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ATOMIC DATA : NEEDS AND PROGRESS

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ABSTRACT We summarize the newly available results which improve both the accuracy and the completeness of atomic data to be used for analysis and modelization of A stars. A major progress is obtained from the large amount of theoretical work that has been performed through the recent revision of stellar opacities. Extensive lists of accurate line data are available and we present their general characteristics. Detailed photoionization cross-sections are now available for many initial states of different atomic ions. They currently show deep resonance structures and strongly depart from the hydrogenic shapes which were often assumed. Their importance is illustrated by the example of the Si II ultra-violet features. Further implications about computation of radiative forces are pointed out.

INTRODUCTION

Because of their chemical differences the peculiar stars are natural laboratories for atomic physics. Their specific properties strongly depend on the spectroscopic data of the elements that appear with anomalous abundances. Atomic data are crucial ingredients in the following steps : (i) calculation of stellar atmosphere models, taking into account the additional opacity of overabundant elements, (ii) analysis of the observed spectral pecularities, either the enhanced lines or the characteristic wide absorption features, (iii) calculation of the radiative forces that drive the elements through the envelope and the atmosphere, which is the starting point to explain their surface accumulation or depletion. The needs for extended atomic data have already been stressed by Michaud (1987). Recent reviews can be found in the proceedings edited by Adelman and Lanz (1988), Hansen (1990), Zeippen (1990) and Crivellari et al. (1991).

This paper will emphasize the actual improvement of theoretical atomic data which has been motivated by the recent revision of the opacity coefficients used for modelling the stellar interiors. First we briefly describe the different approaches which have been adopted for the systematic computation of atomic absorption coefficients. Then we present the example of Si II autoionization to illustrate how the newly available data should improve our capability to analyse and interpret the observed chemical pecularities of stars. Finally we point out some new needs arising when calculating radiative forces due to photoionization.

Many other examples connected to atomic data will appear in this colloquium, about model calculations (Hubeny, Kurucz), abundance analyses (Adelman, Leckrone, Sadakane) and diffusion theory (Alecian, Babel, Michaud). In particular they may recall other important questions about other atomic data, such as collision strength,

line broadening and hyperfine structure, which are not considered here.

NEW CALCULATIONS OF OPACITY COEFFICIENTS

An important work about opacity coefficients in stellar interior and envelopes is being achieved after one decade of a giant collective effort, taking advantage from the most elaborated physical methods, thanks to modern computer performances. The proceedings of the recent International Workshop on Astrophysical Opacities (Lynas-Gray et al., 1992) present a wide panel about this decisive step of the interaction between atomic physics and astrophysics. The original challenge was to revise the stellar models based on the widely-used opacity tables of Los Alamos (Cox and Stewart, 1965; Cox and Tabor, 1976) in order to reconcile observed and predicted pulsation frequencies of variable stars (Simon, 1982). Successful corrections of the previous Rosseland mean opacities have recently been reported by two independant groups : one from Livermore, usually noted OPAL (Rogers and Iglesias, 1992) and the international opacity project, referred as OP, initiated by Seaton (1987, 1992a,b). Meanwhile the continuous activity of Kurucz (1992 and this colloquium) has contributed to improve the opacity coefficients, especially in the outer atmosphere layers, by including more atomic and molecular lines.

A major long-term benefit of this enormous amount of work done for the stellar opacities is to make available a lot of intermediate results of prime importance for astrophysics : extensive atomic data (bound-bound, bound-free and free-free transitions, either radiative or collisional) and improved spectral variations of the opacity coefficients for many absorbing species. Calculations of the atomic absorption by OPAL, Kurucz and OP, follow three different theoretical approaches of atomic physics. A common progress is a realistic computation of atomic spectra, with configuration interaction, instead of the one-electron approximation. They also adopt different methods to improve the equation of state and derive the occupation numbers (Däppen, 1992). Each procedure has specific advantages:

