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Letter to the Editor

Zeeman-split opposite-polarity OH lines in sunspot spectra: Resolution of a puzzle

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Abstract. We present the first synthetic Zeeman-split Stokes I and V profiles of OH lines. They explain the puzzling observations reported by Harvey (1985) of two pairs of lines from the infrared (2, 0) band with Stokes V profiles exhibiting opposite polarities. Our new perturbation calculations of the Zeeman effect in diatomic molecules, which allow states of any multiplicity to be treated, resolve the puzzle. They reveal that the unusual behaviour of these lines stems from the fact that the two pairs have effective Landé factors of similar magnitude, but of opposite signs.

Key words. Sun: sunspots – molecules – polarization

1. Introduction

In the presence of a magnetic field most atomic and many molecular spectral lines exhibit the Zeeman effect, including the production of net circular polarization, i.e. Stokes V (if the magnetic field is not perpendicular to the line of sight). Whereas the V profiles of almost all atomic lines observed on the Sun are nearly antisymmetric and exhibit the same polarity, many Stokes V profiles of molecular lines have strange shapes, while some are of opposite polarity as compared to atomic or other molecular lines (e.g. Nicholson 1938; Harvey 1973, 1985; Rüedi et al. 1995). As we recently showed, the root of such behaviour lies either in the molecular Paschen-Back effect or in the specific changes of the total angular momentum in molecular transitions (Berdyugina et al. 2000; Berdyugina & Solanki 2001).

One particularly interesting case is presented by rovibrational OH transitions in the infrared. In the spectrum of a sunspot umbra Harvey (1985) discovered that lines of the same OH band and of approximately the same strength exhibit opposite polarities. A portion of an FTS (Fourier Transform Spectrometer) spectrum of a sunspot umbra is plotted in Fig. 1, where 4 OH lines are marked. The complete data set is described and discussed by Rüedi et al. (1995). Note that the pair on the right has V profiles of opposite polarity compared with those on the left.

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The fact that two lines each have V profiles of the same polarity, the V profiles are antisymmetric and all lines are otherwise similar rules out possible explanations such as blends, instrumental cross-talk, combined magnetic and velocity gradient or a change in polarity of the magnetic field with height. We propose that the behaviour of the two pairs of lines is due to the fact that they have equal but opposite effective Landé factors.

