 1973; Trujillo Bueno, 1995, in preparation); in practice this means that one may perform a non-LTE solution for a vertical field of suitable strength and afterwards use its results to perform a formal Stokes vector solution for any line of sight and any desired orientation of the magnetic field vector, even for configurations with a gradient in the magnetic field inclination.

4.1. Application to CaII lines

We start with this application, because the validity of the field-free approximation has only been demonstrated for the CaII atom in combination with a depth-independent magnetic field (Auer et al., 1977). Significant sensitivity of the statistical equilibrium to the magnetic field is not to be expected for
Fig. 1. Level population changes, in a quiet Sun model atmosphere, due to a uniform magnetic field of 3000 G, relative to the field-free populations. The curves for the $^2D$ ($^2P$) levels have been shifted down by 5 (10) percent to avoid confusion. Three different cases are compared: all five lines subject to magnetic splitting (solid lines), magnetic splitting only for the H & K lines (dotted), and magnetic splitting only for the IR triplet lines (dashed)

In this case, because these lines are only very weakly split. This weak split—very wide lines in the ultraviolet—implies that the field-free approach should be quite accurate.

We employ the standard 5-level Ca$^+$ atom, with the H & K resonance doublet and the IR triplet lines, together with the Ca$^{2+}$ ground state, which suffices to accurately describe the non-LTE statistical equilibrium. We assume complete frequency redistribution of photons in order to demonstrate the role of the magnetic field, but partial frequency redistribution of photons needs to be taken into account for a more correct description of the resonance lines. Following Auer et al., (1977), we first experimented with rather strong depth-independent fields in a quiet Sun model (Maltby et al., 1986), without accounting for magnetic pressure effects.

Figure 1 shows the population changes of all five Ca$^+$ levels, induced by a magnetic field of 3000 G, relative to their field-free populations. Figure 1 not only displays the population changes for the case that all five lines are subject to magnetic splitting (case A, solid lines), but also the ones that
Fig. 2. POF line source functions in a quiet Sun model atmosphere, for uniform magnetic fields of 1000 and 3000 G, relative to the field-free line source functions. Left part: as functions of the standard continuum optical depth at 5000 Å; right part: as functions of the respective (unsplit) line center optical depths.

Fig. 3. Stokes $I$ and $V$ profiles of the K-line and the strongest member of the IR triplet for a quiet Sun model atmosphere. Only the center parts of the lines are shown and the intensities are normalized to the local continuum values. The solid lines represent the profiles for $B = 0$; the dotted and dashed lines represent the Stokes vector formal solutions obtained respectively from field-free and POF non-LTE statistical equilibrium computations for a LOS inclination of 45° (from vertical) and a 3000 G field with 45° inclination with respect to the LOS.
Fig. 4. POF line source functions, relative to their field-free values, for an umbra model atmosphere, with a magnetic field of 3000 G at $\tau_c = 1$ and an outward decrease of 3 G/km. Left part: as functions of the standard continuum optical depth; right part: as functions of the respective (unsplit) line center optical depths.

Fig. 5. Stokes $I$ and $V$ profiles of the K-line and the strongest member of the IR triplet for an umbra model atmosphere, with a magnetic field of 3000 G at $\tau_c = 1$ and an outward decrease of 3 G/km. Only the center parts of the lines are shown and the intensities are normalized to the local continuum values. The dotted and solid lines represent the Stokes vector formal solutions obtained respectively from field-free and POF non-LTE statistical equilibrium computations for a LOS inclination of 45° (from vertical) and a field with 45° inclination with respect to the LOS.
result if only the resonance lines are subject to magnetic splitting (case B, dotted lines) or if only the IR triplet lines are split (case C, dashed lines). This shows that the population changes in case A are equal to the sum of the changes in cases B and C, and that the largest contribution comes from the IR triplet lines; only where those become optically thin (in the extreme upper atmosphere) does the contribution of the resonance lines become comparable to that of the triplet.

The line opacities, determined by the populations of the lower level of each line, are much less affected than the line source functions (Figure 2), which are determined by the ratios of the upper and lower level populations. By far the largest changes occur in the populations of the \( 4p^2 P \) levels, the upper levels of all five lines, so that all line source functions undergo virtually the same changes. For comparison, Figure 2 also shows the significantly smaller line source function changes due to a field of 1000 G.

