Theoretical schemes for the interpretation of solar polarimetric observations: An overview and some new ideas

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Abstract. The theoretical scheme based on the density matrix formalism, and self-consistently derived from the principles of Quantum Electrodynamics, is presently one of the most solid frameworks for the interpretation of solar polarimetric observations. This scheme has been highly successful, mainly for the interpretation of polarimetric signals that can be described in the so-called limit of complete frequency redistribution (CRD). However, it suffers from the severe limitation that partial frequency redistribution (PRD) effects cannot be accounted for. The metalevel theory can handle PRD effects, but all the attempts for its generalization to account consistently for collisions and lower-level coherences have failed. The redistribution matrix approach is very suitable for taking PRD effects into account. However, it can consistently describe only two-level atoms with unpolarized lower level. New heuristic approaches have been proposed for treating two-term atoms, but they are based on rather crude approximations and their validity and physical consistency are far from being firmly established. Some few reflections that may lead to the establishment of a self-consistent set of equations, fully derived from first principles, are put forward. These reflections are based on the introduction of the Fourier transform of the density matrix.

1. Introduction

New polarimeters with unprecedented sensitivity are nowadays available to the solar community active in the field of spectropolarimetry. The observations from such instruments are arising a serious challenge to the different theoretical schemes developed in the past for the interpretation of polarimetric observations. These schemes are based on the theory of Quantum Electrodynamics (Q.E.). Although Q.E. can nowadays be considered as an "old theory", its main applications have always concerned the description of rather schematic physical experiments and many phenomena in polarization have still to be fully understood within its framework.

The physical problem to be addressed by solar physicists is the one of measuring and interpreting the intensity and the polarization properties (in other words the Stokes parameters profiles) of the electromagnetic radiation originating from the solar atmosphere, and contained in a particular wavelength interval of arbitrary extension. But the solar atmosphere is a very complicated environment. It may still hide some mysteries (we are thinking here mostly about the turbulent behavior of the magnetic field) but, for the moment, we can suppose that we know its structure in the form of a sophisti-

cated model (even tridimensional) giving at each point the chemical composition, the value of the thermodynamic parameters (such as temperature, density, pressure, bulk velocity, etc.) and the value of the magnetic field (even if in the form of a PDF, or Probability Density Function). The selected wavelength interval may contain the signatures introduced, in the form of spectral lines, by one or more atoms present in the medium, whose physical properties we need to describe in terms of their populations and quantum interferences.

For many applications the simple two-level atomic model cannot be applied. On the contrary, one needs to resort to a multi-level or to a multi-term atomic model. Often (but not always), a description in terms of a "two-term atom" may be a satisfactory approximation to the problem. In other cases a "three-term atom" or a "multi-term atom" would be more appropriate. In this situation, things rapidly get to be extremely complicated. Each term splits into different J-levels and each J-level is further split by the presence of a magnetic field into its magnetic sublevels, or M-levels. In many cases, there is a further complication due to the presence of hyperfine structure (HFS).

Just to be concrete on a single example, if we want to investigate the polarization characteristics of the wavelength interval around the sodium D lines, we can stick to a two-term model atom with HFS. In this case we have 24 M-levels in the upper term and 8 M-levels in the lower term. In general, we thus have 32 levels of which we need to know the populations, and all the possible coherences (or quantum interferences) that are present among them. This already complicated model-atom sits in an environment that is characterized by the presence of a radiation field which is at the time anisotropic and polarized. The radiation field interacts with the atom by means of the usual processes of absorption, emission and stimulated emission, though we have to remember that these concepts have to be generalized to take the polarization of radiation and atomic polarization into account. For instance, when a photon excites our atomic model from the ground term to the upper term, not only it contributes to increase the population of one or more magnetic sub-levels of the upper term, but it also creates coherences among them.

