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Inputting hyperfine structure into synthetic spectrum codes

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Abstract. The effects of hyperfine structure for atomic lines can have an important impact upon spectrum analysis, in particular for chemical abundance analyses. Despite this importance, the incorporation of hyperfine structure into synthetic spectrum codes is not automatic even though a significant amount of atomic data exists in the literature. This discussion presents basic information about the occurrence of hyperfine structure and the calculation of its effects upon line wavelengths and oscillator strengths for inclusion into synthetic spectrum codes.

Key words. Atomic data – hyperfine structure – Stars: abundances

1. Introduction

All spectral lines have structure. While this statement is not strictly correct, it is sufficiently accurate to be a starting point when considering whether to include the effects of hyperfine structure into a spectrum analysis.

Early references, and even some found in present day literature, to the term *hyperfine structure* implied structure in a line profile regardless of its origin, here taken to include isotope shift, magnetic hyperfine due to an external field (Zeeman effect), and hyperfine structure arising from nucleon-electron interactions. It is this last process that is most relevant to the present discussion.

If we ignore the influence of external magnetic fields to line structures observable in laboratory and stellar spectra, we uncover the potential for line structure by intrinsic atomic properties. Let us consider only the stable isotopes of the elements no heavier than bismuth (Z = 83). Of these, only 21 are mono-isotopic, implying that for most elements isotope composition may create line structure in atomic lines and molecular bands. In addition, all 21 mono-isotopic elements have odd-valued atomic weights, implying that they may show hyperfine structure. One can therefore say that there are no stable elements for which there can be no line structure. (If we include the long-lived isotopes of Th and U then only for Th is there a mono-isotopic element of even atomic weight.)

There are 11 elements (H, He, C, N, O, Ar, Ca, V, La, Lu, Ta) that have multiple isotopes and for which there exists one prominant isotope, at about the level of 98% of the total isotope composition as measured in solar system objects. Of these, isotope compositions may be measured for H and He from atomic lines due to their great abundances, and the light elements C, N, and O can have mea-

Send offprint requests to: G.M. Wahlgren sureable isotopic compositions from the study of molecular lines. Only for Ar and Ca would it appear that no line structure would be observable for a solar-system abundance distribution, since the remaining four elements (V, La, Lu, Ta) are dominated by a single, odd atomic weight isotope that in all cases shows measureable hfs line broadening.

We must qualify this last statement by saying that there may be circumstances under which a minor isotope has a more prominant role than predicted by the solar-system elemental abundance pattern. For example, the chemically peculiar stars of the upper main sequence are known for their elemental abundance and isotope anomalies. The isotope ^{204}Hg, which accounts for no more than 7% of the solar system Hg abundance, is often the most abundant Hg isotope in HgMn stars (Dolk et al. 2003), and recently it has been suspected that observed wavelength shifts in certain Ca II lines may be interpreted as an isotope anomaly (Castelli & Hubrig 2004).

A second example of minor isotopes becoming prominant in line profiles is provided by metal-deficient galactic halo stars. These stars are considered to be among the oldest in the galaxy and their heavy elements were formed in earlier supernovae. The abundance patterns constructed for these stars points to the prominance of the *r*-process over the *s*-process as a mechanism for nucleosynthesis, which would result in a different relative isotope composition among many elements.

This brief consideration of the stable elements serves to underscore the premise that line structure must be a consideration for the accurate analysis of spectral lines in stellar spectra. The extent to which line structure plays a role in the final result depends upon other factors, some attributed to the atomic structure and others due to observation technique. These are briefly outlined below, along with a means for including the effects of hfs into synthetic spectrum codes.

2. Hfs theory

The theory describing hyperfine structure is well developed and documented in many sources. Here, the discussion only outlines the most prominent equations that define energy level splitting and serve as a background for algorithms written to quantify the problem.

The basic concept behind hyperfine splitting of energy levels starts with the intrinsic spins of individual protons and neutrons in the atom's nucleus giving rise to a net spin angular momentum of the nucleus, designated by the quantum number I. The magnetic moment of this spin is given by the relation

$$\mu_{\mathbf{I}} = \mathrm{g}(\mathrm{e}/2\mathrm{m}_p)\mathbf{I}, \tag{1}$$

where the symbols have their usual meaning. It is the interaction of $\mu_{\mathbf{I}}$ with the magnetic field originating from the combined orbital motion and spin of the electrons, at the location of the nucleus, that gives rise to small adjustments to the fine structure levels.

