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Atomic Data in Non-LTE Model Stellar Atmospheres

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Abstract. We review the sources and the handling of atomic data in NLTE line-blanketed model stellar atmospheres, with an emphasis on our code TLUSTY. Incorporating tens of thousands of energy levels and millions of lines explicitly in NLTE is now feasible, but requires a statistical approach. We discuss our implementation of superlevels, the representation of line opacity by Opacity Distribution Functions and by Opacity Sampling, and the concept of Resonance-Averaged Photoionization cross-sections. We show that different implementations of bound-bound collisional strengths in Fe superlines may result in systematic effects in the predicted emergent spectrum. Finally, we present a short study of the influence of various assumptions in the Fe model data on the resulting model atmospheres.

1. Introduction

NLTE modeling of stellar atmospheres requires extensive sets of atomic data. Contrary to stellar-interiors work where Rosseland mean opacity tables are sufficient to describe the radiative transport of energy, in a stellar atmosphere one needs to model detailed monochromatic opacities and emissivities to solve the radiative transfer in the atmospheric layers where photons escape from the star. Moreover, when we lift the restrictive assumption of LTE, we need data for all relevant processes that will determine the individual atomic/ionic level-populations. Calculating realistic NLTE model stellar atmospheres therefore requires data for radiative and collisional bound-bound, bound-free, and free-free transitions, for all species that are significant opacity sources. One may also need to include autoionization processes, di-electronic recombination, and Auger ionization. Generally, high accuracy (better than 20%) is desirable for radiative data because the reliability of the predicted emergent spectra and of the derived spectral diagnoses is directly influenced by the quality of the radiative data. On the other hand, moderate accuracy (say, a factor 2 or better) is sufficient for collisional data which will determine by how much level populations will depart from their LTE values. Such extensive sources of atomic data exist now for ra-

diative transitions, while the set of collisional data remains more limited, forcing the use of generic formulae. These sources will be discussed below.

TLUSTY and SYNSPEC are user-oriented codes for modeling stellar atmospheres and makeing stellar spectroscopic diagnostics. TLUSTY is a NLTE model-atmosphere code, assuming radiative equilibrium, hydrostatic equilibrium, and plane-parallel geometry. TLUSTY uses a hybrid Complete Linearization/Accelerated Lambda-Iteration Method that allows one to include consistently thousands of NLTE levels and the effect of millions of individual lines (Hubeny & Lanz 1995) in the models. SYNSPEC computes a detailed emergent spectrum using a model atmosphere and the NLTE populations calculated with TLUSTY, and extensive linelists. A description of our NLTE model atmospheres (Hubeny & Lanz) and of a grid of NLTE line-blanketed model atmospheres of O-type stars (Lanz & Hubeny) can be found elsewhere in this volume. These codes are user-oriented in the sense that all opacities included in the models are specified by users, thus making TLUSTY and SYNSPEC very flexible tools to analyze spectra of widely different objects from the X-ray domain to the infrared.

In this paper, we discuss the sources of atomic data and how we handle them in our stellar atmosphere codes, TLUSTY and SYNSPEC, to realize NLTE line-blanketed model atmospheres incorporating thousands of individual levels and millions of lines. We address several issues arising from the inclusion of such an extensive set of atomic data. The details of the data format is left to the TLUSTY user's guide that can be found in TLUSTY's web site (`http://tlusty.gsfc.nasa.gov/`) along with all atomic data files. In a parallel paper in these proceedings, Rauch describes the handling of atomic data in the Tübingen NLTE Model Atmosphere Package. Brief descriptions of the implementation of atomic data in other model-atmosphere codes are also given by their authors (Hauschildt, Hillier, ...). Alexander (these proceedings) addresses the topic of molecular and dust opacities.

2. Sources of Atomic Data

In this section, we list briefly the sources of data for atoms and ions that we currently use in TLUSTY and in SYNSPEC.

The bulk of the radiative data are extracted from Topbase, the database of the Opacity Project (OP; Cunto et al. 1993). This database will soon be superseded by the TipTopbase which, in addition, will include the data of the Iron Project as well as updates to the OP data. OP provides very extensive datasets of energy levels, gf-values, and photoionization cross-sections, which have been obtained from ab-initio calculations for all ions of the most abundant light species ($Z \leq 14$, S, Ca, and Fe); see Nahar (these proceedings) for a description of the current status of this project. OP claims that these data are accurate at the 10% level or better. Level energies measured in laboratory experiments are extracted from the NIST database to improve the theoretical energies.