- OPAL offers the most efficient flexibility to get radiative opacities. The atomic structure calculation (done for all ions of every element up to Z=31) uses an optimized parametric potential, adjusted to fit the experimental levels along the isoelectronic sequences. The basic atomic data are not stored, but they are entirely recalculated for each stellar condition, together with the line broadening effects of the plasma.
- Kurucz has collected a huge line-list, recently extended to nine ionization stages of the iron-peak elements (Kurucz, 1992). The oscillator strengths are calculated from scaled Thomas-Fermi atomic wavefunctions, the Slater parameters being adjusted to fit the experimental levels. He includes the fine structure of atomic levels (other calculations consider LS terms only) and gives the exact wavelengths, whenever laboratory energies are available. Such line lists are priceless for identification of the individual lines in stellar spectra and computation of synthetic spectra. He also provides data on the molecular absorption that occurs at lower temperatures in stellar atmospheres.
- the OP collaboration has succeeded in producing a large-scale set of consistent atomic data, with simultaneous completeness and accuracy that were not reached before. The computations are entirely a priori, without fit to experimental data. A good accuracy is reached thanks to sophisticated theoretical techniques: they combine the use of accurate eigenfunctions of the "target" ion (charge i+1),

calculated by means of atomic-structure codes, with collision methods to obtain the excited and continuum states of the current ion (charge i). The great adavantage of this choice is to give a unified treatment of the bound and free states of the outer electron. Autoionization transitions appear as resonances in the spectral variation of the photoionization cross-sections with the exact shapes (either Lorentz or Fano profiles). Intermediate files containing the basic atomic data are stored for future applications. Present results include thirteen more abundant elements in all ionization stages.

New Rosseland mean opacity cefficients K_R are now currently produced by OPAL and OP for various stellar conditions, in the temperature range 10^4 - 10^7 K. Extensive tables of K_R have already been published by Rogers and Iglesias (1992) who also discuss in details the influence of various approximations and stellar parameters on the K_R value. The comparison between the two independant set of results (Seaton, 1992a,b), shows a good agreement, with differences in K_R generally smaller than 5 %. The main departure from the previous values is a striking enhancement of K_R, beyond a factor of 3 at temperatures of about 2,5 10^5 K in the stellar envelope. It is mainly due to the absorption of highly-charged atomic ions which have strong transitions involving core-excited states, ignored by the hydrogenic approximations.

ATOMIC DATA FROM THE OPACITY PROJECT

Seaton (1992a) describes the large amount of accurate oscillators strengths and photoionization cross-sections that have been obtained by the OP team, through this long-term effort done to revise the stellar opacities. They will be accessible in the future for many other astrophysical applications. Possible developments are pointed out by Hummer (1991) who also stresses the practical difficulties to handle such a volume of data files. Cunto and Mendoza (1992) have built a software to organize and use the corresponding database.

Limited samples of the OP atomic data are published in a series of fifteen papers which are devoted to the physical methods and their performances. They are listed by Hummer (1991) and the last one, by Sawey and Berrington (1992), concerns the first ions of iron (Fe I-IV). These papers present many comparisons with experimental results and other reliable theoretical calculations, which prove the excellent accuracy of the OP values. Relative theoretical energies are generally correct to a few percents, which allows to establish an unambiguous correspondance between the calculated terms and the experimental energies of observed levels. A detailed line analysis requires to recognize each transition by its classification and to replace the predicted wavelengths by the true ones, when available from laboratory data. This has been done for the three spectra C III, N IV and O V, by Allard et al. (1990, 1991) who have compiled all gf-values available for the observed lines. Their comparisons show that the OP oscillator strengths are reliable to better than 10%, except for the weakest transitions (see their Fig.1-3). For these ions the number of observed lines is about one third of the total OP data. Actually the newly available theoretical data, either from OP or from Kurucz, include many more transitions than the observed multiplets and are generally more complete than any previous calculation. Therefore they also provide a basis to extend spectral analyses, from experimental or astrophysical sources. Such simultaneous progress have already been efficient in the case of Fe II (see for

example Adam et al, 1987).
The photoionization cross-sections occupy a great part of the OP files (about 90% of the storage volume). They are given with a variable step in frequency that allows to resolve the resonances. Striking structures are due to photoexcitation of the core (PEC), a process which is discussed by YuYan and Seaton (1987) in the case of C II. They also describe how the OP photoionization data are extended in the region just below a threshold to take into account the continuity between the pressure-broadened lines and the continuum.

