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The Molecular Paschen-Back Effect

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Abstract. The molecular Paschen-Back effect (PBE) lacks a detailed description since the problem was first addressed by Hill in 1929. However, many diatomic molecules exhibit the PBE at field strengths typical of sunspots and active cool stars. Recently we have presented a complete theoretical description of the molecular PBE in Hund's cases (a), (b), and all intermediate cases. This description allows us to compute the splitting of levels of any multiplicity and the transitions between them. We find that in the partial PBE regime strongly asymmetric Stokes profiles are produced, whose strengths and asymmetries depend sensitively on the magnetic field. Also, the strength of the forbidden and satellite transitions increases rapidly with field strength, while the strength of the main branch transitions decreases. These signatures hold promise to form the basis of new diagnostics of solar and stellar magnetic fields.

1. Introduction

A theory of the molecular Zeeman effect in the Paschen-Back regime (PBR) was first considered by Hill (1929), who described the splitting of molecular doublet levels for the intermediate case (a–b) using Hund's case (b) wavefunctions. However, he did not succeed in calculating the theoretical line strengths for this case. This was done much later by Schadee (1978), who repeated the analytical calculation by Hill using Hund's case (a) wavefunctions. He did not give details on line strength calculations, however, as the corresponding analytical expressions would have been too complicated. Both above approaches were limited to doublet states and to the Paschen-Back effect (PBE) on the fine structure of molecular levels. Schadee's theory of the molecular PBE was successfully used to explain peculiar Stokes profiles of molecular doublet transitions observed in sunspots: MgH (Berdyugina et al. 2000) and CN (Berdyugina, Solanki, & Frutiger 2001; Asensio Ramos, Trujillo Bueno, & Collados 2005).

Recently we presented a more general numerical approach to the molecular PBE which is valid for terms of any multiplicity and accounts for interactions of all rotational levels in a molecular electronic state (Berdyugina et al. 2005). We carried out calculations of molecular levels of different multiplicity and Stokes profiles in the PBR, when the magnetic splitting becomes comparable with the fine structure, and extended this further for the rotational structure. This theory was successfully employed for the interpretation of Stokes profiles of CaH lines observed in sunspots (Berdyugina et al. 2006), for simultaneous inversions of

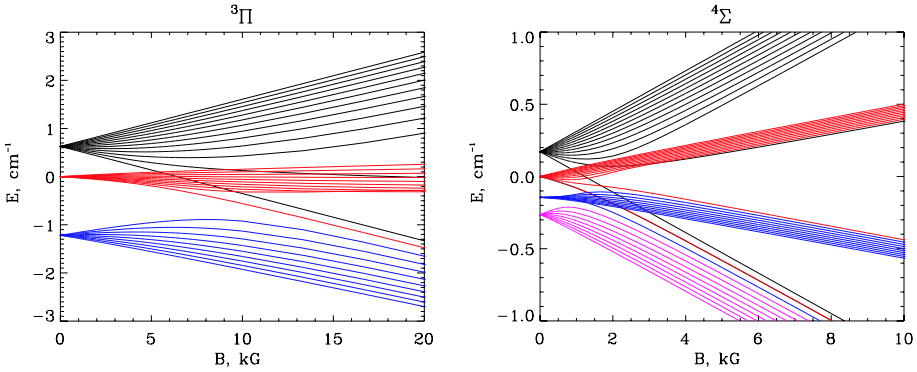

Figure 1. The PBE effect on the fine structure of $^3\Pi$ and $^4\Sigma$ states for $N = 5$ and 4, respectively. The transition to the PBR in Σ-states occurs generally at field strengths below 1 kG.

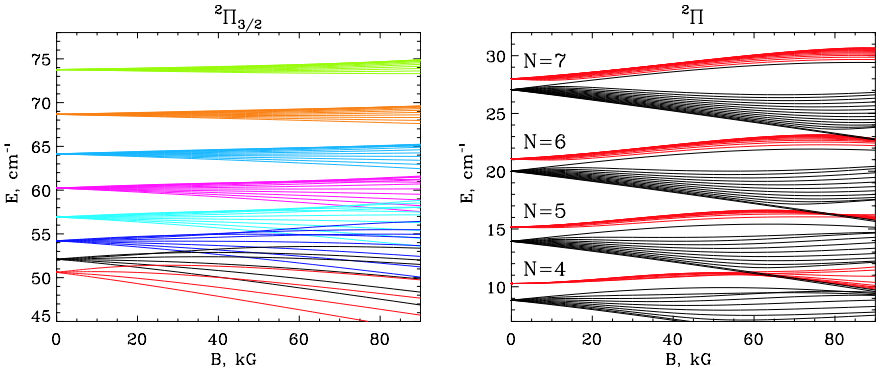

Figure 2. The PBE effect on the rotational structure of a $^2\Pi$ state in Hund's case (a) (left; $J = 1.5$ to 8.5) and in Hund's case (b) (right).

Fe I and MgH Stokes profiles (Afram et al. 2006), and for developing the theory of the molecular Hanle effect in the PBR (Shapiro et al. 2006). As a parallel effort, Asensio Ramos & Trujillo Bueno (2006) presented their calculations of the molecular PBE, while neglecting interactions between rotational levels.

Here we discuss major peculiarities of the PBE on both fine structure and rotational structure of molecular electronic states. These peculiarities, when properly modeled, hold promise to form the basis of new diagnostics of solar and stellar magnetic fields.

