NEEDS FOR ATOMIC DATA FOR QUANTITATIVE ANALYSIS OF STELLAR SPECTRA

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I. Introduction

The goal of a quantitative analysis of a stellar spectrum is to derive the physical and chemical state of the stellar atmosphere, <u>i.e.</u> by definition the region emitting the spectrum. Of particular interest are the element abundances, they have to be determined together with the temperatures and densities (pressures) in the atmosphere. A detailed analysis usually is an iterative procedure: a model atmosphere is constructed from reasonable starting values of the parameters (effective temperature, surface gravity, element abundances,...) and used to calculate a theoretical, "synthetic" spectrum. By comparing the observed with the theoretical spectrum, improved stellar parameters are gained for the next iteration step.

Ideally, all atomic data entering the analysis should be known with sufficient accuracy, <u>i.e.</u> errors in the analysis should be due to uncertainties in the assumptions of the models, in the treatment of the velocity fields etc., and not due to insufficient atomic data. In the last decade, the ultraviolet portion of the spectrum below $\lambda \leq 3200$ Å has become accessible by satellites such as Copernicus and the International Ultraviolet Explorer (IUE) with high spectral resolution. Studies of stellar spectra in this new range have revealed the needs for a large amount of atomic data required for the analyses.



Fig. 1a: Solar spectrum at the center of the disk from the atlas by Kurucz and Avrett (1981). Heavy lines: photoelectric spectrum scans taken from a rocket by the Harvard group; thin line: theoretical synthetic spectrum (cf. §IV).

781

Richard M. West (ed.), Highlights of Astronomy, Vol. 6, 781-787. Copyright © 1983 by the IAU. In this overview, the needs for atomic data arising from ultraviolet spectra will be emphasized. The discussion will be restricted to the photospheric parts of stellar spectra, characterized by a continuum with absorption lines. Typical temperatures range from a few 10^3 K to almost 10^5 K, and densities in excess of about 10^{11} cm⁻³. Stellar chromospheres, coronae and winds which require consideration of a larger variety of atomic processes (X-ray spectra!) will not be covered here.

II. Illustration of Stellar Ultraviolet Spectra

In Fig. la - lc are exhibited three examples of parts of solar and stellar spectra in the ultraviolet which may serve as illustration of type and quality of the observational material presently available for ultraviolet spectrum analyses.

III. Stellar Absorption Coefficients

For the interpretation of a photospheric spectrum a fairly large number of atomic processes has to be taken into account even in the simplest case, i.e. assuming local thermodynamic equilibrium (for a compendium of the physics of stellar atmospheres see e.g. Baschek and Scholz, 1982). The crucial quantity is the absorption (and scattering) coefficient κ_{λ} describing the interaction of photons with matter. At any position λ in the spectrum, it consists of continuous and "resonant" line contributions by several species β (with κ_{β} line transitions):

$$\kappa_{\lambda} = \sum_{\beta} \kappa_{\lambda} \text{ (cont)} + \sum_{\beta} \sum_{\beta} \kappa_{\lambda} \text{ (line)}.$$

Over the entire spectrum, the total number of lines contributing to the absorption usually is of the order of 10^6 .



Fig. 1b: High resolution (0.05 Å) scan of the bright standard BO V star τ Sco ($m_V = 2.8 \text{ mag}$), obtained with the Princeton spectrometer aboard the Copernicus (OAO-3) satellite (Rogerson and Upson, 1977).



Fig. 1c: Eschelle-spectrum, integrated by a television camera, of the faint horizontal-branch B star Feige 86 ($m_V = 10.0$, <u>i.e.</u>, 760 times fainter than τ Sco). Observed in the high-resolution mode (0.1 -0.2 Å) of the IUE satellite by J. Köppen in 1981 for our blue halo star project, exposure time 2 hours.

A. CONTINUOUS ABSORPTION

Photo-ionization (bound-free transitions) and electron-ion bremsstrahlung (free-free transitions) together with Thomson scattering by free electrons (and in some cases Rayleigh scattering) are the dominant processes for the formation of photospheric continua.

The available data for the relevant constituents seem to be reasonably complete and accurate. I will not discuss the continuous processes in detail, but only mention two examples of open questions concerning negative ions.

There is still some uncertainty in the (free-free) opacity of H⁻ due to systematic differences ($\langle 25\% \rangle$) of two relatively recent sets of calculations, as is discussed by Frisk et al. (1982) in their study of the cool giant Arcturus.

The existence of a <u>bound</u> 1s2s2p ⁴P state of He⁻ with an electron affinity of 0.08 eV (Brehm <u>et al.</u>, 1967) would have important consequences for the spectra of white dwarfs so that its confirmation would be desirable (see Wehrse and Liebert, 1980).

