THE INFLUENCE OF HYPERFINE STRUCTURE ON SOME MANGANESE LINE PROFILES IN THE SOLAR SPECTRUM

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SUMMARY: Taking into account effects of hyperfine structure, we calculated the synthetic solar spectrum for wavelength intervals around nine neutral manganese lines. To estimate values of hyperfine components we used the Oxford total absorption oscillator strength measurements (Booth et al, 1983). We compared observed profiles (Photometric Atlas of the Solar Spectrum from 3000 to 10000Å (Delbouille et al, 1973)) of selected manganese lines with synthesized profiles in two cases: when hyperfine structure is not and when it is taken into account. By comparing the calculated with observed spectrum, we corrected the total oscillator strengths of all nine selected manganese lines.

Key words. Sun: photosphere - Line: profiles - Techniques: spectroscopic

1. INTRODUCTION

One of the fundamental methods used to obtain information about the physical and chemical properties of celestial bodies is spectroscopy. However, the observed spectrum itself is not sufficient. It has to be compared with the theoretically obtained spectrum, and their similarities and/or differences are the basis for conclusions about the nature of the studied object. To be able to calculate correctly the theoretical spectrum, it is necessary to adopt the model and to select the basic parameters of the object study, but also to know the values of atomic parameters of relevant elements. One of possible causes for the significant deviation of the observed from the synthetized lines in the spectrum may be due to neglecting of the hyperfine structure effects in the calculation of line profiles of some elements.

Hyperfine structure (**hfs**) of spectral lines is a consequence of splitting of the fine structure of energy levels, caused by the interaction of nuclear spin magnetic or charge moments and the unfilled electron shells, or caused by atomic isotopes. The typical order of magnitude of hyperfine structure energy differences is 0.02 cm^{-1} which corresponds to the difference of wavelengths of components 0.5 pm at 500 nm. Due to thermal and pressure broadening of spectral lines we usually do not see specific components (for example, typical width of thermally broadened spectral lines in the solar photospheric spectrum is several pm), but only the integral line resulting from their superposition (convolution of component profiles). This line has a significantly different profile shape than the lines not affected by hyperfine structure. Abt (1952) first pointed out the possibility of strong influence of hyperfine structure on the line shapes in the solar spectrum. He studied hyperfine structure effects on the curve of growth for the el-ements V, Mn, Co, Cu, Sc and La, and also the systematic changes of measured wavelengths with respect to their laboratory values. In the calculation of spectrum, the **hfs** effect on the line can be calculated by superposing individually synthetized **hfs** components. This procedure is possible for the lines with known laboratory or theoretical data about the components' relative intensities and wavelengths. Edmunds (1973) provided a detailed description of a theoretical model for an approximate evaluation of **hfs** constants for the levels whose splitting was not measured in the laboratory.

Booth et al. (1983) carried out precise laboratory measurements of textbfhfs for about fifty lines of neutral manganese in the visible range of the spectrum. Those are the results, which we accept in this paper as starting values for the calculation of profiles of nine selected manganese lines. Manganese has only one stable isotope, thus the hfs of its spectral lines is only due to the interaction of electron angular momentum with the nuclear spin. Obviously, every line has its own characteristics. For example, the measured cyclic variation of equivalent width of the MnI 539.47 nm line of the full solar disc is about 2% (Livingston, 1992). This line pertains to photospheric lines that are very sensitive to temperature changes, as theoretically proved by Erkapić and Vince (1995), but its unusually high amplitude of equivalent width variation cannot be explained only by photospheric temperature change. Therefore, this line will give wrong diagnostics of temperature variation without taking into account its hfs and the non-LTE effects due to its optical coupling with the MgII k line (Doyle et al. 2001). Recently, the Zeeman effect of hyperfine structure of this line has been proposed for diagnostics of the solar photospheric magnetic field (López Ariste et al. 2002). On the other hand, determining of the effects of magnetic field of various strengths on the MnI 539.47 nm line has shown that the observed relative intensity variation in plage region is not due to the magnetic field change (Vince et al. 2000), but to the change of other parameters (Vitas et al. 2002). In addition, the hfs can significantly influence the abundance determination, too. From these examples, it is evident that the precise determination of hyperfine structure of spectral lines is very important. In this paper we compared observed profiles of nine manganese lines with synthesized profiles in two cases: when hfs is not included and when its effect is taken into account, and of improved the total oscillator strength

by comparing the observed and calculated line profiles.