Since the line source functions only change in the upper atmosphere, largest line profile changes are to be expected for oblique lines of sight (LOS). Figure 3 therefore shows a comparison between field-free and POF profiles for the K-line and the strongest IR triplet line (8542 Å) obtained through a formal Stokes vector solution for a 45° inclination of the line of sight and a 3000 G field with 45° inclination with respect to the LOS. These profiles are also compared to the line profile that results in the absence of any field, from which they differ only very little. For the K-line the maximum difference between field-free and POF results occurs near the K₂ peaks and it is at most about 1% of the continuum intensity or about 6% percent of the intensity at those wavelengths. The degrees of linear and circular polarization (Stokes \( Q, U \) and \( V \)) differ only by a few tenths of a percent. For the triplet lines the profile differences are enhanced due to their longer wavelengths and near the line core they amount to about 3% of the continuum intensity or 12% of the actual core intensity. The differences in Stokes \( V \) are somewhat smaller, but most important is the shift in the position of the peaks.

Two-level atom computations show that gradients in the magnetic field can produce significantly larger changes in the populations. A realistic application would be a superpenumbral canopy, but unless one assumes its location extremely high in the atmosphere, the strong CaII lines are not affected at all. Unfortunately, a high location implies a smaller field strength jump, so that again the impact is limited.

Another obvious case with a field-strength gradient is provided by an umbra; there one may expect a magnetic field gradient \( \partial B/\partial z \) of several Gauss per kilometer to exist over a significant height interval. We use the Maltby et al. (1986) umbra model M and assume a field gradient of 3 G/km. Figure 4 shows the line source function changes for this case, as function of continuum optical depth and of non-magnetic line-center optical depth. The differences are very similar in character to the ones for a uniform magnetic
field, but the maximum deviations from the field-free values are only about 9% as compared to 12% for the above case with uniform field of 3000 G. The line profile differences (Figure 5) are nevertheless larger than in the previous case and they are now more pronounced for the K-line than for the IR triplet, up to 8% difference in Stokes $I$ at the $K_2$ peaks; the linear and circular polarization do not change significantly.

We conclude that the field-free approach is sufficiently accurate for the CaII H & K lines in case the magnetic field is homogeneous. In the presence of magnetic field gradients, especially for oblique lines of sight, a better approximation, such as the polarization-free approach, is desirable. The IR triplet lines call for a more accurate method in the presence of homogeneous magnetic fields, but are already described accurately by the field-free approach for the umbra field model used here.

4.2. Application to MgI 12 $\mu$m lines

The interest in this application is based on the presence of a number of lines in the near and far infrared, some of them rather strong, that as a whole contribute significantly in setting the statistical equilibrium of neutral magnesium. Due to the nature of their emission, the 12 $\mu$m lines are very sensitive to even small changes in the populations that may be induced by magnetic fields. The 12 $\mu$m lines themselves are weak and will not markedly influence the statistical equilibrium, even though they are completely split at field strengths of only a few hundred Gauss. We use the full 66-level model atom of Carlsson et al. (1992), with a few typing error corrections as noted by Bruls et al. (1995). Given that the 12 $\mu$m lines disappear in umbrae, penumbrae are a prime choice here. We performed non-LTE radiative transfer computations using the line-blanketed radiative equilibrium model atmosphere T5000 (Kurucz, 1991) with effective temperature $T_{\text{eff}} = 5000$ K, and a magnetic field of 1500 G at the 12 $\mu$m line formation height ($\tau_c \approx 10^{-3}$) with a gradient of 3 G/km, which is close to the maximum observed penumbral field strength gradient.

Differences between the field-free and POF results can best be expressed in terms of line source function ratios. Figure 6 shows these ratios for the 12.32 $\mu$m line and for the lines identified by Carlsson et al. (1992, Figure 12) as the ones to which the 12.32 $\mu$m emission is most sensitive. In this case line source function changes (top panel) are more instructive than population changes (bottom panel), because the role of stimulated emission increases with wavelength: small population changes may induce large line source function changes. Population changes of all neutral Mg levels, except for a few low-excitation ones which are irrelevant, are very similar, but the 12.32 $\mu$m line source function is clearly more enhanced than the ones of the driving lines, which all have shorter wavelengths.
Fig. 6. Line source functions, relative to their field-free values, for the T5000 model atmosphere and a magnetic field of 1500 G at $\tau_c = 10^{-3}$ with a gradient of 3 G/km. The dashed line refers to the MgI 12.32 $\mu$m line source function and the solid ones to the source functions of the lines to which the amount of emission in the 12.32 $\mu$m line is most sensitive (Carlsson et al., 1992). The lower part of the figure shows the populations, relative to their field-free values, for all but the lowest 8 levels of Mg which behave slightly differently.