B. LINE ABSORPTION

The line absorption coefficient of a transition $i \neq j$ is proportional (i) to the number density N₁ of particles in the lower state i which in turn is proportional to the element abundance ε_{α} of element α , (ii) to the oscillator strength $f \equiv fij$ (or equivalently to the Einstein coefficient A_{ji}), and (iii) to the profile function ϕ_{λ} which depends on the damping constant γ :

The depth r_{λ} of an absorption line in the stellar spectrum is determined not only by

 κ_{λ} (line) but also by the continuous absorption coefficient κ_{0} (cont) at the position λ_{0} of the line and on the temperature structure of the atmosphere. For $r_{\lambda} <<1$, <u>i.e.</u> neglecting saturation effects,

$$r_{\lambda} \propto \frac{\epsilon_{\alpha} f \phi_{\lambda}}{\kappa_{0} (\text{cont})} | \text{grad T} |$$

The (relative) total absorbed energy in the line i . j, i.e. the equivalent width is

$$W_{\lambda} = \int_{-\infty}^{+\infty} r_{\lambda} d(\lambda - \lambda_{o}).$$

In practice, the requirement for data of the spectral lines is twofold:

- (1) In order to calculate the model atmosphere, a great number (≥ 10⁶) of lines has to be taken into account. Since these lines essentially enter only as bulk line absorption, a statistical treatment of the many lines is sufficient, and the individual f-values need not have very high accuracy. However, it is crucial, that the available lists of relevant line transition have to be fairly complete. As will be discussed below, the present state in the ultraviolet spectral range is far from being satisfactory.
- (2) In order to determine the element <u>abundance</u> from a selected individual line, in contrast to (1), an accurate f-value and an accurate profile function has to be known. In addition the data for neighboring overlapping lines (blends) may be required, especially in line-rich spectra.

In principle, (1) and (2) are only different aspects of the ideal spectrum synthesis technique, <u>i.e.</u> a perfect analysis should comprise both cases self-consistently. This is, however, not tractable at present.

IV. Remarks on the Completeness of Line Identification Lists

Obviously, the premise for any quantitative line analysis is the proper identification: to each observed line a known transition within the energy level diagram of an ion has to be assigned. This requires extensive lists of atomic transitions which should be as complete as possible. In high-resolution stellar spectra usually the fine structure transitions within a multiplet are well separated whereas the hyperfine splitting is masked by the broadening mechanisms.

Frequently more than one transition is offered for the identification of a spectral line. In particular in line-rich spectra line identification may thus not be straightforward. Since in general the element mixture of the atmosphere is not known a priori, a reliable identification, including estimates of the strengths of the various contributors to a line, requires support by the quantitative analysis.

The needs for atomic data for line identification are discussed in the contribution by C. R. Cowley at this session. I will supplement his discussion by a few further examples, demonstrating the need for more extensive lists of atomic transitions.

(A) Even in the well-studied <u>solar spectrum</u>, synthetic spectrum calculations fail to reproduce the observations in the ultraviolet by a considerable amount, as is shown in Fig. 1a. According to Kurucz and Avrett (1981) about 50 percent of the lines are missing, they are probably due to atomic transitions of iron-group elements and molecular transitions involving high rotational and vibrational quantum numbers (CO, SiO, Hydrides).

(B) In their analysis of cool giant atmosphere, Gustafsson and Bell (1979) and Frisk et al. (1982) have to introduce an adjusting factor

784

 $\kappa_{\lambda} \cdot \{1 + 2 \ (1 - \frac{\lambda[\Lambda]}{5000 \ \Lambda})\}$

below $\lambda \leq 5000$ Å to obtain agreement between the observed and calculated fluxes. Thus, e.g. at λ 4000 Å, an increase of the absorption coefficient by 40 percent is required, either due to numerous faint lines or due to an unknown continuous opacity. At longer wavelengths, their model describes the observations well.

(C) In the ultraviolet spectra ($\lambda \leq 3200$ Å) of 0 and B stars, which are now available with high spectral resolution from satellites, not more than about 50 percent of the observed lines can be identified. This holds for standard stars of (roughly known) chemical composition such as τ Sco (Rogerson and Upson, 1977) as well as for peculiar stars. The majority of the missing lines may perhaps be transitions in twice to three-times ionized 3d-transition elements.

As an illustration, some more details are given from our analysis of the (chemically peculiar) OB subdwarf HD 149 382 with an effective temperature around 35000 K (Baschek et al., 1982). The entire spectral range observed with the IUE satellite, $\lambda\lambda$ 1160-3230 Å, contains about 1500 absorption lines stronger than 40 mÅ (corresponding to a depth larger than 0.2 in units of the continuum). A preliminary identification, based on correlations between relative laboratory intensities and observed stellar strengths, could be achieved for only \lesssim 50 percent of these lines.



Fig. 2: Curve-of-growth (of the uv Fe III λ 1531.6 Å line in a B star) as illustration of the saturation of stellar absorption lines. (a) Equivalent width W_{λ} , (b) central depth r_c as functions of f-value times level population N.

Of these, about 500 lines are reasonably undisturbed in the stellar spectrum, i.e. in principle are suited for the analysis, but for only about 250 of these lines f-values are known.