EXAMPLE : THE PHOTOIONIZATION OF Si II

The photoabsorption of Si II has been computed in the context of the opacity project (OP). In Fig.1 is shown the spectral variation of the cross-sections corresponding to three excited initial states of Si II (Le Dourneuf, 1992). Such newly available data has an important astrophysical application, since it confirms that the Si II autoionization can produce the wide ultra-violet absorption features observed in the spectra of Ap-Si stars. This explanation was first suggested by Jamar et al. (1978) and investigated by Artru et al. (1981). A definite confirmation was given by the synthetic calculation of Artru and Lanz (1987) which reproduces the typical depression at 140 nm. They have identified the stellar feature as one wide autoionization line of Si II (transition $3s^23d\ ^2D$ - $3s3p(^1P)3d\ ^2F^o$) on the basis of revised atomic data (Artru, 1986) which were still incomplete. It can be seen in Fig.1 that the curve corresponding to the $3s^23d\ ^2D$ initial state of Si II, exhibits a strong resonance at the expected wavelength of 140 nm, with characteristics (total intensity and profile) in agreement with the previous identification. On the $3s3p^2\ ^2P$ curve appears an other peak at 154 nm which should explain the smaller feature observed near this wavelength on the spectra of Ap-Si stars. The curves of Fig. 1 also show why the spectral jump observed at 130 nm was not completely reproduced in the synthesis of Artru and Lanz (1987): it must be the due to the combination of the steep variations of the the three cross-sections shown in Fig.1, and not only to the $3s3p^2\ ^2D$ threshold at 130 nm.
This example shows that the OP data offers a significant advance for understanding the spectral features of Ap stars. Autoionization is at the frontier between line and continuum absorption: instead of increasing the natural broadening for autoionization lines, it is more correct to include the corresponding resonances in the photoionization cross-section. Resonances from excited states are likely to produce the most important features in stellar spectra: for example in Si II, the ground-state threshold at the wavelength of 76 nm is not observable, while an excitation energy of 10 eV gives a threshold at 190 nm, the corresponding 140 nm feature being observed in spite of the weak population factor. For many other ions, the photoionization of excited levels was previously unknown.

FURTHER NEEDS FOR COMPUTATION OF RADIATIVE FORCES

Michaud (1987) has recalled to the atomic physicists the amount of basic data that are required to compute radiative forces. Hopefully the newly available theoretical data should fulfill a large part of these needs. The OP data have been already used to compute the radiative forces on iron (Alecian, this colloquium). The example of

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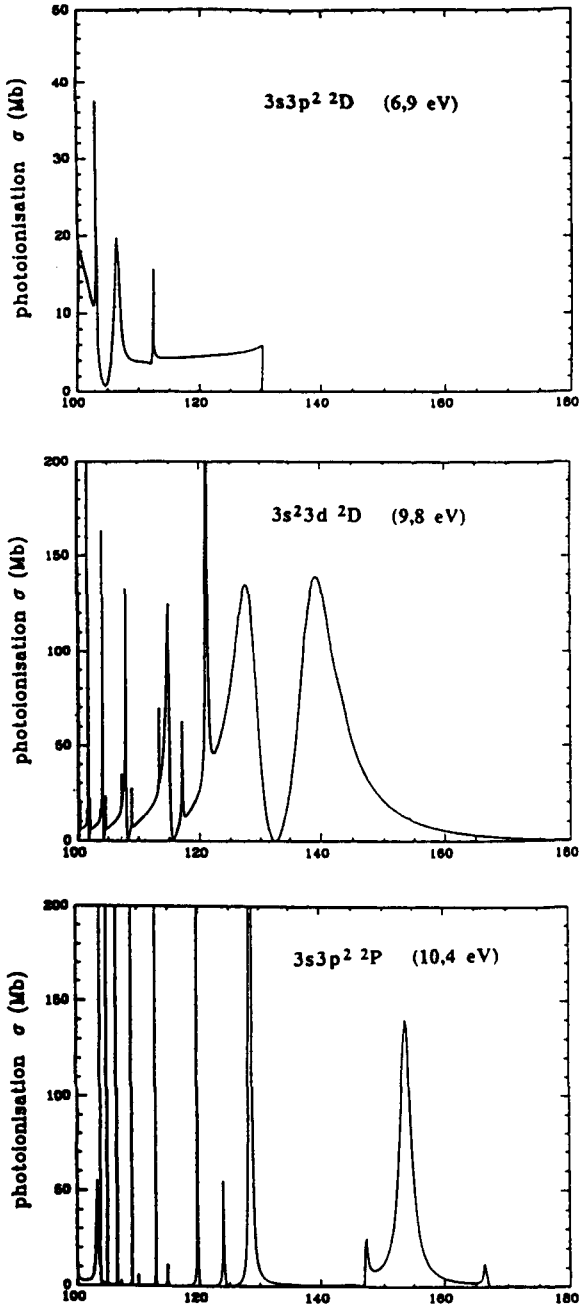

Fig. 1 Photoionization of Si II: the theoretical cross-sections from Le Dourneuf (1992) are plotted versus the photon wavelength (in nm) for three initial excited states.