The second extensive dataset is extracted from Kurucz's web site and CD-ROMs (Kurucz 1993). His large semi-empirical calculations for iron-peak elements provide the energy levels and line data for the model atoms of Fe and Ni in TLUSTY, whereas we use an updated version of his line list with SYNSPEC.

We list here a few useful web sites from which we have extracted atomic data. This list is by no means exhaustive, but may serve as a good starting point.

Opacity Project Database:
`http://heasarc.gsfc.nasa.gov/topbase/`
(also accessible through `telnet vizier.u-strasbg.fr`
`username: topbase , password: Seaton+`)

NIST Atomic Spectra Database:
`http://physics.nist.gov/cgi-bin/AtData/main_asd`

Kurucz Model Atmospheres and Data:
`http://kurucz.harvard.edu/`

Vienna Atomic Line Database:
`http://www.astro.univie.ac.at/~vald/`

Databases for Atomic and Plasma Physics:
`http://plasma-gate/weizmann.ac.il/DBfAPP.html`

Tlusty Web site:
`http://tlusty.gsfc.nasa.gov/`
(select "Data" to get to the atomic data files page)

3. Energy Levels and Superlevels

The NIST and the OP databases typically list tens to a few hundreds individual energy-levels for each ion of light elements ($Z < 20$), while the Kurucz data may contain over 10,000 levels for some individual ions of iron-peak elements. Therefore, a different approach must be adopted for these two datasets and a statistical approach is required in case of very large number of levels. We start with the case of the light elements, then introduce the concept of superlevels and its application to iron; finally, we tackle the topic of level-identification in TLUSTY and in SYNSPEC.

For most ions of light elements, all levels below the ionization limit can, in general, be incorporated in the model atoms, while levels above the limit are assumed to be in LTE with respect to the ground state of the next ion. The populations of the latter levels are taken into account by the LTE partition function. If needed, they may also be treated explicitly. Level-energies of light elements are extracted from Topbase, and energies are reset to their empirical values listed in the NIST database. Missing, high-l levels are added to the list of levels. OP does not provide fine-structure data, but fine structure is usually ignored in NLTE calculations (that is, fine-structure sublevels share the same b-factor). We include fine-structure data in a few special cases, e.g. strong resonance doublets, where we have found small changes in the resulting model atmospheres.

To manipulate these large model atoms easily, we have developed MODION, an IDL-based graphic tool that works directly with Topbase data files (Lanz et al. 1996; Varosi et al. 1996). MODION displays a Grotrian diagram from which one can select interactively the explicit NLTE levels, and/or build superlevels