In the solar environment the atom also experiences collisions with the particles present in the medium. The most important collisions are those with electrons (in some cases also with protons) and those with neutral hydrogen atoms. The effect of collisions is only marginally known. Indeed, this is a very complicated matter, and only few theoretical results are available. On the other hand, there is an almost complete lack of experimental results. In many applications, a distinction is made between anelastic (or superelastic) collisions (mainly due to electrons) that induce transitions between different J-levels, well separated in energy, and elastic collisions that induce transitions between different M-levels of the same J-level (mainly due to neutral hydrogen atoms). Unfortunately, this distinction becomes rather vague when treating the case of multi-term atoms because the energy difference between M-levels is often comparable with the energy difference between J-levels. Much work has still to be done on this subject which is extremely important because collisions act on our model-atom basically with three distinct (but correlated) effects: line broadening, depolarization, and frequency redistribution in scattering events.

2. An overview of the present theoretical schemes

One of the most fruitful theoretical approaches that have been used to cope with the formidable problem outlined in the Introduction is the one based on the density matrix operator. Introduced in the scientific literature by Von Neumann (1927), it was systematically applied to atomic physics since the seminal paper by Fano (a pupil of Fermi) "*Description of States in Quantum Mechanics by Density Matrix and Operator Techniques*" (1958). Astrophysical applications started with the work of Litvak (1975) for the interpretation of the polarization properties of astrophysical masers and continued with the work of Bommier & Sahal-Bréchot (1978) on solar prominences.

Starting from the simplifying assumption that the single processes of absorption and emission are independent (Markovian approximation), and following the methods of Q.E., it is possible to find the statistical equilibrium equations for the density matrix elements of the selected model atom. The different rates appearing in the equations (transfer rates and relaxation rates) depend on the local properties of the radiation field illuminating the atom. Moreover, within the same theoretical approach, one can also find the radiative transfer equations for polarized radiation along any particular direction. These equations contain the absorption coefficient (in the form of a matrix) and the emission coefficient (in the form of a vector) which depend on the local values of the density matrix elements (see Landi Degl'Innocenti & Landolfi 2004). The coupled set of equations can thus be solved numerically or, in some few cases, analytically.

The main strength of this theoretical approach is that the statistical equilibrium equations for the density matrix and the radiative transfer equations for the Stokes parameters are derived in a self-consistent way from the principles of Q.E.. Moreover, the formalism allows the possibility of taking lower level polarization into account, to treat multi-level and multi-term atoms, to include HFS in the calculations, and to account for the interaction of the atom with a magnetic field in any regime (from the Zeeman effect regime to the complete Paschen-Back effect regime). Through this formalism it is also possible to account simultaneously for the polarizing effect of a magnetic field (due to Zeeman splitting) and for its depolarizing effect on resonance polarization (due to the Hanle effect). Finally, rather unfamiliar mechanisms, such as the so-called "level-crossing", "anti-level-crossing", and "alignment-to-orientation" mechanisms are well contained in the formalism and suitably described by it.

This approach has been successfully applied for the solution of a rather large number of problems concerning spectro-polarimetric profiles observed in the second solar spectrum and in solar structures. Here we just mention some of the most relevant applications (see Belluzzi 2010, for further details): a) diagnostics of the magnetic field in solar prominences (Leroy et al. 1983, 1984); b) modeling of the b-lines of magnesium (Trujillo Bueno 1999, 2001); c) modeling of the infrared triplet of ionized calcium (Manso Sainz & Trujillo Bueno 2003); d) interpretation of spectro-polarimetric observations in prominences and filaments (e.g. Trujillo Bueno et al. 2002); e) interpretation of the second solar spectrum of Ti i (Manso Sainz & Landi Degl'Innocenti 2002) and of Ce ii (Manso Sainz et al. 2006); f) differential magnetic sensitivity of the Ba ii 4554 Å line (Belluzzi et al. 2007).

