The Molecular Zeeman Effect and Solar Magnetic Fields

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Abstract. The potential of molecular lines as diagnostics of solar magnetic fields is not yet known. We present here a short overview of major properties of the molecular Zeeman effect and demonstrate, using fits to observed molecular Stokes profiles, that we now possess the tools to apply such profiles to obtain a better understanding of solar and stellar magnetic fields.

1. Introduction

Lines of diatomic molecules observed in sunspot spectra are good temperature and pressure indicators. They are also useful for determining elemental and isotopic abundances, while little is known about their diagnostic capabilities for solar magnetic studies. The fact that the effect of the applied magnetic field in molecular lines is smaller and less striking than that observed in the most Zeeman sensitive atomic lines has significantly delayed their use for diagnosis of solar magnetic fields. With developing observational facilities, though, reports on puzzling polarization of molecular lines compared to atomic lines have appeared (e.g. Harvey 1973, 1985; Rüedi et al. 1995). These have not been understood, however. The scarcity of theoretical works which would be able to explain both the splitting and polarization patterns of molecular lines for different coupling cases was another reason for the slow progress in this field. For instance, two latest theoretical investigations of the molecular Zeeman effect were separated by five decades (Kronig, 1928; Schadee, 1978). Moreover, in spite of the major advance which the latter work represents, giving the treatment of the molecular Paschen-Back effect for the weak coupling case, till now there has been only a single attempt to utilize this theory for sunspots (Illing 1981). Recently, we have presented the first spectral synthesis of molecular Stokes parameters, based on

Schadee's theory, and provided first successful fits to molecular Stokes I and V profiles observed in sunspots (Berdyugina et al. 2000). This gives the opportunity for further, more thorough investigations of the diagnostic properties of molecular lines and for their applications in studies of solar and stellar magnetic fields.

Here we present some details of the splitting and polarization patterns of lines of the TiO γ-system and MgH green system. The two band systems represent two coupling cases, which cover most of the molecular transitions observed in sunspot spectra from near UV to near IR. They are good examples of the molecular Zeeman and Paschen-Back effects, whose peculiarities we discuss.

2. The Molecular Zeeman and Paschen-Back effects

The magnetic splitting of energy levels in the case of molecules occurs due to the same fundamental causes as in atoms. If the molecule possesses a non-zero magnetic moment, the external magnetic field interacts with the magnetic moment and causes a precession of the total angular momentum, $\mathbf{J}$, about the field direction (Herzberg 1950). The space quantization of $\mathbf{J}$ results in $2J+1$ magnetic components with different energies. The largest contribution to the magnetic moment of a diatomic molecule is due to the magnetic moment associated with the orbital and spin angular momenta of the electrons. If they are zero or small, the contributions from the rotational motion of the molecule and the spins of nuclei should be taken into account.

The energies of the magnetic components depend on how the electronic angular momenta are coupled to the rotation of the molecule.

In *Hund's case (a)* the electronic angular momenta (both spin and orbital) are strongly coupled to the internuclear axis. Thus, the splitting is determined only by the quantum numbers of the transitions and independent of the molecular constants. This behavior is analogous to the Zeeman effect of atomic lines. In this case, the splitting and strengths of the Zeeman components are described by rather simple analytical expressions (Kronig 1928).

An example of such a splitting is shown in Fig. 1 for the line of the TiO γ-system ($A^3\Phi - X^3\Delta$). Both electronic states of the system are under strong spin-orbit coupling and, thus, represent the ordinary molecular Zeeman effect. The splitting of the levels is symmetrical and proportional to the field strength for a given total angular momentum number J. It is larger for low J and decreases with increasing J. The partial sums of the strengths of the Zeeman patterns for transitions with $\Delta M = 0, +1, -1$ (π and σ components) are equal, so that the line itself undergoes symmetrical splitting. For lines of the γ-system, the symmetry holds up to very strong fields, such as $10\,\mathrm{kG}$, hence one can use these calculations for interpretation of the Stokes parameters observed in sunspot spectra.