We normally consider the hfs to be comprised of two terms in the expansion of the nuclear multiploe moment, those being the magnetic dipole moment and the electric quadrupole moment. Other terms in the expansion are possible; however, they contribute negligible amounts to the level splitting and are usually ignored for quantitative purposes. The energy shift due to the magnetic dipole term is given by

$$\Delta E_{mhfs} = -\mu_{\mathbf{I}} \cdot \mathbf{B_J} = A(\mathbf{I} \cdot \mathbf{J})/\hbar^2, \tag{2}$$

where $\mathbf{B}_J$ is the magnetic field from the electrons as measured at the nucleus, and A is a proportionality constant.

We introduce the total quantum number **F** as the sum of the nuclear and electron angular momentum vectors,

$$\mathbf{F}\!=\!\mathbf{I}\!+\!\mathbf{J} \tag{3}$$

and note that the range in F is given by

$$F = I + J, I + J\text{-}1, ..., |I\text{-}J|. \tag{4}$$

The number of sub-levels into which each fine structure level is split is given as 2I+1 if

I<J, or 2J+1 if I > J. The product of **I** and **J** can be found to be

$$< \mathbf{I}\cdot\mathbf{J} >= (\hbar^2/2)[\mathbf{F}(\mathbf{F}+1)-\mathbf{I}(\mathbf{I}+1)-\mathbf{J}(\mathbf{J}+1)], \quad (5)$$

and by substitution into eq. 2, the magnetic hfs splitting is written as

$$\Delta E_{mhfs} = (A/2)[F(F+1)-I(I+1)-J(J+1)], \quad (6)$$

where A can now referred to as the magnetic dipole constant, or, the A constant.

The hfs electric quadrupole component is related to the surface charge of the nucleus, and it can be expressed as

$$\Delta E_{ehfs} = B\frac{(3k/4)(k+1) - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)}, \quad (7)$$

where

$$k = F(F+1) - I(I+1) - J(J+1). \quad (8)$$

B is related to the electric quadrupole moment, Q, and the gradient of the electric field from the electrons at the location of the nucleus, and is referred to as the electric hyperfine constant, or, the hfs B constant.

The total hfs level splitting is the sum of the magnetic dipole and electric quadrupole terms and is often found written as

$$\Delta E_{hfs} = A\frac{k}{2} + B\frac{(3k/4)(k+1) - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)}. \quad (9)$$

Equation 9 brings to mind an important caution: that there exists more than one expression for ΔE_{hfs} in the literature, due to different formulations for B. To alleviate any potential confusion in the use of the A and B constants, it is incumbent upon the data providers to state the version of the equation that was used in deriving the A and B constants, along with the units (typically either MHz or mK). Data users need to assure themselves that the algorithm used by them to create line lists is appropriate for the constants taken from the literature.

From the general equation for the energy level differences in the presence of hfs (eq. 9), we can draw general insights into anticipating the influence of the magnetic and electric hfs on a spectral line. This is often helpful since tables of atomic data can be found that include these line data. Since the hfs is proportional to the magnetic dipole moment, $\mu_{\mathbf{I}}$, electric quadrupole moment, Q, and quantum numbers I or J, we anticipate that it will scale with these values.

To check the intuitiveness of this statement, we can compare the value I with elements known to display hfs, independent of other considerations. There are 102 isotopes of odd atomic weight for which their solar-system isotope composition is more than 2% of their respective element. This 2% limit is a rather arbitrary one chosen for the purpose of this exercise, and only acts to discriminate against isotopes not likely to be detected. The distribution by number over I is found to be (I = 1/2, 3/2, 5/2, 7/2, 9/2) = (27, 28, 22, 16, 9), respectively. A minority of elements have I as large as 7/2 or 9/2, but all of the associated elements are known to have noteable hfs line splitting based upon laboratory spectra, where it exists. Large hfs patterns are observed for elements having I = 5/2 if, for instance, they also have a large value for $\mu_{\mathbf{I}}$. The most noteable elements in this case are Mn, Pr, Eu, and Re.

The angular momentum quantum number J also has a bearing on the line width. As for I, a large value for J is associated with broader hfs patterns. The J values are those associated with the levels of individual transitions. We draw no general association with individual elements other than to note that heavier elements can have higher values of J.

Just as we used eq. 9 to anticipate large hfs patterns, we can also use it to state when we would not expect energy level shifts. No hyperfine splitting of a level will occur if I or J is equal to 0, and no electric quadrupole if I or J is equal to 1/2. There is also no electric quadrupole splitting (B = 0) for spherical nuclei (Q = 0). Twenty elements have Q = 0 for all of their odd isotopes, which makes for a nice simplication when either determining hfs constants or using them.