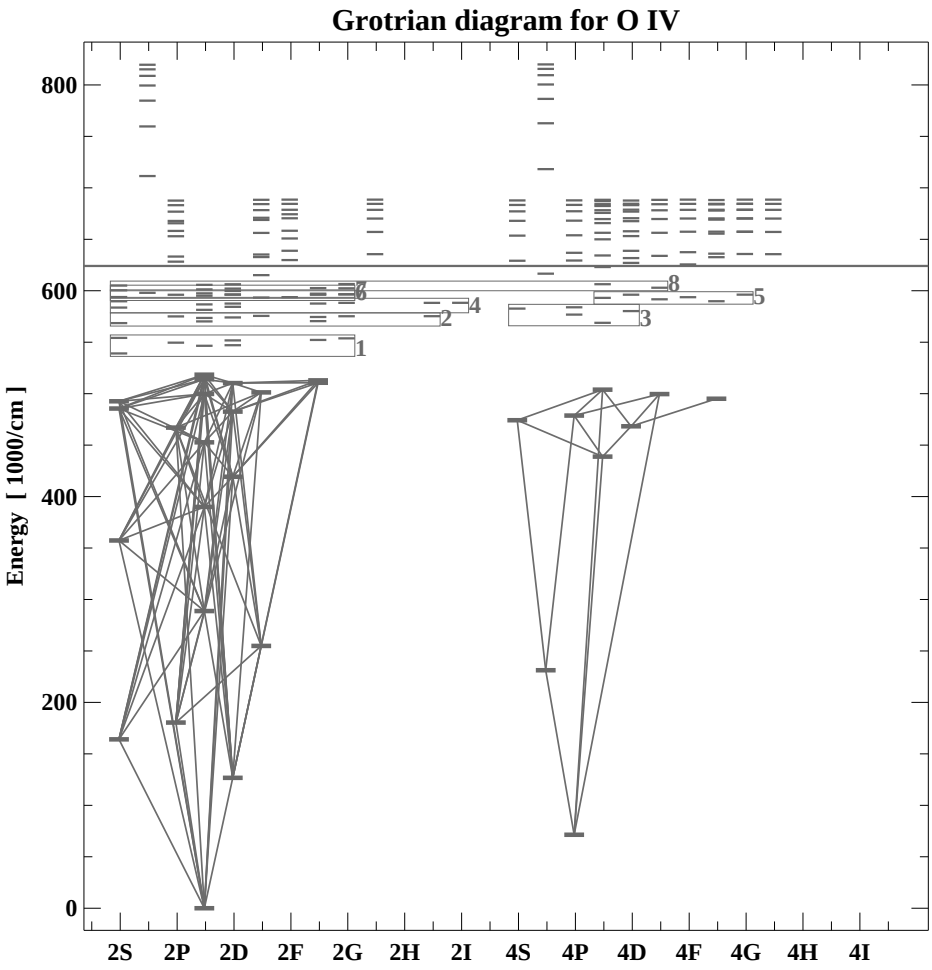

Figure 1. Example of MODION output: the O^{3+} model ion. The lowest 30 individual levels are selected as explicit NLTE levels. 63 high-excitation levels are grouped into 8 superlevels represented by boxes. The line across the diagram corresponds to the ionization energy of O^{3+}, $E_{\rm ion} = 624,382\,{\rm cm}^{-1}$. All 270 transitions between selected levels and superlevels, representing about 900 individual lines, are included. For better clarity, transitions connecting to superlevels have not been displayed.

(see Fig. 1). Next, MODION automatically builds an array of bound-bound and bound-free transitions between the selected levels (with the proper averaging if required). Finally, MODION saves the selected data in the appropriate format for a selected model-atmosphere code. With MODION complicated model atoms can be prepared in a few minutes with a few mouse clicks, thus saving a great deal of painstaking work.

High-excitation levels are often grouped into superlevels in view of their very close energies (see Fig. 1). The underlying assumption is that the populations of individual levels inside a given superlevel follow the Boltzmann distribution. While the populations of superlevels could depart from their LTE values, all sublevels in a given superlevel share the same b-factor. To make sure that this is a reasonable aproximation, one should group levels with very close excitation energies (thus having large collisional rates between levels) into a superlevel. This concept was first introduced by Anderson (1989), and developed further by Dreizler & Werner (1993) and Hubeny & Lanz (1993). Detailed expressions for the mean energies of superlevels, statistical weights, and transition cross-sections between superlevels, may be found in Hubeny & Lanz (1995). We stress that superlevels provide a good statistical approach for calculating the atmospheric structure. However, this is not the case when one aims at understanding the detailed behavior of the radiation field, e.g. radiative pumping mechanisms. Detailed model atoms are then obviously required.

We have applied the concept of superlevels to Fe and Ni ions. We have adopted a second criterion besides energy when grouping levels: we demand that all levels in a given superlevel share the same parity. This requirement avoids radiative transitions within a superlevel; and, more importantly, it enhances the validity of the assumption of equal b-factors because parity will be correctly taken into account for radiative transitions between superlevels and the ground state of the ion (i.e., metastable states, and transitions into and out of them are treated properly). We have built model atoms in which all level-data calculated by Kurucz (typically, a few thousand, and up to 13,000, levels per ion) are grouped into about 40 - 60 superlevels per ion.

Additional ways to reduce the number of levels in the calculation includes grouping levels and superlevels during the linearization step (i.e. in a group, levels do not have to share the same b-factor: an exact solution is calculated, but the ratio between these b-factors is kept fixed during the linearization step). Populations of some levels can also be set to zero automatically whenever they become very small. See Hubeny & Lanz in this volume for additional details.