In *Hund's case (b)*, the orbital angular momentum of the electrons is coupled to the internuclear axis, whereas the spin is coupled to the rotational axis. It often also happens that the spin-rotational coupling is so weak that these two angular momenta are uncoupled even by a small field. This is the molecular analogue of the atomic Paschen-Back effect. Then, the spin is space quantized independently, and the total splitting for large J is approximately independent of
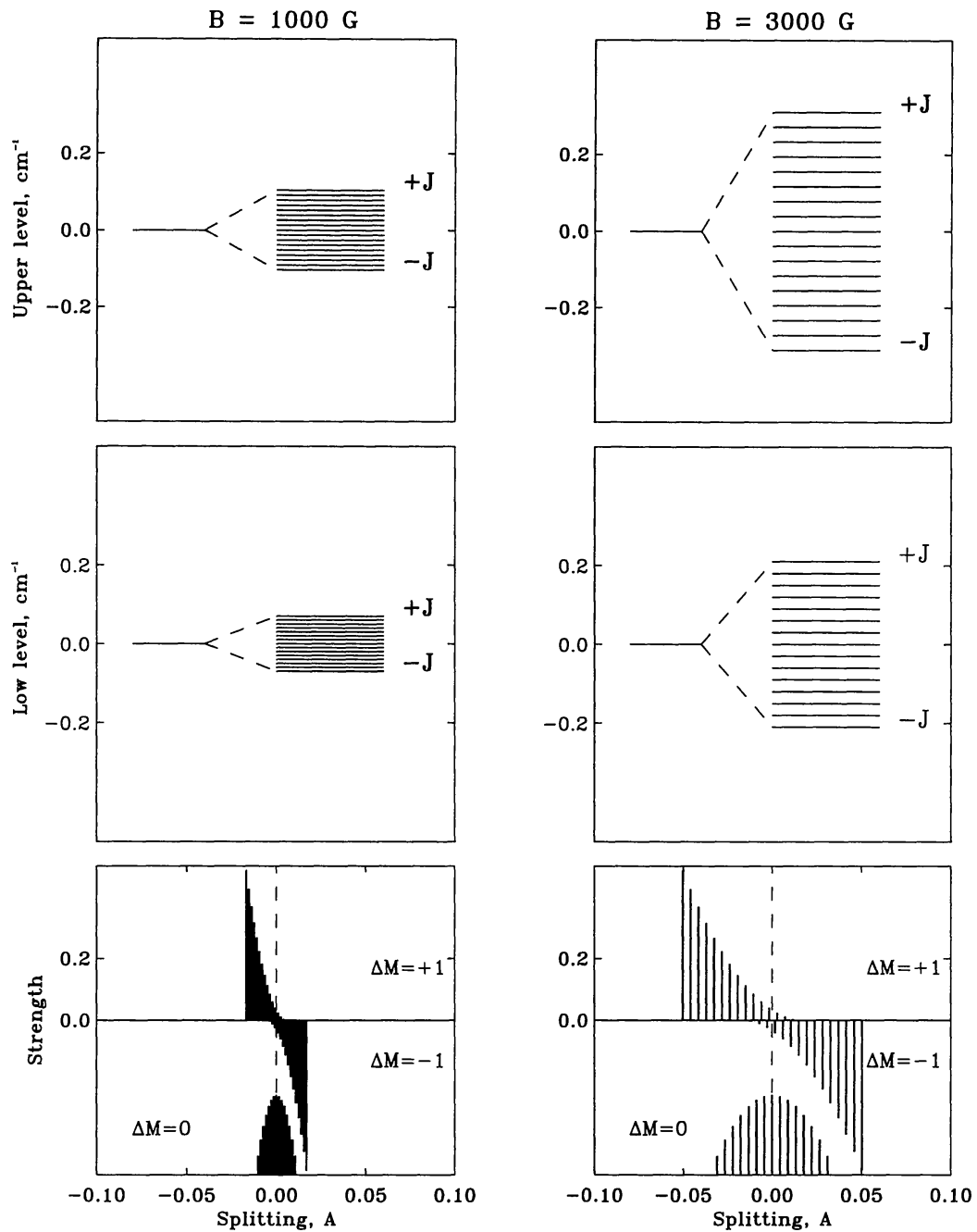
Figure 1. Splitting of TiO $\gamma(A^3\Phi-X^3\Delta)$ (0,0) $R_3(7)$ 7055.5Å at field strengths of 1000 G (left) and 3000 G (right). The energy levels of the upper and lower states are plotted in the top and middle rows, the Zeeman splitting patterns of the transition are plotted in the bottom panels. The symmetry holds up to very strong fields.

J and is of order of magnitude of the normal Zeeman splitting. This case holds as long as the multiplet splitting is small compared to the Zeeman splitting. Computation of the splitting and strengths of the Zeeman components in the Paschen-Back effect can be done only numerically (Schadee 1978).