This explanation may at first sight appear surprising, since negative Landé factors are extremely rare among atomic lines (see, e.g., Stenflo et al. 1984). However, explaining polarization patterns of molecular lines is more complex than for atomic lines. This partly explains why there are relatively few investigations of the molecular Zeeman effect in the literature. A theory of the molecular Zeeman effect was derived at the end of the 1920s (see the review by Crawford 1934). It explained the Zeeman splitting of molecular lines in its basics, but left the calculation of the intensities and polarization patterns of the Zeeman components for later treatment. Five decades later, this problem was successfully solved by Schadee (1978), but only for doublet terms. Recently, we extended the solution to terms of any multiplicity in the Zeeman regime (Berdyugina & Solanki 2001). This has now created the possibility of tackling the problem of the odd behaviour of the OH lines shown in Fig. 1. Here we present the first successful synthesis of Zeeman-split Stokes parameters of OH lines and provide an explanation of their puzzling Stokes V profiles.
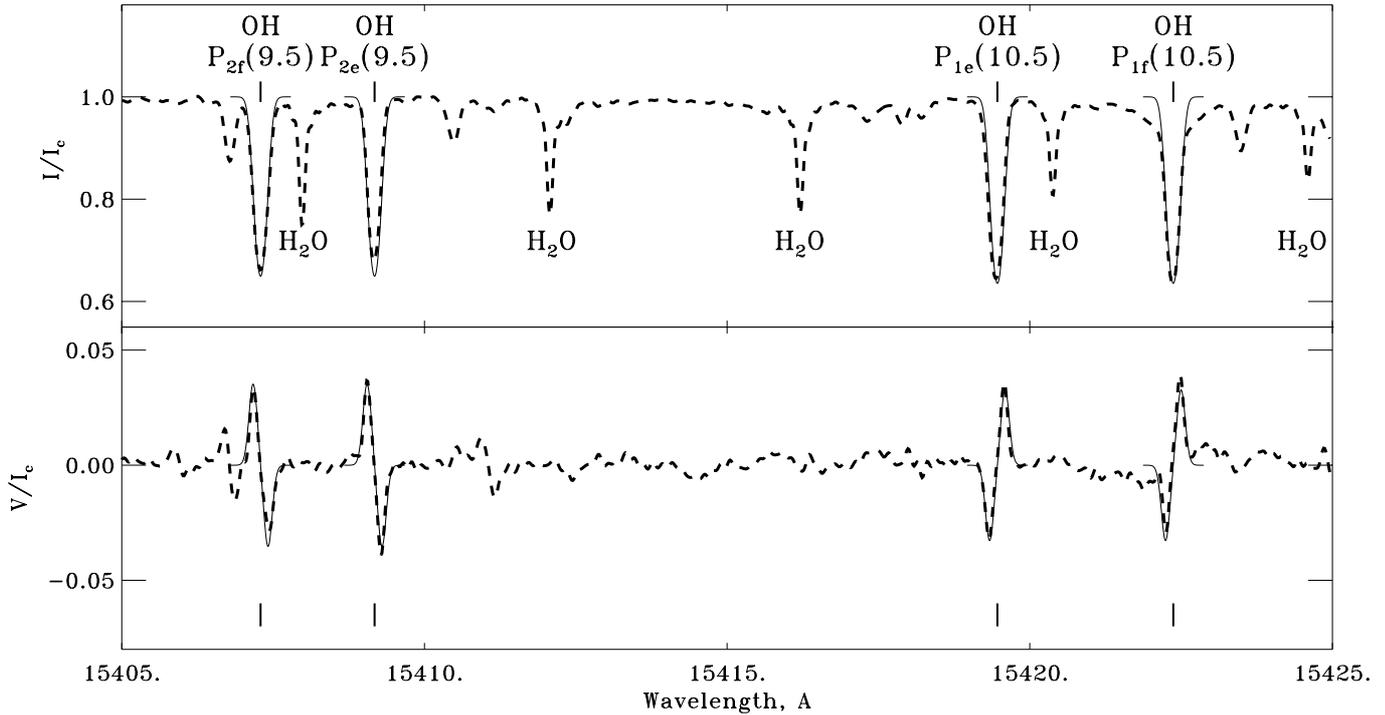
Fig. 1. The observed (dashed line) and synthesized (solid lines) Stokes I and V spectra of the two pairs of OH lines pointed out by Harvey (1985). Plotted are the profiles normalized to the local continuum intensity I_c. Note that the magnetic field in the spot is directed away from the observer and, thus, the reversed polarization is present in the left pair of lines. The weaker reversed-polarity V profiles, e.g. at $15\,407$ Å, are also due to OH.

2. The Zeeman effect in the infrared OH lines

The successful synthesis of the Zeeman pattern of molecular lines basically depends on the correct choice of the momentum coupling scheme and the accuracy of measurements of the coupling constants. In contrast to the atomic case, three angular momenta determine the coupling scheme in a diatomic molecule: the electronic orbital angular momentum $\boldsymbol{L}$, the electronic spin $\boldsymbol{S}$, and the molecular rotation $\boldsymbol{R}$. One distinguishes between a few coupling cases of the three momenta with respect to each other and the so-called internuclear axis (e.g. Herzberg 1950). In Hund's case (a), the electronic angular momenta, both $\boldsymbol{L}$ and $\boldsymbol{S}$, are strongly coupled to the line joining the nuclei and interact very weakly with the rotation. In Hund's case (b), the orbital angular momentum is coupled to the internuclear axis, whereas the spin is coupled to the rotation. In Hund's case (d), the orbital angular momentum is uncoupled from the internuclear axis and is coupled to the rotation. The description of the Zeeman effect in the pure cases is relatively simple: for cases (a) and (b) see, e.g., Landau & Lifshits, while for case (d) the explicit formula can be easily obtained in a similar way, but is of little practical interest.

It often happens, however, that the uncoupling of $\boldsymbol{L}$ and $\boldsymbol{S}$ from the internuclear axis is incomplete and increases gradually with increasing rotation. In such cases an intermediate coupling scheme must be considered. This is the case for OH lines of the Meinel system observed in

the infrared which arise due to transitions between rovibrational levels of the ground state $X^2\Pi$.

To first order, however, the Zeeman effect in the infrared OH lines is well described by pure Hund's case (b), especially for higher rotational levels, $J \geq 10.5$ (see Berdyugina & Solanki 2001). Lines of the R and P branches show rather moderate splitting, with effective Landé factors $|g_{\mathrm{eff}}| \leq 0.37$. Of particular interest is the relation between the effective Landé factors of lines from different sub-branches which may be deduced from the computations of Berdyugina & Solanki (2001): $g_{\mathrm{eff}}(P_1) = -g_{\mathrm{eff}}(P_2)$ and $g_{\mathrm{eff}}(R_1) = -g_{\mathrm{eff}}(R_2)$, i.e. lines in different sub-branches of the same rotational branch exhibit polarization of opposite sign (although they do not need to have the same splitting patterns – see below). This might form the basis for an explanation of the observations of Harvey (1985). For lower rotational levels, the perturbation due to the uncoupling of spin from rotation causes some deviations from case (b) and slightly reduces the maximum of $|g_{\mathrm{eff}}|$ down to 0.33 in the P branches and 0.27 in the R branches.