2. THE METHOD

The nine lines studied in this paper are selected according to the following criteria: (1) they do not show significant blending with other lines, (2) they have noticeable hyperfine structure in the observed spectrum and (3) known laboratory data for **hfs** are at disposition. We calculated the synthetic spectra in the vicinity of the selected lines using the program package SPECTRUM (PC-based Stellar Spectral Synthesis Program) by R. O. Gray. This package works under the LTE assumption. We first calculated profiles of lines without considering **hfs**. Results obtained in this way (Fig.1, dashed line) significantly deviate from the observed spectrum taken from the High Resolution Solar Spectrum Atlas and normalized to the local continuum (Fig.1, solid line).

Data given in the paper by Booth et al. (1983) mentioned are taken as a starting estimate for the relation of components' relative intensities and their mutual positions. Further synthesis is carried out when the line in the input of SPECTRUM is replaced by a set of corresponding hfs components. The shapes of line profiles obtained in this way are much closer to the observed, but they usually have a different equivalent width and longer wavelength, (Fig 1. dotted line). A shift in the wavelength of the integral line profile is mainly due to an unsufficiently starting value of the wavelength of the first hfs component. New profiles of these lines, showing a good agreement with the observations, are obtained by correcting the wavelength, varying the total value log(gf) and by repeating the calculation (Fig.1, small circles). The value of the microturbulent velocity assumed in all calculations was 1.5 km/s, and for the abundance of manganese in relation to hydrogen in logarithmic scale 6.65. The initial and the corrected values of the total $\log(gf)$ and of the first components' wavelength, as well as the number of components of hyperfine structure for each line, are presented in Tab. 1.

number of components	multiplet number	λ ' (nm)	$\log(\mathrm{gf})$	$\lambda(\mathrm{nm})$	$\log(gf)$
6	20	500.4892	-1.795	500.4874	-1.725
11	32	525.5326	-0.794	525.5276	-0.950
6	1	539.4677	-3.453	539.4624	-3.650
10	4	542.0355	-1.492	542.0274	-1.530
6	1	543.2546	-3.740	543.2500	-3.965
10	4	547.0637	-1.702	547.0573	-1.750
7	27	601.3513	-0.397	601.3457	-0.380
7	27	601.6646	-0.216	601.6586	-0.160
7	27	602.1787	-0.084	602.1747	-0.070

Table 1. Selected manganese lines: number of **hfs** components, multiplet number, wavelength of the first component and total log(gf) before correction (λ ' and log(gf)') and after correction (λ and log(gf)).

The procedure described here is based on a subjective estimate of the achieved matching of calculated and observed profiles. Satisfactory result has been obtained by different number of steps, usually by varying λ and log(gf) five to ten times for each studied line. The practice showed that a mutual approach of profiles is reached when total log (gf) is changed by 0.005, that may be considered as a limit of uncertainty in our procedure.

3. RESULTS AND COMMENTS

a) MnI 500.49 nm (Fig.1. a)

Table 2. Component positions with respect to the most intense, are relative intensities, $\log(gf)$ before correction $(\log(gf))$, and after correction $(\log(gf))$.

$\Delta\lambda(\text{nm})$	relative intensity	$\log(\mathrm{gf})$	$\log(gf)$
0.00000	100.0	-2.341	-2.271
0.00128	79.0	-2.444	-2.374
0.00232	68.0	-2.509	-2.439
0.00323	54.0	-2.609	-2.549
0.00387	36.0	-2.785	-2.715
0.00440	15.0	-3.165	-3.095

For the MnI 500.49 nm line, the fitting in the line's core is very good, while in the wings the synthetized profile better fits the observed one on the blue wing, where the influence of neighboring lines in absents, and the local continuum is well defined (Fig. 1. a).

b) MnI 525.53 nm (Fig.1. b)

Table 3. The same as Table 2.