Up to now this discussion has pertained to energy level splitting, and not the hyperfine structure measured from spectral lines. This is because the line structure is related to the energy difference between the levels that we associate with the wavelength of a line. The patterns associated with hfs for a line are understood as transitions between the split levels, following the selection rules of quantum mechanics. If transitions occur between two fine structure levels having identical hyperfine splittings, then no line structure will be seen. In general, similar splittings for both upper and lower levels yield narrow line structures, often undetectable in the laboratory and even less so at the effective spectral resolution of astronomical objects.

Line structure is often broadest when one level is associated with an *s* orbital. It is for these orbitals that the electron - nucleus interaction is greatest, as the *s* electron may penetrate into the nucleus. Transitions involving configurations with different numbers of *s* electrons would therefore be considered important for hfs.

3. Determining hfs constants

Hyperfine structure is usually analysed from laboratory spectra by fitting line profiles with synthetic profiles that are generated under certain assumptions. For maximum accuracy, the spectra need to be of high spectra resolution and high signal-to-noise (S/N). High spectral resolution allows for analysing line blending, by either the components themselves or with other lines, while high S/N allows relative intensities of the various components to be accuaretly determined, as well as to identify weak components that can lead or trail the main hfs pattern and be lost in the noise. Subtle distinctions in line intensity or the presence/absence of a component can lead to confusion in choosing among the possible *J*-values of levels.

The desire for high spectral resolution in studies of hfs has lead to the use of Fourier transform spectrometers and laser techniques as the instruments of choice. Also, since the analysis of hfs *A* and *B* constants is best done using many lines in order to have redundancy among lines from a specified energy level, the data should have a broad wavelength coverage and large dynamic range. Light sources are usually of a hollow-cathode design, which has limitations in terms of the ionization states created. Current day studies of hfs for stellar astronomy have prioritized observations of neutral atoms and the lowest ionization states, which is a good match to the capabilities of hollow-cathode light sources in producing narrow line profiles.

Starting from a high quality emission line spectrum, one must first identify lines of the ion under study. Typically, a number of lines are already known from previous studies and lines can be predicted from known energy levels. Theoretical calculations are often useful in predicting line intensities for identification purposes. Useful information for the analysis includes line the wavelength, and *J*-value, energy, and parity for both upper and lower levels. These data are needed to perform checks of the analysis as it progresses, and they may be improved by the line profile fitting of the hfs pattern.

Simple profile fitting procedures (Karlsson & Litzen 2001) have been developed to analyse the hfs patterns, and require the fitting parameters: *A* and *B* values for both levels, the center of gravity wavelength of the transition, the intensity of the strongest component in the hfs pattern, and the width of individual components in the pattern. All components of the pattern are assumed to have the same shape and width (FWHM). Unfortunately, the number of free parameters is too great to produce a unique solution for both sets of hfs *A* and *B* values, which is the primary purpose of the line fitting. Therefore, it is usually necessary to have one level for which the *A* and *B* values are known, either from previous experiment or from the good fortune of having a level having no hyperfine splitting.

The fit to the line Ho II λ3810 is presented in Fig. 1. The laboratory spectrum was taken with the Lund UV FTS and hollow cathode light source. This line has 21 hfs components, which blend together at this resolution to produce about nine visible components. At a resolving power of R = $\lambda/\Delta\lambda$ = 10^5, typical of many high-resolution astronomical spectrographs, all of the components blend together to create the asymmetric feature presented in Fig. 2 for the case of a giant star of T_{eff} = 4750 K, log g = 1.5, turbulent velocity of 2 km s^{-1} and a rotational velocity of 6 km s^{-1}. In this figure the abundance of holmium ranges from solar to a +2 dex enhancement.

The inclusion of hfs has the effect of increasing the line breadth and the equivalent width for the larger enhancements, and shifting the center of gravity wavelength. Measurement of the equivalent width (W_λ) results in a curve of growth (Fig. 3), which shows the remarkable result that the inclusion of hfs can actually decrease W_λ for low abundances. This result occurs because the weakest components of the pattern may be too weak to register any significant absorption.

For larger abundance enhancements the calculation including hfs (solid) is continuously enhanced in its equivalent width from the calculation excluding hfs (dotted). A straight line (dashed), offset by +0.13 dex in log (W_λ), is presented to guide the eye. This line follows that excluding hfs for the weakest enhancements. Note that for this spectral line the two cases (with and without hfs) produce the same equivalent width at an abundance enhancement near +0.6 dex.

Therefore, ignoring hfs in a stellar spectrum analysis may either increase or decrease the derived abundance from a particular line. When the abundance derived from a number of lines from the same element/ion are averaged together, the abundance uncertainty when not including hfs will tend to be larger than if hfs was included for all lines.