If $L \neq 0$ then, because of the interaction of the orbital angular momentum with rotation and its partial decoupling from the internuclear axis, gradual transition to Hund's case (d) occurs. As a result the levels of the fine structure split into two sublevels and lines in the rotational branches appear as close doublets. This phenomenon is called Λ-type doubling, since the projection of the orbital angular momentum onto the internuclear axis can have
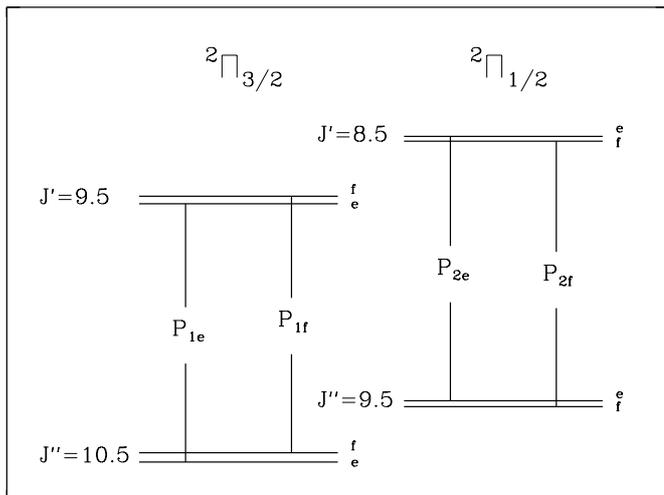
Fig. 2. Schematic representation of the transitions underlying the two pairs of OH lines, for one of which the puzzling reversed polarization was reported by Harvey (1985). The small Λ-type doubling intervals between levels denoted by e and f are exaggerated for clarity.

two values: $+\Lambda$ and $-\Lambda$. The two sublevels are denoted as e and f (Fig. 2), the eigenfunctions of these levels being combinations of the eigenfunctions corresponding to the two projections of $\boldsymbol{L}$. The intensities and Zeeman patterns of lines of the Λ-doublets are equal if no perturbation due to $\boldsymbol{L}$ uncoupling is taken into account in their calculation. The effect of such a perturbation is very small. For the OH lines, for instance, it is an order of magnitude smaller than the effect due to spin uncoupling (Radford 1962). Therefore, by neglecting perturbations due to $\boldsymbol{L}$ uncoupling we introduce an error that is only of the order of 10^{-3} for the Landé factor of a given level. For astronomical purposes this accuracy is quite adequate. In Fig. 3, we present the Zeeman patterns of the two OH lines from the P_1 and P_2 branches, which will be the same for the corresponding Λ-doublet components shown in Fig. 2. Note that the splitting patterns of the two transitions are different, although they have almost the same $|g_{\mathrm{eff}}|$.

3. Line synthesis

Using the theoretical Zeeman patterns calculated as described in the previous section, we carried out the forward spectral synthesis of the Stokes parameters of the OH infrared transitions. The radiative transfer calculations were performed with an extended and improved version of the code STOPRO (Solanki et al. 1992; Frutiger et al. 2000), which solves the set of radiative transfer equations in the formulation given by Rees et al. (1989). This code has been updated to enable computations of lines of diatomic molecules in the presence of a magnetic field, i.e. calculate the wavelength shifts of the Zeeman components and their theoretical strengths as well as molecular number densities. As a model umbra we used a radiative equilibrium atmosphere tabulated by Kurucz (1993) having
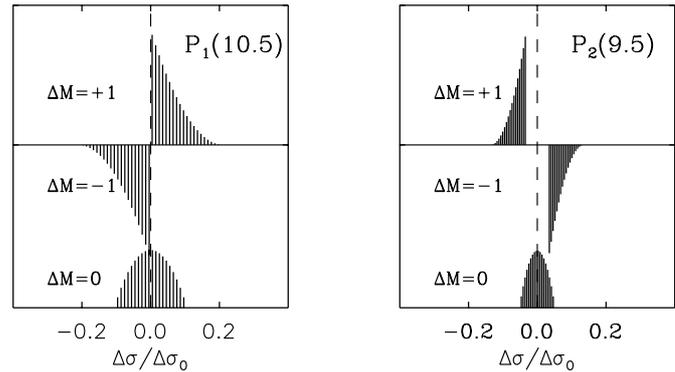

Fig. 3. The Zeeman patterns of the two pairs of OH lines of interest. In spite of rather different Zeeman patterns, the two plotted lines have almost identical absolute values of the effective Landé factors: 0.11 and –0.12 for $P_1(10.5)$ and $P_2(9.5)$, respectively.