$\Delta\lambda(\text{nm})$	relative intensity	$\log(\mathrm{gf})$	$\log(gf)$
0.0000	100.0	-1.427	-1.583
0.0208	82.5	-1.511	-1.666
0.0287	5.7	-2.671	-2.827
0.0397	68.5	-1.591	-1.747
0.0467	10.0	-2.427	-2.583
0.0567	56.5	-1.675	-1.831
0.0622	9.9	-2.431	-2.587
0.0711	45.0	-1.774	-1.930
0.0756	8.8	-2.483	-2.639
0.0828	37.0	-1.859	-2.015
0.0863	5.6	-2.679	-2.835

The blue wing of the MnI 525.53 nm line shows a more significant deviation from the corresponding line in the Atlas, a fact can be partly explained by influence of the adjacent CrI 525.51 line and lower local continuum (Fig. 1. b.). c) MnI 539.47 nm (Fig.1. c)

Table 4. The same as Table 2.

$\Delta\lambda(\text{nm})$	relative intensity	$\log(\mathrm{gf})$	$\log(gf)$
0.0000	100.0	-4.002	-4.199
0.0347	81.4	-4.092	-4.289
0.0638	65.8	-4.184	-4.381
0.0877	50.4	-4.300	-4.497
0.1052	35.1	-4.457	-4.654
0.1168	21.4	-4.672	-4.869

Lines MnI 539.47 nm and MnI 543.25 nm show very good agreement between observed and calculated profiles after correction of the first components wavelength and total log(gf).

d) MnI 543.25 nm (Fig.1. d)

Table 5. The same as a Table 2.

$\Delta\lambda(\text{nm})$	relative intensity	$\log(\mathrm{gf})$	$\log(gf)$
0.0000	100.0	-4.222	-4.447
0.0321	75.4	-4.345	-4.570
0.0575	57.4	-4.463	-4.688
0.0762	39.9	-4.621	-4.846
0.0881	21.4	-4.892	-5.117
0.0923	9.5	-5.245	-5.467

e) MnI 542.04 nm (Fig.1. e)

Table 6. The same as a Table 2.

$\Delta\lambda(\text{nm})$	relative intensity	$\log(\mathrm{gf})$	$\log(\mathrm{gf})$
0.0000	100.0	-2.058	-2.096
0.0270	8.7	-3.118	-3.156
0.0546	75.0	-2.183	-2.221
0.0774	16.5	-2.840	-2.878
0.0995	52.5	-2.337	-2.376
0.1166	20.2	-2.752	-2.790
0.1323	35.7	-2.505	-2.543
0.1462	18.5	-2.790	-2.828
0.1565	22.3	-2.709	-2.747
0.1677	18.4	-2.793	-2.831

The lines MnI 542.03 nm and MnI 547.06 nm belong to the fourth multiplet of manganese and have the same number of the **hfs** components, and a similar arrangement of relative intensities among them. With these lines, we notice a very similar deviation of the theoretical model from the observed line. While the red wing of the calculated line shows good fitting, on the blue side of the profile we notice a conspicuous bump, resulting perhaps from the non-precisely determined intensity and/or position of the first and the most intensive **hfs** component with respect to the others (Fig 1, e and f).

f) MnI 547.06 nm (Fig.1. f)

$\Delta\lambda(\text{nm})$	relative intensity	$\log(\mathrm{gf})$	$\log(\mathrm{gf})$
0.0000	100.0	-2.276	-2.324
0.0223	16.1	-3.069	-3.117
0.0285	16.6	-3.056	-3.104
0.0510	57.8	-2.514	-2.562
0.0714	48.4	-2.591	-2.639
0.0921	26.9	-2.846	-2.894
0.1075	47.5	-2.599	-2.647
0.1230	7.9	-3.378	-3.426
0.1329	35.5	-2.725	-2.773
0.1480	18.0	-3.020	-3.068

Table 7.Same as a Table 2.

g) MnI 601.35 nm (Fig.1. g)

Table 8.Same as a Table 2.