The dramatic transformation from almost normal Zeeman splitting to the Paschen-Back case is demonstrated in Fig. 2 with the help of transitions of the MgH green ($A^2\Pi - X^2\Sigma$) system. At a field strength of 1000 G, the magnetic splitting is less than, although comparable to, the multiplet splitting in the lower state. The transitions in the main rotational line $P_1(5.5)$ and the satellite line $Q_{12}(4.5)$ are still distinguishable. With increasing field strength, the perturbation by the approaching magnetic sublevels results in abnormal shifts of the sublevels and modification of the strengths of the Zeeman patterns and the lines themselves, so that the main line becomes weaker, while the satellite line strengthens. At a field of 3000 G, the splitting of individual rotational levels is no longer symmetrical and the Zeeman patterns of the main and satellite lines are mixed. As a result, the partial sums of strengths of π and σ components for individual lines are not equal. The two lines together start to imitate a normal Zeeman splitting, in which however the transitions in the main and satellite lines dominate different σ-components.

2.1. TiO and MgH lines in solar umbral spectra

As was shown by e.g. Livingston & Berdyugina (2001), there is no unique spectrum of the solar umbra. For instance, strong TiO lines appear only in spectra of bigger spots, while MgH lines are always observed in umbral spectra, getting stronger in cooler regions. High temperature sensitivity makes these molecular bands attractive for probing the structure of the coolest parts of sunspot umbrae. As the first step in such a study, a comparison of observed and synthetic Stokes parameters of molecular lines should be made. For this purpose, we have obtained observations of two spectral regions with TiO and MgH lines, discussed below, with the technique described by Livingston & Berdyugina (2001). The Stokes profiles were calculated by solving the set of radiative transfer equations with the code STOPRO (Solanki et al. 1992, Frutiger et al. 2000) updated for molecular line computations and for accounting the effect of blends. The calculations were carried out with the radiative equilibrium model by Kurucz (1993) having T_{eff}=3750 K and log g=4.5.