Notwithstanding its numerous successes, the theoretical scheme based on the density matrix suffers from the severe limitation that, due to the Markovian approximation, partial frequency redistribution (PRD) effects cannot be taken into account. Indeed, referring to the intensity spectrum, PRD effects result to be important mainly for reproducing the wings of very strong resonance lines, such as the calcium H and K lines, the

magnesium b-lines, the sodium D lines, Hα, Hβ, Lyα, and few others. The importance of PRD effects on polarization was put forward by the pioneering work of Dumont et al. (1977), who pointed out that such effects might be the key ingredient to model the typical triplet-peak structure observed in the Q/I profile of the "champion" Ca I line at 4227 Å (the one that shows the largest limb polarization and the first one to be observed for this phenomenon by Redman 1941). We now believe that without including such effects it would not be possible to interpret those linear polarization profiles that have been classified as of "M-type" by Belluzzi & Landi Degl'Innocenti (2009). Indeed, without invoking PRD effects it seems impossible to explain the physical origin of such multi-peak structures.

To handle PRD effects, different theoretical schemes have been proposed. One of them, due to Bommier (1997a,b), generalizes the theoretical approach previously described by including higher order terms in the perturbative expansion of the atom-radiation interaction, under the hypothesis of a two-level atom with unpolarized lower level. Other schemes are based on the introduction of suitable redistribution matrices but are generally restricted to the case of a two-level (or two-term) atom with unpolarized lower level (Omont et al. 1972; Domke & Hubeny 1988). Generalizations to model atoms having more than two levels are difficult. In the scalar case such generalizations have been proved to be possible, though extremely complex. For instance, Hubeny & Oxenius (1987) succeed in defining generalized redistribution functions, but to treat a 3-level model atom 11 such functions are needed, and this number increases to 36 for a 4-level model atom. Such generalizations have never been attempted in the "polarized world". Moreover, phenomena of lower-level polarization (differences in populations among the sublevels and coherences between any pair of them) are difficult to incorporate in the theory.

Another approach is based on the so-called metalevel theory (Landi Degl'Innocenti et al. 1997). This is a heuristic approach which was developed for the scalar case by several authors (Ehrenfest 1914; Weisskopf & Wigner 1930; Woolley & Stibbs 1953; Milkey & Mihalas 1973; Milkey et al. 1975; Oxenius & Simonneau 1994). The main idea is that the energy levels can be considered as a collection of internal "sublevels" or "metalevels" having a certain distribution in energy. This distribution has a Lorentzian profile whose width is inversely proportional to the lifetime of the level. The metalevel theory has the advantage of keeping the same scheme as the theory based on the Markovian approximation, with the difference that a single matrix element ρ_{nm} becomes a function $\rho_{nm}(\zeta)$, ζ being a parameter related to the energy of the single metalevel. For the rest, the scheme of the theory remains the same, in the sense that two sets of equations are established, the statistical equilibrium equations for the density matrix function and the radiative transfer equations, containing the density matrix function in the absorption matrix and in the emission vector. In its present status, without the introduction of collisions, the metalevel theory is capable of correctly describing a rather large number of scattering phenomena (including those where the ground level has a definite amount of atomic polarization). When lower level polarization is neglected, it brings to the same results as the well-known Kramers-Heisenberg equation.

The metalevel theory was successfully applied by Landi Degl'Innocenti (1998, 1999) in order to explain the peculiar interference profile observed in the second solar spectrum around the sodium D-lines, though this result was subsequently criticized because of the rather large amount of ground level atomic alignment needed to explain the observations. However, notwithstanding its partial success, the metalevel approach

never reached the status of a completely satisfactory theory for two main reasons. From one side, the introduction into the theory of the effect of collisions has revealed to be rather problematic, and it has not been achieved so far in a consistent way. From the other side, the broadening of the metalevels distribution is introduced in a somewhat heuristic way and a "rule" for obtaining its value has never been found.