Another practical issue is to transfer the assignment of explicit NLTE levels in model-atmosphere calculations to the detailed spectrum synthesis. The NLTE populations of the lower and the upper energy-levels of each line in the spectrum synthesis must be set up from the (super)level populations obtained in the model-atmosphere calculations. With few lines and levels, this correspondence could be done by hand, but with thousands of levels and millions of lines, the spectrum synthesis code needs to do it automatically. While one can construct superlevels in many different ways, some may be impractical for this reason. In particular, we stress that the level-correspondence in SYNSPEC is based on level-energies and parities (for iron-peak elements). Any other type

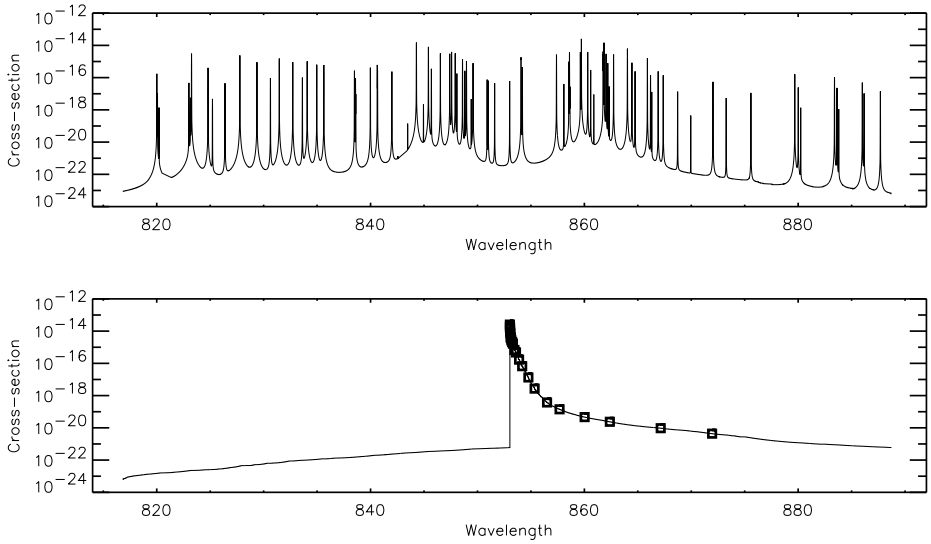

Figure 2. Absorption cross-section of a typical transition between two superlevels of Fe III ($T \approx 19,200\,\mathrm{K}$, $n_e \approx 10^{14}\,\mathrm{cm}^{-3}$). The cross-section has been evaluated at 15,485 frequency points. The lower panel shows the corresponding ODF, which is represented by 24 points (squares) in the model-atmosphere calculations.

of level grouping is not recognized by the current version of SYNSPEC and would require additional coding.

4. Lines

Fully line-blanketed model atmospheres incorporate the opacity of millions of atomic lines. Therefore automation is needed to set up the data files, and statistical methods are required to represent the opacity reliably. Data are extracted from Topbase and set up automatically by MODION, including the necessary averaging for lines involving superlevels. Such transitions are represented by a single line profile with the appropriate f-value. Doppler profiles are used for most lines of the light elements in TLUSTY. Stark profiles are assumed for the first four series of hydrogen and ionized helium, and Voigt profiles are used for the strongest lines of heavier elements (typically, for 50 - 100 lines). In some instances, accounting for Stark broadening may result in significant changes in the model atmosphere (Werner 1996). Data for the Stark widths are extracted from the literature; see the bibliography at the NIST web site.

Transitions between Fe superlevels may involve hundreds or thousands of individual lines. The resulting absorption cross-section is then very complex and a detailed representation may require a very large number of frequency points (Fig. 2). Two approaches have been implemented to limit the number of frequencies. First, we used Opacity Distribution Functions (ODFs): the total opacity from all lines in a given transition (computed using Voigt profiles for