2. Level Splitting in the PBR

The PBE on the Fine Structure. The behavior of the electronic states in a magnetic field depends on how strongly the electron spin is coupled to the internuclear axis and the orbital moment. In the case when $\Lambda = 0$, with Λ the projection of the electronic orbital momentum on the internuclear axis, the spin is completely uncoupled from the internuclear axis and only weakly coupled to the rotation (Hund's case (b)). This implies that even a very weak magnetic

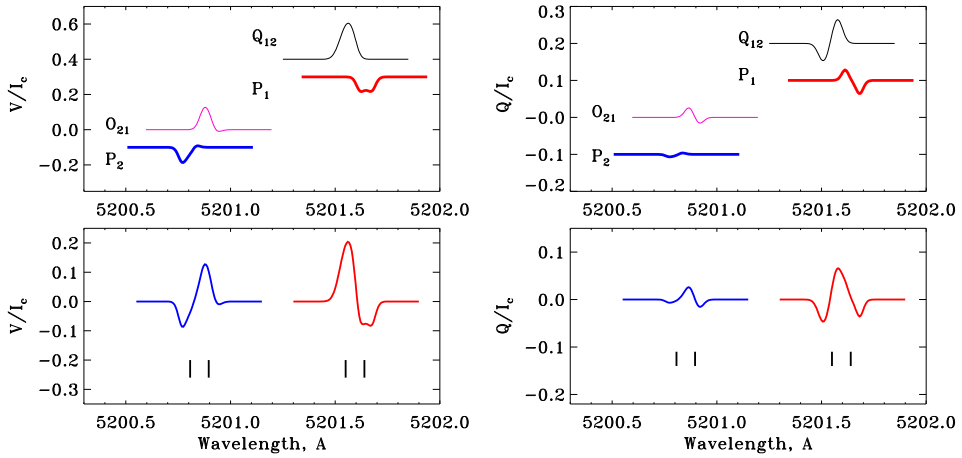

Figure 3. Stokes profiles of the MgH A–X (0,0) $P_1 + {}^PQ_{12}$ and $P_2 + {}^PO_{21}$ transitions for $N'' = 6$ for a longitudinal (left) and transversal (right) magnetic field of 2 kG. Top plots present individual line profiles separately (shifted in the vertical scale). In the bottom, composite profiles of line pairs are shown. Vertical dashes indicate the position of lines at zero magnetic field.

field can significantly perturb the fine structure of molecular levels. This effect is demonstrated for a $^4\Sigma$ state in the right panel of Fig. 1. Significant perturbation of the level structure occurs when the magnetic splitting becomes comparable to the fine structure splitting. For many Σ-states the perturbation becomes noticeable at field strengths well below 1 kG.

In the case when $\Lambda \neq 0$, the fine structure is defined by the spin-orbital interaction. An example of the level splitting for a $^3\Pi$ state in the intermediate case (a-b) is shown in the left panel of Fig. 1. Here the field strength at which the PBE becomes significant is determined by the spin-orbital interaction constant A: the magnetic splitting should be of the order of $A\Lambda$. For $A \sim$ 1–10 the transition to the PBR occurs at magnetic fields of a few kG.

The PBE on the Rotational Structure. In Hund's case (a), the electronic angular momenta are strongly coupled to the line joining the nuclei and only weakly to the rotation of the nuclei. The electronic term structure is characterized by larger multiplet splitting compared to the rotational splitting. When magnetic shifts become comparable with the rotational splitting, levels corresponding to the same magnetic numbers start to interact. This is illustrated in the left panel of Fig. 2 for a $^2\Pi_{3/2}$ state with strong spin-rotational interaction. In this example, the second state in the doublet, $^2\Pi_{1/2}$, is separated by about 100 cm^{-1} and remains magnetically insensitive, in accord with Hund's case (a). These two substates start to interact significantly only at very large field strengths. Then, the PBE occurs on the fine structure as well. In Hund's case (b), for an increasing magnetic field strength, the PBE occurs first on the fine structure, i.e. levels with the same M and N numbers. When magnetic shifts exceed the multiplet splitting and become comparable with the rotational splitting, a mixture of levels with different N occurs. This is illustrated in the right panel of Fig. 2 for a $^2\Pi$ state. The increasing magnetic splitting and the repulsion of interacting levels

lead to complete smearing of the rotational and multiplet structure, indicating the complete PBE within a given electronic state. A special case is represented by Σ states ($\Lambda = 0$). Their rotational structure is not further perturbed by an increasing magnetic field. Consequently, a pseudo-multiplet structure of the levels results from the complete PBE on the fine structure. Only additional perturbations by other electronic states would change this picture.

3. Stokes Profiles in the PBR

The most striking signature of the PBE is that Stokes profiles are strongly asymmetric and their spectral shape depends sensitively on the magnetic field. Also, the strength of forbidden and satellite transitions increases rapidly with field strength in the partial PBR, while the strength of main branch transitions decreases.

Typical Stokes-V profiles in a longitudinal field are shown in the left panels of Fig. 3. Individual lines are essentially single-lobed but when Stokes-V profiles of the main and satellite lines are calculated together the profiles look more antisymmetric, especially for lower N numbers. The antisymmetry slowly disappears with N. This results in an increasing net circular polarization signal with N in the beginning of the band. For even larger N numbers, the net signal goes to zero because of the reduced PBE (see Berdyugina et al. 2005).

Typical Stokes-Q profiles in the transversal magnetic field are shown in the right panels of Fig. 3. Again, the individual line shapes are very different from what is normally observed in the Zeeman regime. Instead of being symmetric, the profiles are essentially antisymmetric and are reminiscent of normal Stokes-V profiles. The polarization signal of satellite lines is larger than that of main branch lines, and their sign of polarization is opposite. Because of wavelength shifts between main and satellite lines, the resultant Stokes-Q signals from pairs of lines look almost symmetric, as observed in the Zeeman regime. This visible symmetry is however very sensitive to the magnetic field strength.

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