$\Delta\lambda(\text{nm})$	relative intensity	$\log(\mathrm{gf})$	$\log(gf)$
0.0000	100.0	-0.891	-0.874
0.0214	61.0	-1.106	-1.089
0.0419	39.0	-1.300	-1.283
0.0561	38.0	-1.311	-1.294
0.0676	33.5	-1.366	-1.349
0.0755	18.5	-1.624	-1.607
0.0878	22.0	-1.549	-1.532

The three lines of muliplet 27, MnI 601.35 nm, MnI 601.66 nm and MnI 602.18 nm have been selected for their relatively high intensity and especially for their surroundings with no other strong lines that could significantly affect their profiles. For these lines, the profile with included **hfs** and corrected wavelength and $\log(gf)$ shows the expected good fitt to the observed profile, but it can also be noticed that the synthetized profiles are narrower than the observed in the wings, and deeper in the core. Such behaviour of lines in multiplet 27 is different from other selected lines.

h) MnI 601.66 nm (Fig.1. h)

Table 9. Same as a Table 2.

$\Delta\lambda(\text{nm})$	relative intensity	$\log(\mathrm{gf})$	$\log(\mathrm{gf})$
-0.0272	12.5	-1.613	-1.557
0.0000	100.0	-0.710	-0.654
0.0212	65.5	-0.894	-0. 838
0.0389	40.5	-1.103	-1.046
0.0524	34.5	-1.172	-1.116
0.0664	57.0	-0.954	-0.898
0.0805	2.0	-2.409	-2.353

i) MnI 602.18 nm (Fig.1. i)

Table 10. Same as a Table 2.

$\Delta\lambda(\text{nm})$	relative intensity	$\log(\mathrm{gf})$	$\log(gf)$
-0.0319	13.0	-1.521	-1.508
-0.0095	16.0	-1.431	-1.417
0.0000	100.0	-0.635	-0.621
0.0092	16.0	-1.431	-1.417
0.0180	84.0	-0.711	-0.697
0.0314	71.0	-0.784	-0.770
0.0423	56.0	-0.887	-0.873



Fig. 1. Comparative view of the Solar Atlas (solid line), synthetized spectrum with out hfs (dashed line), synthetized spectrum with hfs according to the data from Booth et al. (1983; dotted line), and synthetized spectrum with hfs after the correction of the overall log(gf) and wavelength (open circles). Series of vertical lines represent relative intensities and positions of hfs components.



Fig. 1. (continued).

4. CONCLUSION

This paper presents the results of synthesis of nine manganese lines with a conspicuous hyperfine structure. The comparison of calculated and observed line profiles shows that it is necessary, in the calculation of the synthetic spectrum, to take hfs into account, so that model provides good fit of theory and observation. Deviations of the svnthetized profile from the Atlas can be classified in two groups. Deviations in the first group are the result of influence of surrounding lines which were not taken into account in the synthesis, or whose parameters have not been precisely determined. These deviations manifest themselves mainly through the fact that observed profiles have broader wings then the theoretical ones. Deviations of the second group are most clearly seen in the cores of the lines. The source of such deviations should be searched for the hfs data, in widening to which some components have been exposed, as well as in the program used for the synthesis. These deviations must be studied with particular care. Similar result was already obtained for the lines of the first manganese multiplet, MnI 539.47 nm and MnI 543.25 nm (Vitas et al. 2002). The question remains how these lines would behave if deviations from the local thermodynamical equilibrium are taken into account, and how would the inclusion of the hfs affect the determination of formation depths of the manganese lines with significant hfs.

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УТИЦАЈ ХИПЕРФИНЕ СТРУКТУРЕ НА ПРОФИЛЕ НЕКИХ ЛИНИЈА МАНГАНА У СУНЧЕВОМ СПЕКТРУ

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UDK 523.9 Оригинални научни рад

Узимајући у обзир ефекте хиперфине структуре израчунат је синтетички спектар Сунца у интервалима таласних дужина око девет линија неутралног мангана. За процену компонената хиперфине структуре користили смо Oxford total absorption oscillator strength measurements (Booth et al, 1983). У овом раду извршено је поређење посматраних профила изабраних линија мангана (Photometric Atlas of the Solar Spectrum from 3000 to 10000Å (Delbouille et al, 1973)) са синтетисаним профилима у два случаја: када хиперфина структура није урачуната и када је узета у обзир. Поређењем израчунатог и посматраног спектра извршена је корекција укупне снаге осцилатора за девет изабраних линија мангана.