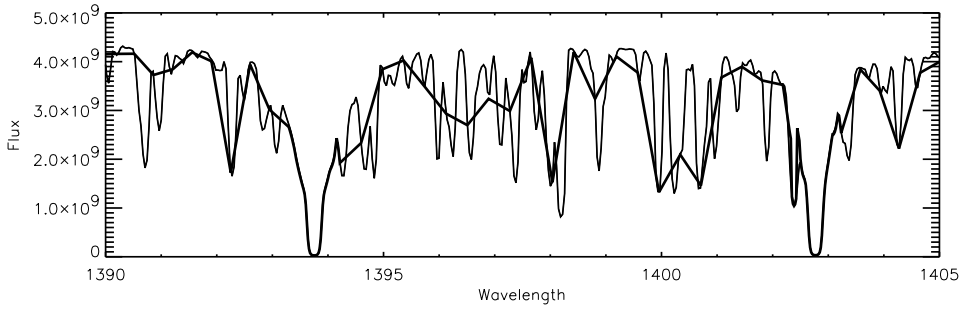

Figure 3. Opacity Sampling in Tlusty: UV spectrum of a 35000K, $\log g = 4.0$, model atmosphere with a zoom in on the region of the Si IV resonance lines: two sampling steps are shown: 0.75 and 30 Doppler widths; notice that the Si IV lines are sampled in the same way in both cases; all other lines are iron lines.

each line) is sorted; the sorted opacities could be represented with a limited number of frequencies, typically 15 to 30 per transition (Fig. 2), or 30,000 to 50,000 frequencies for the whole spectrum. Exact details of line blends are lost; some care should thus be exercised in checking that unintentional blends between strong lines of light elements and Fe ODFs are not affecting the results.

The second method is Opacity Sampling (OS), which is a simple Monte Carlo-like sampling of the superline cross-sections. It has the advantage to treat exactly the blends. However, the cores of important strong lines might be missed if too few frequency points are used. We use a variant of OS, sampling the whole spectrum at prescribed intervals in frequency. Our model atmospheres are sampled with a typical step of 0.75 Doppler widths, thus using close to 200,000 frequency points for an O-star model. While costly in terms of computing requirements, we can sample the spectrum with sufficient resolution to ensure that every line is accounted for. This is the current standard mode in TLUSTY. Fig. 3 illustrates the frequency sampling. We can adopt a larger step to represent the opacity of iron lines and decrease the number of frequency-points to about 60,000 for the same model with a step of 30 Doppler widths; in this case, however, we keep a small frequency-step to sample accurately the lines of light elements (e.g. the Si IV lines in Fig. 3). In Sect. 7 we show the differences in a typical model atmosphere resulting from the method adopted to represent the line opacity.

5. Photoionization

Detailed photoionization cross-sections are also extracted from the OP database by MODION, which performs the necessary summations to set up the cross-sections of superlevels. Most cross-sections have a complicated structure with many autoionization resonances. How should we represent these data in TLUSTY?

In an early implementation, we picked the low envelope of the cross-section, basically skipping the resonances. This approach aimed at getting reasonable estimates of the photoionization rates with a limited number of frequency points,

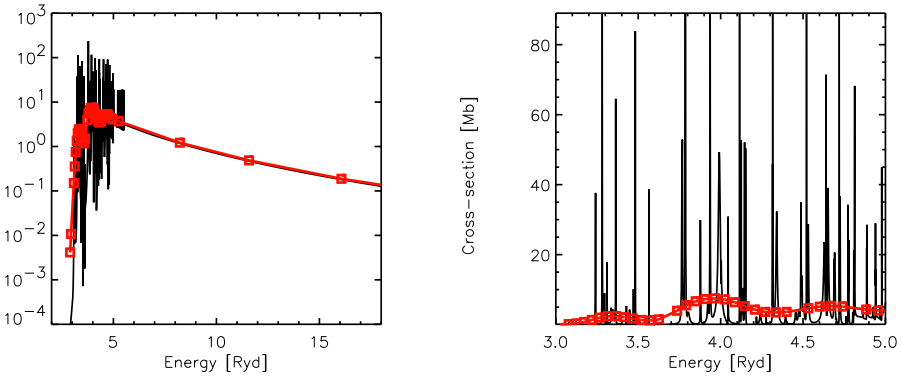

Figure 4. OP (thin line) and RAP (squares and thick line) photoionization cross-sections of the level $2p^3\ ^2P^0$ of O IV.

but was not fully satisfactory because we could not estimate the effects of autoionization and dielectronic recombination.