3. Conclusions and new ideas

The theoretical approach based on the density matrix formalism, and self-consistently derived from the principles of Q.E. is presently one of the most solid theoretical frameworks in the field of spectropolarimetry. This theoretical approach has been highly successful, mainly for the interpretation of signals which can be described in the so-called limit of complete redistribution in frequency (CRD). However, it suffers from the severe limitation that PRD effects cannot be accounted for. The metalevel theory can handle PRD effects, but all the attempts for its generalization to account consistently for collisions and lower-level coherences have failed. The redistribution matrix approach is very suitable for taking PRD effects into account. However, it can consistently describe only two-level atoms with unpolarized lower level. New heuristic approaches have been proposed for treating two-term atoms, but they are based on rather crude approximations and their validity and physical consistency are far from being firmly established. In this scenario, some new ideas for treating the problem through a self-consistent set of equations, fully derived from first principles, would be highly desirable. Here we would like to put forward some few reflections that may lead to the establishment of such a theory.

Consider a physical system having total Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}^{\mathrm{I}} \ , \tag{1}$$

the sum of the unperturbed Hamiltonian $\mathcal{H}_0$ and of the interaction Hamiltonian $\mathcal{H}^{\mathrm{I}}$. The physical system evolves in time according to the Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = (\mathcal{H}_0 + \mathcal{H}^{\mathrm{I}})|\psi(t)\rangle \ . \tag{2}$$

To solve this equation one can use the method referred to as "method of the variation of the constants". Suppose to have solved the stationary Schrödinger equation for $\mathcal{H}_0$

$$\mathcal{H}_0 |\alpha\rangle = E_\alpha |\alpha\rangle \ . \tag{3}$$

One can develop the wave-function in series of the eigenvectors of $\mathcal{H}_0$ by writing

$$|\psi(t)\rangle = \sum_\beta c_\beta(t)\,\mathrm{e}^{-\mathrm{i}E_\beta t/\hbar}|\beta\rangle = \sum_\beta f_\beta(t)|\beta\rangle \ . \tag{4}$$

The coefficients $f_\beta(t)$ are functions of time and they reduce to a constant multiplied by an exponential in the absence of perturbations. In the traditional method of the variation of the constants, a differential equation is established for the coefficients $c_\beta(t)$ that multiply the exponential. Now, following an approach often called of "coarse-graining", we introduce a variation of the traditional method by directly developing the

coefficients $f_\beta(t)$ in Fourier series and thinking that the Fourier components are function of time.

The coarse-graining technique, some times also refereed to as "multiscale technique", consists in separating the time scales on which the physical phenomenon evolves in two separate sets: the short timescales and the long timescales. This corresponds, in the Fourier domain, to make a distinction between high and low frequencies, respectively. Typically, one develops the time-varying signal (in our case the coefficients $f_\beta(t)$ appearing in Eq. [4]) through a Fourier integral. The frequency domain is however restricted to an interval (Ω, ∞) containing all the relevant information about the spectral characteristics of the signal. The coefficients of the Fourier development are then functions of time that evolve according to the frequency domain that is outside the interval chosen (frequencies smaller than Ω). This approach is connected with the mathematical difficulties that are met when trying to define, for instance, the spectrum of any non-stationary radiation source. In mathematical terms, the exact definition of the spectrum would imply to measure the electric signal at any time t from $-\infty$ to $+\infty$, which is obviously impossible in practice. If the time interval in which the sampling of the signal is performed is $\mathcal{T}$, one can obtain the spectrum only for frequencies larger than $\simeq 1/\mathcal{T}$, and the same spectrum is a function of time. An illustrative example is the spectrum of the electromagnetic radiation emitted by a variable star.