The obvious effects of hfs on line profiles will be diminished by the line blending arising from star and the instrument. The star will contribute to line blending through its rotational velocity and atmospheric turbulence, and the instrument by its inherent resolution limits. However, symmetrizing the line profile may not hide its slightly broader or shifted nature.

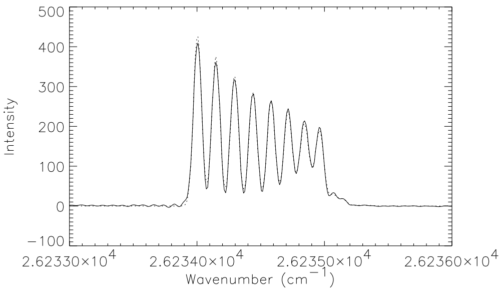

Fig. 1. Hyperfine structure in the line Ho II λ3810. The laboratory spectrum (solid) is compared with a fitted profile (dotted) computed under assumptions described in the text.

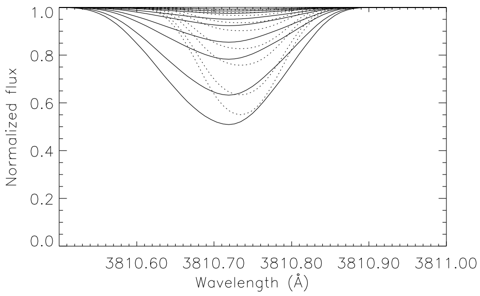

Fig. 2. The spectral line of Fig. 1 is modeled using SYNTHE for a cool, giant star. The inclusion of hfs in the calculation (solid) accounts for additional line breadth and equivalent width, along with a wavelength shift relative to a calculation that excludes the line structure (dotted). The holmium abundance ranges from the solar system value to an enhancement of +2.0 dex in alternating steps of 0.2 and 0.3 dex.

4. HFS in synthetic spectrum

Including the effects of line structure into synthetic spectrum calculations must take into consideration both the position (wavelength) and intensity (log gf) of the line components. The spectral line must be represented by all of its components and each component by its proper oscillator strength, and could involve all three line structure mechanisms: hfs, isotope shift, and magnetic broadening.

The program LINESTRUC has been created to account for hfs effects in line profiles.

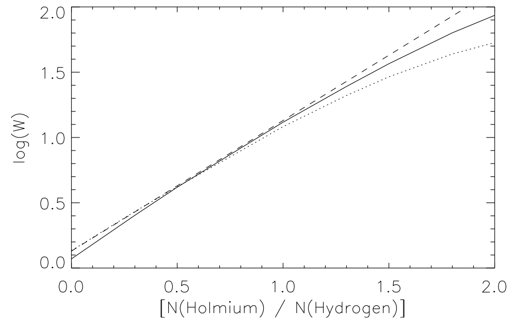

Fig. 3. The equivalent width behaviour of the Ho II $\lambda 3810$ line is plotted, based on the computed line profiles in Fig. 2. The calculations either include hfs (solid) or do not (dotted). The straight line (dashed) is to guide the eye.

The total number of line components and their wavelengths are computed from the rules of quantum mechanics and energy level splitting that were outlined in section 2. The gf value for each hfs component is computed from the input gf value in the case of no hfs, following the description in Wahlgren (1995).

The program is written in FORTRAN and runs under UNIX/LINUX systems. The required inputs include the wavelength, total gf value to be distributed amongst the hfs components, the J value and hfs A and B constants for the transition upper and lower levels, and nuclear spin I. The results can be chosen to be output in either of two formats: one that provides only the hfs parameters for the line and a second that is suitable for direct incorporation into the SYNTHE code (Kurucz 1993). The latter format also requires as input the lower level energy of the transition and the ionization potential for the ionic state of the line. The formalism for the calculation of line broadening parameters (radiative, Stark, and van der Waals) is taken from auxiliary SYNTHE codes.

LINESTRUC currently produces line structure components only for hfs. It is my intention that in the future this program will be expanded to include structure from isotope shift and magnetic broadening. The code can be obtained from the author or from the web site of this workshop.

5. Final comments

So when is hfs important for spectrum analysis? A quick answer is to say that it should always be included if the level splittings are known or the individual line components are measured from laboratory spectra. As additional hyperfine structures become measured or calculated this question will become moot since hfs will eventually be incorporated into lists of atomic line data as one today includes oscillator strengths and wavelengths, since the characterization of both of these parameters is influenced by hfs.

Much more work needs to be conducted on atomic structure for many ions before a comprehensive approach to treating line broadening by hfs can be fully incorporated into synthetic spectrum codes. But for present day analyses of stellar elemental abundances sufficient information usually exists to either include these effects directly for individual lines or form generalizations about correction factors that would account for hfs.

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