Recent TLUSTY models use extensive frequency grids and, therefore, the number of points is no longer a constraint. We could thus simply adopt the full cross-sections as provided by OP. However, an examination of the cross-sections reveals that the sharp resonances are not fully resolved by the OP calculations. Moreover, the theoretical energies have an accuracy of 2-3%, and the resonances are therefore shifted off their exact wavelengths. Following Bautista et al. (1998), we have therefore adopted the idea of resonance-averaged cross-sections. The cross-sections are convolved with a Gaussian that smoothes the sharp resonances:

$$\sigma_{\rm RAP}(E) = \int_{E_0}^{\infty} \sigma(x)\ \exp[-(x-E)^2/2(\delta E)^2]\ dx, \qquad (1)$$

We have also adopted a width, $\delta E/E = 0.03$, that corresponds to the typical uncertainty of the resonance positions. This approach addresses the two problems of the original OP cross-sections. Moreover, a few tens of points are sufficient to represent the RAP cross-section accurately. Fig. 4 illustrates the RAP approach with an example of an O IV level.

For Fe II-V, we use the OP cross-sections updated by the Ohio State group (see Nahar, this volume) for the lowest 15 - 20 superlevels of each ion. We have summed up the contributions of all sublevels and applied the RAP convolution. For higher-excitation superlevels, we cannot assign an OP cross-section to every sublevel (the Kurucz list of energy levels is 5 to 10 times more extensive than the number of levels in the OP calculations), so we have to resort to the hydrogenic approximation.

The RAP cross-sections conserve the integral of each cross-section, thus yielding the correct photoionization rate including the effect of autoionization. However, the contributions from direct photoionization and autoionization to the total cross-sections cannot be separated. Therefore, dielectronic recombination is treated in only an approximate fashion.

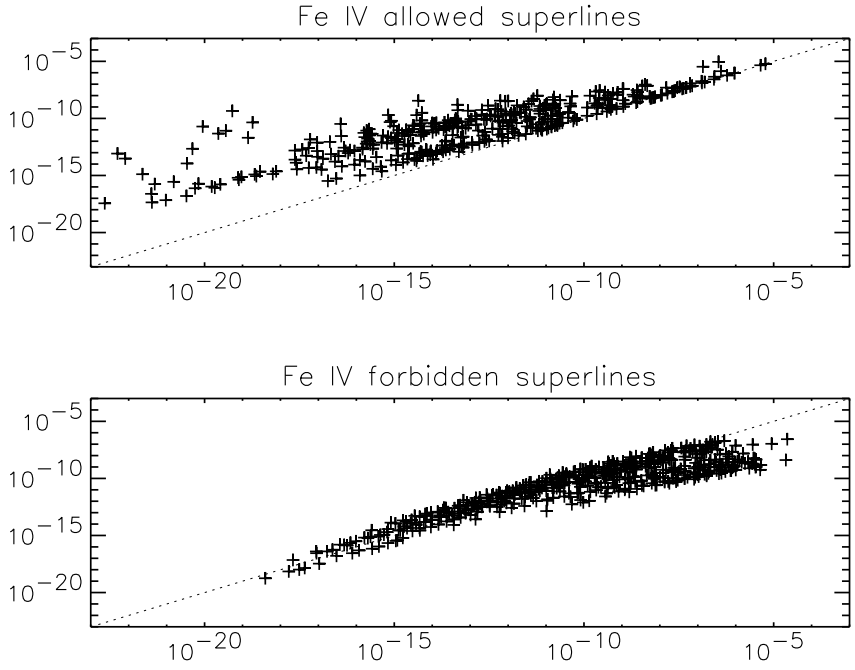

Figure 5. Comparison of collisional strengths of Fe IV bound-bound transitions computed from the superline data or from the sum of the contributions of each transition between the sublevels of the superline. Top: radiatively-permitted superline; bottom: forbidden superline.

6. Collisions

Data sets for collisional strengths are not as extensive as those for radiative data. The work of calculating collisional strengths has mainly concentrated on inter-system transitions that are important for diagnostics at low densities. This situation is starting to change with the Iron Project, which is providing a large number of collisional strengths for iron ions. We plan to adopt these collisional data as they become available; at present, however, we have to resort to approximate formulae for collisional strengths in most cases. TLUSTY models use Seaton's formula extensively for collisional ionization, the Van Regemorter formula for radiatively-permitted bound-bound transitions, and the Eissner-Seaton formula for forbidden transitions [with an ad hoc strength parameter $\gamma(T) = 0.05$].