$T_{\mathrm{eff}} = 3750$ K and $\log g = 4.5$, into which we introduced a height-independent magnetic field of strength 2500 G.

The calculations presented here were carried out for lines of the (2, 0) band with molecular constants and line positions taken from Abrams et al. (1994) and the band oscillator strength from Mies (1974). The rotational dependence of the latter was taken into account.

4. Comparison with observations

OH lines of the Meinel system are observed in sunspot spectra as two main band sequences extending up to 4.2 μm and starting at 1.4 μm and 3.1 μm, for the difference between the upper and lower vibrational state numbers $\Delta v = 2$ and $\Delta v = 1$, respectively (Wallace & Livingston 1993). Pure rotational transitions within the $v = 0$ vibrational state are observed in the solar spectrum at $10-13$ μm (e.g. Sauval et al. 1984).

The two OH line pairs at about 1.54 μm showing opposite Stokes V polarities represent the Λ-type doublets arising due to transitions in the P_1 and P_2 branches. As was noted in Sect. 2, lines in these branches have Landé factors of opposite signs, while the Λ-doubling does not change the sign of polarization. Therefore, within each pair the polarization is of the same sign, but the two pairs display opposite polarity V profiles. This effect is repeated for all OH lines observed in sunspots (e.g. Rüedi et al. 1995). In Fig. 1 we plot synthesized (solid lines) Stokes I and V profiles for the pairs of lines pointed out by Harvey (1985) on the top of the observed spectrum (dashed line). Within the uncertainties of the used model atmosphere, the observation is very well reproduced. Our computations also confirm the result of Rüedi et al. (1995) that reversed polarity is also exhibited by the other lines belonging to the P_2 sub-branch (the P_1 transitions have $g_{\mathrm{eff}} > 0$).

5. Conclusions

The successful synthesis of the polarization patterns of the rovibrational OH lines in the infrared achieved with the current state of our understanding of the molecular Zeeman effect opens up a number of astrophysical applications. Now that the unusual Stokes V signature of these lines has been shown to be the natural outcome of the properties of the OH molecule, they can be employed to investigate solar and stellar magnetism. OH is a molecule with a small dissociation energy (4.4 eV), so that OH lines can be used to probe the cooler parts of sunspots, which are otherwise not easily accessible due to stray light from brighter regions.

The lines studied in this paper also possess a rare and useful property in that they allow instrumental cross-talk (from Q, U and I into V) to be identified and removed even in the presence of a Stokes V asymmetry of solar origin. The idea is simple: if an asymmetry of the V profile is solar in origin then all 4 OH lines will be almost equally asymmetric, since their properties, except for the sign of their Landé factors, are almost identical. An asymmetry caused by cross-talk from Q, U and I into V, however, is of opposite sign in the P_1 and P_2 sub-branch lines, respectively.

The success of the present synthesis may also help to improve the diagnostic capability of atomic lines. In sunspots, strong OH lines are observed in the vicinity of the Zeeman sensitive Fe I 15 648.5 Å line and are blended with Fe I 15 652.9 Å. Together, these Fe I lines are excellent diagnostics of the solar magnetic field (e.g. Solanki et al. 1992) and are being increasingly widely used. Inverting the Stokes parameters of the blending Fe I 15 652.9 Å OH lines along with the Fe I lines greatly improves the reliability of magnetic, thermal and dynamic quantities deduced from these lines in sunspot umbrae (Lagg et al., in preparation).

In late-type stars, vibration-rotation and pure rotation lines of OH have been primarily used as indicators of the oxygen abundance (e.g. Lambert et al. 1984). Relatively recently, for the first time OH lines formed in starspots have been detected (O'Neal & Neff 1997). Polarimetric observations of these lines combined with profile synthesis calculations of the type presented here could therefore provide first direct measurements of the magnetic field inside spatially unresolved spots on stellar surfaces, if spots of one polarity dominate the stellar disc at the time of observations or when rapid rotation disentangles the Stokes V signals from different spots.

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