We thus put

$$|\psi(t)\rangle = \sum_\beta \int_{\Delta\Omega} \hat{f}_\beta(\omega, t) |\beta\rangle \, \mathrm{e}^{-\mathrm{i}\omega t} \, \mathrm{d}\omega \ , \tag{5}$$

where $\Delta\Omega$ is a frequency interval sufficiently large to contain all the relevant spectral information for the coefficients f. Substituting in the Schrödinger equation we obtain

$$\mathrm{i}\hbar \sum_\beta \int_{\Delta\Omega} \left[\frac{\mathrm{d}}{\mathrm{d}t}\hat{f}_\beta - \mathrm{i}\omega\hat{f}_\beta \right] |\beta\rangle \, \mathrm{e}^{-\mathrm{i}\omega t}\mathrm{d}\omega =$$

$$= \sum_\beta \int_{\Delta\Omega} \hat{f}_\beta \, E_\beta \, |\beta\rangle \, \mathrm{e}^{-\mathrm{i}\omega t}\mathrm{d}\omega + \sum_\beta \int_{\Delta\Omega} \hat{f}_\beta \, \mathcal{H}^{\mathrm{I}} \, |\beta\rangle \, \mathrm{e}^{-\mathrm{i}\omega t}\mathrm{d}\omega \, . \tag{6}$$

We now multiply both sides by the vector $\langle\alpha|$ to get

$$\int_{\Delta\Omega} \left[\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{f}_\alpha + (\hbar\omega - E_\alpha)\hat{f}_\alpha \right] \mathrm{e}^{-\mathrm{i}\omega t} \, \mathrm{d}\omega = \sum_\beta \int_{\Delta\Omega} \hat{f}_\beta \, \mathcal{H}^{\mathcal{I}}_{\alpha\beta} \, \mathrm{e}^{-\mathrm{i}\omega t} \, \mathrm{d}\omega \ , \tag{7}$$

where

$$\mathcal{H}^{\mathrm{I}}_{\alpha\beta} = \langle\alpha|\mathcal{H}^{\mathrm{I}}|\beta\rangle \ . \tag{8}$$

From the integral equation one then gets the final equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{f}_\alpha(\omega, t) - \mathrm{i}\left(\omega - \frac{E_\alpha}{\hbar}\right)\hat{f}_\alpha(\omega, t) = \frac{1}{\mathrm{i}\hbar}\sum_\beta \mathcal{H}^{\mathrm{I}}_{\alpha\beta} \, \hat{f}_\beta(\omega, t) \ . \tag{9}$$

This is an exact equation for the Fourier transform of the state vector (expressed on the basis of the eigenvectors of the unperturbed Hamiltonian). When applying these ideas to the interaction between a material system and the radiation field, the eigenvectors of the Hamiltonian are indeed of the form

$$|\alpha\rangle \rightarrow |a\rangle|\{n_k\}\rangle \qquad\qquad |\beta\rangle \rightarrow |b\rangle|\{n'_k\}\rangle \ , \tag{10}$$

where, in Dirac's notations, $|a\rangle$ and $|b\rangle$ are the eigenvectors of the atomic Hamiltonian and $|\{n_k\}\rangle$ and $|\{n'_k\}\rangle$ are the eigenvectors of the radiation field Hamiltonian expressed in the formalism of second quantization ($\{n_k\}$ is the set of integer numbers specifying the number of photons present in each mode of the radiation field). The Fourier transform of the "traditional" density-matrix element between the atomic states a and b can be obtained by tracing over the radiation field states to get an expression of the form

$$\hat{\rho}_{ab}(\omega, t) = \sum_{\{n_k\}} p_{\{n_k\}} \, \hat{f}^*_{a,\{n_k\}}(\omega - E_{\{n_k\}}, t) \, \hat{f}_{b,\{n_k\}}(\omega - E_{\{n_k\}}, t) \ , \tag{11}$$

where $p_{\{n_k\}}$ is the probability of finding the radiation field in the eigenstate $|\{n_k\}\rangle$, and $E_{\{n_k\}}$ is the corresponding energy.

We hope that these ideas, and in particular the introduction of the Fourier transform of the density matrix may reveal to be well-founded and that they may lead to the establishment of a set of equations really capable of handling the general problem outlined in the Introduction. Obviously, there will be a price to pay because one will be obliged to deal not with the density-matrix elements of atoms, but with the Fourier transforms of such density-matrix elements. We also hope that this approach may lead to some simplifications in the theoretical treatment of collisions for which working in the Fourier domain may result in being more appropriate.

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