The strongest and least blended TiO band head of the γ-system in the visual spectrum of sunspot umbrae is $(0,0)R_3$ λ 7054.4 Å (Wallace et al. 1998). In this band head, lines of low rotational numbers coincide with those of high numbers, and, thus, the amplitude in Stokes V increases, resulting in a measurable signal. Our calculations were carried out with the molecular constants and line wavelengths from Ram et al. (1999) and band oscillator strengths from Davis et al. (1986). With reasonable values of the field strength (3000 G) and filling factor (0.75), we found an excellent agreement between the observed and calculated Stokes V, though some problems with unidentified blends in Stokes I have been encountered (Fig. 3). The blends, however, being magnetically insensitive, do not contribute to Stokes V. Since the structure of the band in Stokes V is well reproduced by our calculations, we conclude that the approach we use is appropriate.
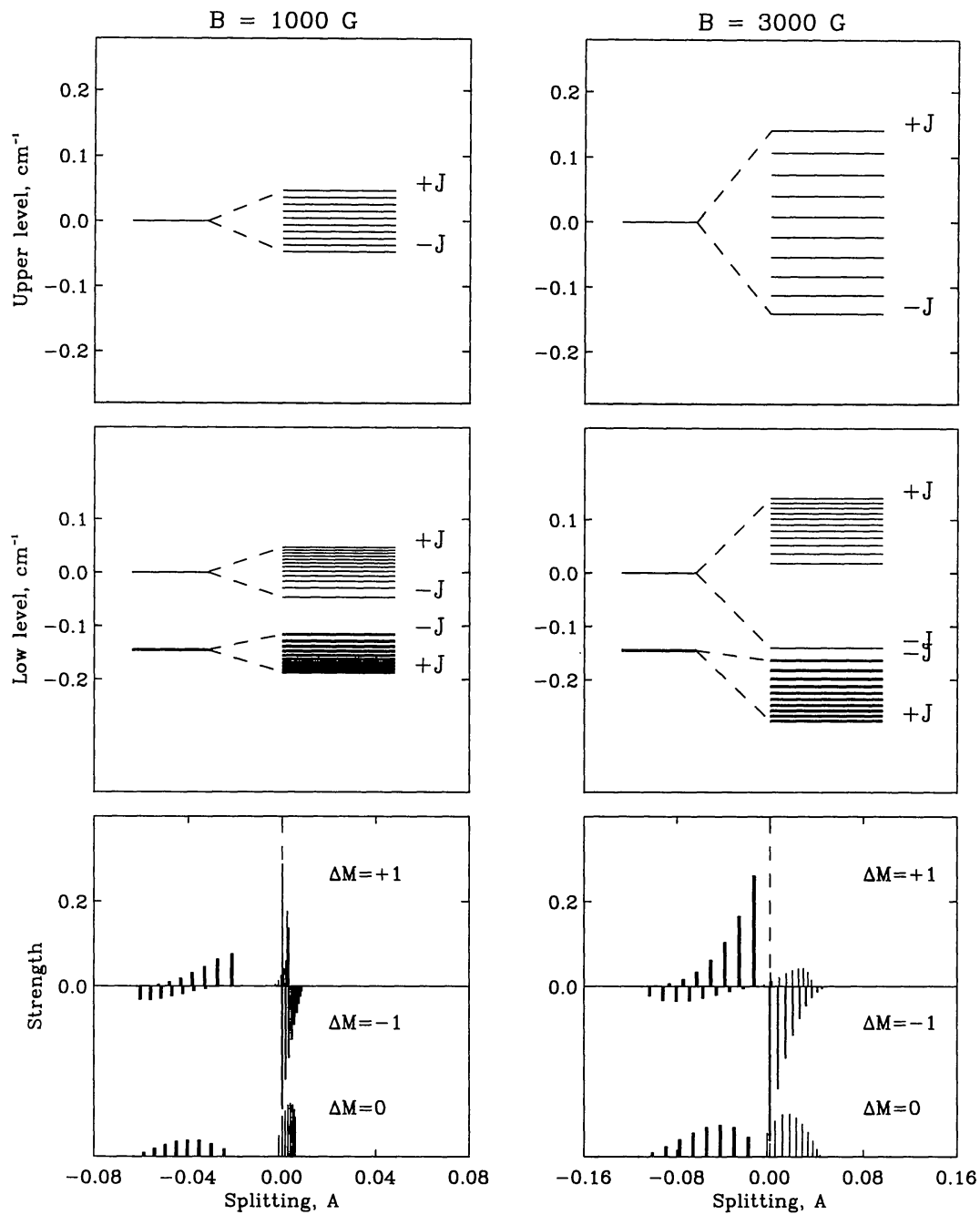
Figure 2. The same as Fig. 1 for MgH $A^2\Pi - X^2\Sigma$ (0,0) $P_1(5.5)+Q_{12}(4.5)$ 5199.6Å. Two terms, $F_1(5.5)$ and $F_2(4.5)$, of the lower state are shown. Thicker lines present patterns of the satellite line $Q_{12}(4.5)$. At stronger fields the two lines imitate a normal Zeeman splitting.
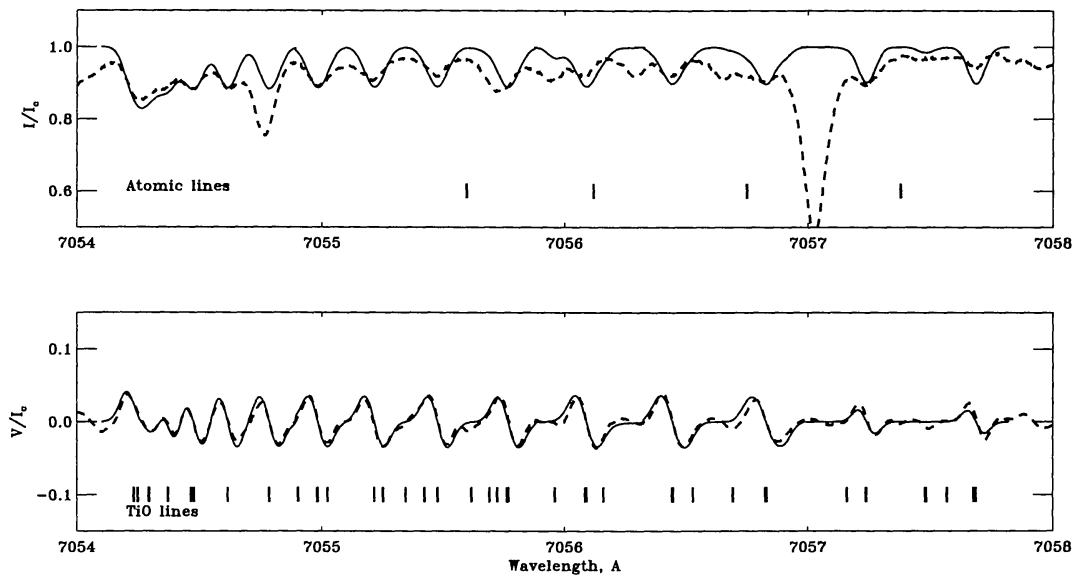
Figure 3. Calculated (solid line) and observed (dashed line) Stokes I and V of the TiO $\gamma(0,0)R_3$ band head. The field strength is 3000 G and the filling factor is 0.75 for an angle between the magnetic vector and the line of sight of $0°$. Vertical dashes indicate positions of lines included in the spectral synthesis. The two strongest absorption features seen in Stokes I are atmospheric water lines.
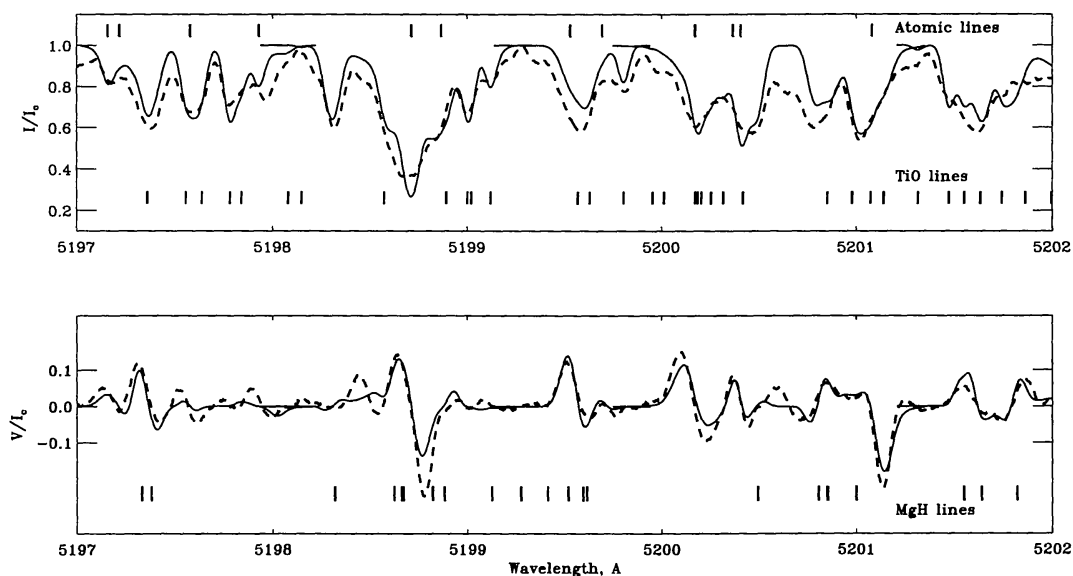
Figure 4. The same as Fig. 3 for the MgH $(0,0)$ band. The field strength is 3000 G and the filling factor is 0.95 for an angle between the magnetic vector and the line of sight of $0°$.