In HD 149 382, the following ions presently lack f-values for the majority of their observed ultraviolet lines: N IV, N V, O III, S II, S III, Sc IV, Cu IV, Zn IV. Furthermore, for Mg III, Al IV, Ca III, V III, Cr III, Cr IV, Mn IV, Fe IV we could not find experimental oscillator strengths (for the lines suitable in the star), the only sources being the extensive calculations by Kurucz and Peytremann (1975) and Abbott (1978).

V. Specific Needs for Atomic Data

In general, it is difficult for the stellar spectroscopist to express <u>specific</u> needs to atomic physicists. The above examples show that extensive, sufficiently complete lists of line transitions including f-values is the prime desideratum for stellar spectrum analyses. However, the more an analysis progresses, the more specific the inquiries concerning missing data can be made.

The almost insatiable needs for atomic line data arise mainly from two facts characteristic for stellar spectroscopy. On the one side, there are many interesting, chemically peculiar stars which may show strong enhancement of lines of "exotic" elements (which are not abundant in the normal composition). On the other side, a stellar atmosphere acts like an optically very thick absorption tube, the possibility of enormous saturation effects is demonstrated by the well-known curve-of-growth. For example, easily observable lines in the ultraviolet of a B star, from central absorptions $r_{\rm C}$ of about 0.2 up to the strongest lines $(r_{\rm C} \lesssim 1.0)$ correspond to a range in f-values of 3 to 4 decades (see Fig. 2). Thus numerous lines which are very faint in optically thin emission line sources come out considerably enhanced in stellar spectra.

In the following, a somewhat more detailed discussion of the need for atomic line data is given. Although molecular lines are not dealt with at this session, we may note in passing that for many electronic transitions accurate f-values are desired. For example, for the electronic oscillator strength of the $\phi(b^{-1}\pi - d^{-1}\Sigma)$ transition of the important TiO molecule which occurs at λ 11045 Å near the flux maximum of cool stars only an estimated value is available (Krupp <u>et al.</u>, 1978). Concerning the <u>strong</u> (atomic) lines in stellar spectra, we are mainly faced with sparse data of the damping constants

 $\gamma \simeq \gamma_{rad} + \gamma_e + \gamma_{vdW}$.

While there is no difficulty to obtain data for the radiation damping γ_{rad} (e.g. beam-foil measurements) many constants for quadratic Stark broadening γ_e and in particular for van der Waals broadening γ_{vdW} by neutral hydrogen are not known.

Considerable improvement for astrophysical applications has been achieved for the broadening of neutral hydrogen lines (Lo-Lô, Ho-Hô) since unified path calculations have become available (see Vidal et al., 1973). Calculations for higher transitions, also for He II lines such as $\overline{\lambda}$ 1640 Å, are desirable.

For many He I lines (e.g. λ 4471 and 4026 Å) detilaed calculations of their broadening have been carried out. No theoretical profiles are available for the well observed stellar lines λ 4387 (2 ¹P° - 5 ¹D) and higher members.

For the <u>medium strong</u> lines any mechanism competing with the (thermal and "microturbulent") Doppler broadening is to be taken into account. For several elements which have nuclei of non-zero spin, such as V, Mn, Co, and Cu, unresolved <u>hyperfine structure</u> acts as an additional broadening mechanism. To my knowledge, no data on hyperfine structure for the many ultraviolet lines of once to three-times ionized atoms, located on the flat part of the curve-of-growth are available as yet.

QUANTITATIVE ANALYSIS OF STELLAR SPECTRA

For <u>all</u> lines, in particular for numerous medium to faint lines in the ultraviolet, the number of known oscillator strengths is not sufficient in order to evaluate all stellar lines of interest quantitatively. In the last decade available data of f-values, mostly for higher ions, has greatly increased due to the beam-foil technique. It should be noted, however, that many of these life-time measurements are of only restricted value for application in stellar spectroscopy, since the life-time of a level is equivalent only to the sum of the A_{ji} coefficients of all downward transitions. For more complex level diagrams, the splitting into the individual lines is not obvious, at least not for an average astrophysicist, so that additional measurements or calculations of the <u>branching ratios</u> are urgently needed.

More sophisticated analyses of stellar spectra which take into account the kinetic rate equations for the occupation of energy levels (the so-called non-LTE analyses) require further atomic data in addition to that of absorption coefficients (see, <u>e.g.</u> Baschek and Scholz, 1982). In particular, knowledge of the cross-sections for <u>collisional excitation</u> and <u>ionization</u> by electrons of thermal energies is essential. For the treatment of strong resonance lines (<u>e.g.</u> of the ultraviolet resonance lines of C IV, N V, Si IV,...) the collisional data are mostly available.

For transitions "higher up" in the Grotrian diagram, however, only very few data are available. For specific ions and transitions, atomic processes such as charge-exchange reactions, two electron excitations, Penning ionization etc. may have to be considered. In contrast to nebulae or coronae, however, such processes are in general not very important for the interpretation of stellar absorption line spectra although a systematic study has yet to be done.

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