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C III shown in Fig.2 (Gonzalez, 1992) shows that the new cross-sections may significantly increase the radiative pressure due to the photoionization.

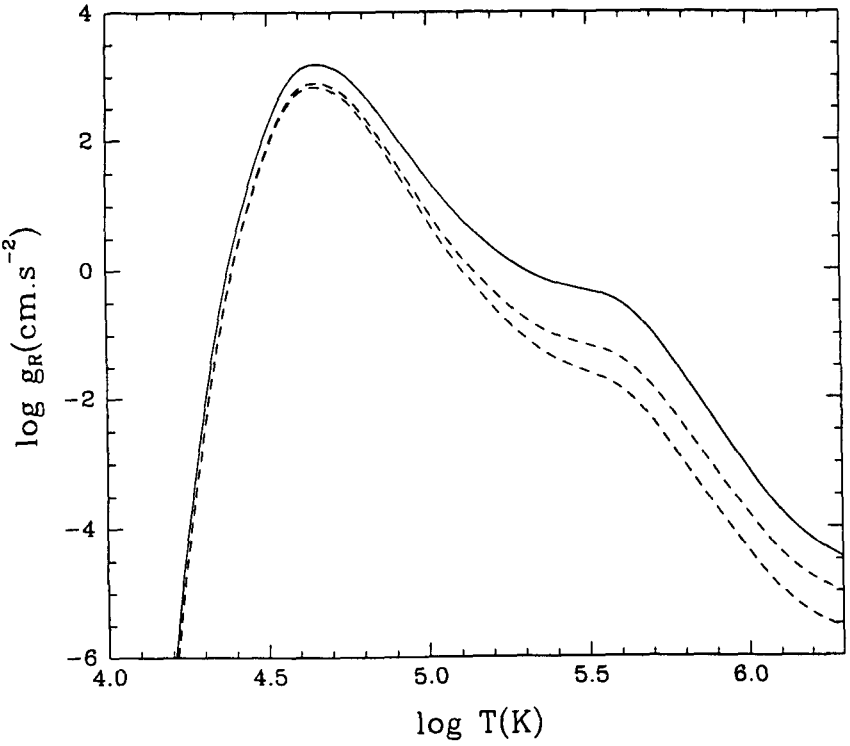

Fig. 2 Contribution of the C III photoionization to the radiative acceleration on carbon, in the envelope of a F-type star : calculation with the OP data (solid line) and calculations with hydrogenic cross-sections (dashed lines); the fraction of the photon momentum transferred to the ion is assumed to be one, excepted for the lower curve where an approximate hydrogen-like value was used.

Michaud also stressed an additional demand which appears in calculating the transfer of momentum from photons to ions, in the case of photoionization. The electron is ejected from the initial ion (charge i) with a relative velocity v and it takes a part of the photon momentum which depends on its escape direction θ. Since we are interested in the fraction F of the momentum that pushes the remaining ion (charge i+1), it is necessary to know the angular distribution $\sigma(\theta)$ of the cross-section. The factor F depends on the odd terms of $\sigma(\theta)$ in $\cos\theta$ (mainly the first-order term in v/c due to the "retardation" effect, see Bethe and Salpeter, 1957). The value of F is always +1 at threshold. When the photon energy is much larger than the ionization energy, F can be simply evaluated in the hydrogenic case; a backwards effect.is found for the n=1 orbital (F=-0.6). But a correct calculation of F requires the complete knowledge of the asymetry of $\sigma(\theta)$ (which also depends on the photon energy, with steep variations near a resonance) and the first-order

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corrections to the Born approximation which are difficult to evaluate at intermediate energies. Introduction of the F factor will reduce the radiative force, as shown in Fig. 2 for C III with hydrogenic approximations. Therefore an uncertainty still remains in the calculation of the contribution of photoionization to the radiative forces, although they should be improved thanks to the newly available cross-sections.

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