The strongest lines of the MgH green system are observed in the (0,0) band. We searched for the least blended early rotational lines in the branches of this band using the sunspot atlas by Wallace et al. (2000) and found the P-branch of the band to be most suitable. It starts at 5192 Å, develops first to the red, forms the head at 5211 Å and, then, degrades toward shorter wavelengths. Six lines of the P-branch are useful for the analysis (on the basis of strength and blending): P_1 J=4.5–8.5 λ 5197.4, 5199.6, 5201.6, 5203.5, 5205.2 Å and P_2 J=5.5 λ 5200.8 Å. One must note that this region is also plagued by many lines of the TiO α-system, which are not Zeeman sensitive. Thus, these lines do not contribute to other Stokes parameters besides Stokes I, but they can still influence the Stokes profiles of lines which they blend.

In Fig. 4 we present the observed and calculated Stokes I and V for the spectral region with four selected MgH lines of the P-branch. A number of atomic and TiO lines have been included into the calculations, though not all blends have been identified. The calculations were carried out with the molecular constants, line positions and band oscillator strengths from Bernath et al. (1985) and Kirby et al. (1979). The fit to the MgH lines under investigation with the field strength of 3000 G and filling factor of 0.95 is rather acceptable, taking into account the simplicity of the spot model used. Thus, we conclude that the theory of the Paschen-Back effect used is adequate.

3. Conclusions

We have discussed the peculiarities of the molecular Zeeman and Paschen-Back effects and examined the magnetic sensitivity of the two band systems, TiO and MgH, observed in sunspot spectra. We showed that the synthetic Stokes parameters fit reasonably well the observed profiles, so that the applied theory can be used in future investigations. The magnetic splitting of the TiO γ-system is typical for band systems of other molecules with strong internal momentum coupling, such as TiO γ'- and α systems, C_2 Swan and FeH Wing-Ford (infra-red) systems. Also, the red systems of CN and CaH are of the same electronic transition as the considered MgH system. Lines of these molecules are observed in spectra of the umbra (TiO, FeH, MgH, CaH, CN) and penumbra (MgH, CN, C_2). Thus, being formed at different height in the atmosphere, they can be used to probe the thermal and magnetic structure of sunspots.

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