Figure 7 displays the profile of the 12.32 $\mu$m and 9412 Å lines for a 80° inclined line of sight, to exploit the increase of the source function differences with height. The 9412 Å line (6f–3d) is one of the few observable ones of the 'driving lines'. The behavior displayed by both lines is typical of the whole set of lines: small changes in all Stokes parameters, but no remarkable changes of the profile shapes. For the 12.32 $\mu$m lines the effect on $Q$ and $V$ seems to be comparable to a multiplication by a factor close to unity, whereas for the 9412 Å line the differences are more subtle, including a slight wavelength shift of the Stokes $V$ peak positions. Given the significant changes of the 12.32 $\mu$m line emission, diagnostic applications that rely on the absolute
Fig. 7. Stokes I, Q and V profiles for the 12.32 μm line (left column) and for the 6f–3d 9412 Å line, one of the most important ‘driving lines’ and one of the few that are actually observable (Wallace et al., 1993), for the T5000 model atmosphere and a magnetic field of 1500 G at $\tau_c = 10^{-3}$ with a gradient of 3 G/km. The dotted and solid lines represent the Stokes vector formal solutions obtained respectively from field-free and POF non-LTE statistical equilibrium computations for a LOS inclination of 80° (from vertical) and a field with 80° inclination with respect to the LOS.

amount of emission in this line should be analyzed taking into account the magnetic field.

For a canopy type field configuration (in this case $B = 800$ G above $\tau_c = 10^{-3}$ and $B = 0$ below that height) populations change by no more than 5% due to the magnetic field. The 12.32 μm line source function increases by up to 5%, and even for a 45° inclined LOS the Stokes Q and V peak values, which are small anyway, increase by 5% only. The size of the emission peaks
in Stokes $I$, however, increases by about 20%, which is easily measurable on observed profiles.

5. Discussion

We have implemented the polarization-free approximation, which describes in an approximate way the influence of a magnetic field on the radiative transfer, in Carlsson's (1986) multi-level non-LTE radiative transfer code. This required relatively few modifications to the existing code and the performance is only slightly degraded: the initialization of the line absorption profiles is more involved and has to be performed for each grid point of the angle-frequency quadrature instead of only once per frequency point. In addition, a slightly higher total number of frequency points is generally needed in the presence of a magnetic field, with significant increases only required for lines in the far infrared. The CPU-time per iteration scales linearly with the number of frequency points and the convergence rate is not affected.

Furthermore, since this approximation can also easily be implemented in 2-D or 3-D multi-level radiative transfer codes, such as the one recently developed by Auer et al. (1994), it provides a fast and sufficiently reliable means of computing non-LTE Stokes profiles as long as a fully consistent 3-D multi-level non-LTE Stokes vector transfer code is not available, and even beyond that time it may prove to be the preferred method.

The most important reason why for realistic model atoms the differences between the field-free and the polarization-free approximation are so small, is given by the presence of strong (interlocking) ultraviolet lines that are crucial in setting the statistical equilibrium. Those lines are rather insensitive to magnetic fields and they also strongly suppress population changes induced by more sensitive (infra)red lines. This property is inherent to multi-level atoms and has nothing to do with the polarization-free approximation: consistent solution of the Stokes vector radiative transfer and statistical equilibrium equations, which will ultimately be necessary to evaluate the accuracy of the polarization-free approximation, will not change this situation.

The applications to realistic multi-level radiative transfer problems show that the differences between POF and field-free line profiles, though much smaller than for the two-level atom case, are still important enough to warrant a critical look and that the decision whether or not to use POF instead of field-free depends on each particular problem considered.

We finally conclude that the present work presents a valuable tool that for many problems may turn out to be preferable above consistent Stokes vector solutions (due to its simplicity and accuracy), but that it also supports the validity of the field-free approximation, for the CaII and MgI problems we have studied here, given a reasonable error margin.
Acknowledgements

Partial support of the Spanish DGICYT (project PB 91-0530) is gratefully acknowledged.

References