We have implemented two different ways to compute the collisional strength of superlines. The original implementation applied the Van Regemorter formula using the total f_{IJ}-value of the superline, $\Omega_{IJ} \propto f_{IJ}$, or the Eissner-Seaton formula if the superline is forbidden. A more recent implementation considers all individual transitions between the sublevels, and sums up each contribution to the total collisional strength, $\Omega_{IJ} = \sum_{i,j} \Omega_{ij}$. Fig. 5 displays a comparison of the collisional strengths evaluated using both implementations, for permitted and forbidden superlines. The sum of individual contributions is larger than

the first estimate for allowed transitions because it includes all the individual forbidden lines between the sublevels, while the original implementation neglects all these contributions. The second approach therefore seems physically more sensible. For forbidden superlines, there is no systematic effect, because only the Eissner-Seaton formula is used and the differences reflect a distribution of the individual level energies with respect to the averaged energy of the superline.

We found a systematic difference between the iron line strengths predicted by the CMFGEN (see, e.g., Hillier in this volume) code and TLUSTY when using our earliest estimates of the collisional strengths. The Fe lines were predicted to be deeper with TLUSTY, which translated to deducing a systematically lower Fe abundance, up to a factor of two. This discrepancy disappeared when we started using the new collisional strengths computed as the sum of all the individula contributions. However, the situation is still far from perfect, essentially because of the lack of reliable data for collisional strengths for optically forbidden transitions.

7. Model Atmospheres

We compare the effect of different Fe model data on the resulting model atmospheres. As a test case, we adopted the parameters, $T_{\rm eff} = 35,000\,{\rm K}$, $\log g = 4.0$, solar composition, and $V_t = 10$ km/s. The reference model is extracted from our new grid of NLTE model atmospheres, see Lanz & Hubeny in this volume for a description of these models.

Table 1. Assumptions and characteristics for the test case models.

Model		Levels	Freqs	Fe lines
G35000g400v10	Reference model (OS, 0.75)	907	184,136	1,176,853
Ga35	OS, 30 Doppler widths	907	65,398	1,176,821
Gb35	ODF	907	40 759	7 459 416
Gc35	Fewer selected Fe/Ni lines	907	184,136	88,009
Gd35	More Fe IV-V superlevels	965	65,493	1,221,466
Ge35	Less Fe IV-V superlevels	874	65,366	952,051
Gf35	No levels above ioniz. limit	804	184,226	1,168,764

The first three models deal with the representation of line opacity: OS with larger frequency step, ODF, and line strength selection (Fe and Ni lines are dynamically selected depending on a strength criterion). In the case of the ODF model (Gb), all the Fe and Ni lines are used to set up the ODFs. In the second set of models, we have built different Fe IV and Fe V model atoms (they are the dominant ions). All individual levels are included in models Gd and Ge, but grouped in more (74 and 69 vs 43 and 42) or less (33 and 19) superlevels. In the last model, all the Fe and Ni levels above the ionization limits are ignored.

Fig. 6 illustrates the effect of different ways of including the Fe data on the model atmosphere's temperature structure. First, differences are larger in the case of ODFs than in the case of a large sampling step, which we interpret as reflecting incorrect blends between ODFs and other lines. The larger sampling step is probably appropriate in most cases ($\Delta T \approx 100\,{\rm K}$), and reduces the

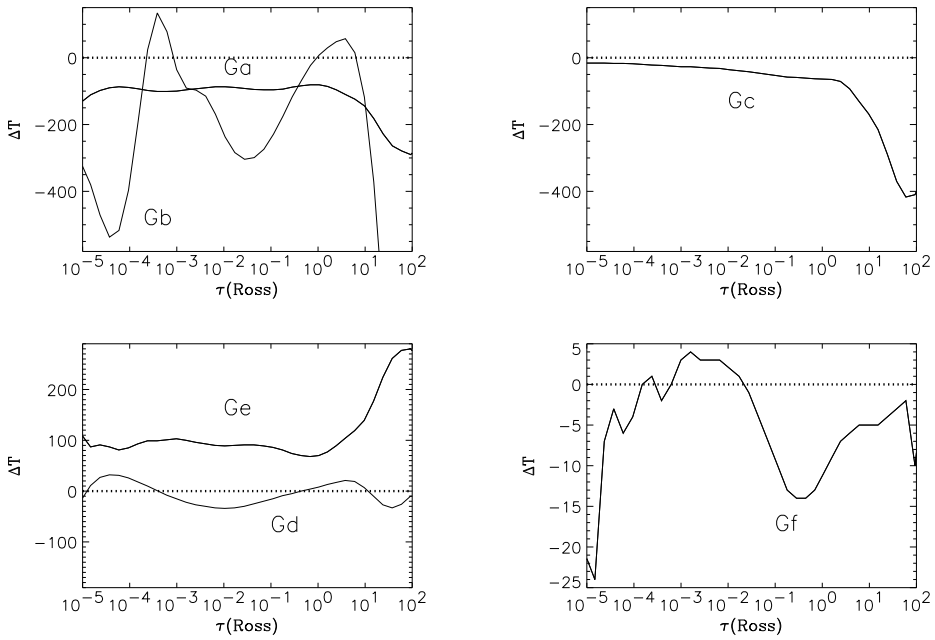

Figure 6. Changes in the model temperature-structure with repect to the reference model depending on the treatment of Fe lines and model atom (see Table 1 for model keys).

computing time by a factor of three (CPU time is essentially proportional to the number of frequency points). The largest difference arising from the line-strength selection criterion is seen at depth, because of a large change in the number of selected Fe VI lines (upper right). However, this does not affect the predicted spectrum. Differences in the layers where the spectrum is formed are small ($\Delta T < 100$ K) showing that most of the line-blanketing effect results from the strongest 10^4 to 10^5 lines rather than the millions of weaker lines. The lower part of Fig. 6 shows the results related to the model atoms. First, we see that increasing the number of superlevels results in small changes, while the model with less superlevels shows a larger systematic temperature difference. This result indicates that we have adopted Fe model atoms of reasonable sizes for our reference model. Finally, the levels above the ionization limits have a minimal effect on the model-atmosphere structure.

Hillier & Lanz (2001) have presented a brief comparison of CMFGEN and TLUSTY (see their Fig. 1). The agreement in the predicted spectra is excellent. While the Fe data are the same, the independent implementations of the Fe data in two NLTE model atmosphere codes yielding such an excellent agreement increases our confidence that these data are properly handled.

8. Conclusion

Extensive sets of atomic data can now be routinely incorporated in NLTE model stellar atmospheres. We are thus able to take advantage of the latest, most accurate atomic calculations to improve our description of the total opacities, therefore of radiative rates. Generally, these models reproduce well most details of high-quality UV and optical spectra of hot stars. In particular, we point out that consistent fits of lines of several ions of different species can be achieved for main-sequence O stars, hot subdwarfs, and hot metal-rich white dwarfs. This result indicates that the ionization structure of the model atmospheres is basically correct, showing that the claim of high accuracy of the OP data (seen as a whole set) is well justified and that our handling of these data (Opacity Sampling, Resonance-Averaged Photoionization cross-sections) is also adequate.

There are still several areas where a further progress is desirable. First, we need improved cross-sections for Fe I, which is an important continuous opacity source for intermediate-temperature stars. Use of the current OP dataset produces a number of sharp features in the near and mid-UV spectrum of F stars which are not observed. We can observe the restframe UV spectrum of these stars, which trace intermediate-age populations, from the ground in $1 < z < 3$ galaxies. Improvements in the Fe I photoionization cross-sections will have a direct impact on the analysis of these galaxies, and thus on the understanding of stellar populations in the early Universe, as well as on the chemical evolution of these galaxies. Fortunately, the Ohio State group has informed us of their intention to improve this work.

Second, we need to know how realistic the general formulae for collisional strengths are. In addition to implementing the large amount of collisional data expected from the Iron Project, we will be able to assess the accuracy of these formulae and determine if their continued use in stellar-atmosphere modeling

is justified. Finally, an extension of these atomic calculations to other species (e.g. P, Ni, Cr, and other iron-peak elements) is highly desirable.

Acknowledgments. As a community, we are greatly indebted to the physicists who provided, and are still providing, all these atomic data, in particular the OP team, Bob Kurucz, and the NIST team. The present sophistication of current model atmospheres would simply not been achievable without all their work during many years. This work was supported by several NASA grants.

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