May 2007

THE HAO SPECTRAL DIAGNOSTIC PACKAGE FOR EMITTED RADIATION (`HAOS-DIPER`) Reference Guide (Version 1.0)

P. G. Judge

HIGH ALTITUDE OBSERVATORY

NATIONAL CENTER FOR ATMOSPHERIC RESEARCH
BOULDER, COLORADO

THE HAO SPECTRAL DIAGNOSTIC PACKAGE FOR EMITTED RADIATION (`HAOS-DIPER`) Reference Guide (Version 1.0)

P. G. Judge (HAO)

Contents

List of Figures

List of Tables

Acknowledgments

This work is a compilation of efforts made sporadically over a period of several years. The author wishes to thank HAO director, M. Knölker, for his encouragement and for his willingness to hire R. Meisner to help in the initial phases of this project.

I also wish to express sincere thanks to E. Landi and the entire CHIANTI[1] project for permission to import their carefully compiled database. Similar thanks go to the OPACITY and NIST atomic spectroscopy database projects for making their data so freely available. M. Arnaud is gratefully acknowledged for sending electronic forms of ionization and recombination data. Some very useful procedures from the solarsoft library have been used.

Work in the 1980s and 1990s with Prof. Mats Carlsson prompted this project and the package contains many of his ideas and routines.

I would like to thank the NCAR organization for their support, patience and understanding over the last four difficult years dealing with my illness and its complications, during which this project reached some level of maturity while working mostly from home. The flexitime policy has been enormously helpful to me.

Most importantly, I would never have made it this far without the love, support and understanding of my lovely wife, Terri. Different and better indeed.

Overview

This document is a reference guide for HAOS-DIPER, an IDL-based database and software system for working with data from atoms and atomic ions. HAOS-DIPER grew out of a need to work with and manipulate data for neutral atoms and atomic ions to understand radiation emitted by some space plasmas, notably the solar atmosphere and stellar atmospheres. An early version was described by Judge and Meisner (1994). Since then, other packages have become available which substantively perform many of the tasks originally intended for HAOS-DIPER. These include CHIANTI (Dere et al. 1997, Landi et al. 2006, and references therein), and ADAS (Summers 2003, Badnell et al. 2003). However, HAOS-DIPER has some properties which together make it unique:

– It is based upon the fast, flexible database software system written by D. Lindler[2] for IDL, and takes some advantage of this system.

– It works with quantum numbers for atomic levels, enabling it to perform tasks otherwise difficult or very tedious, including a variety of data checks, calculations based upon the atomic numbers, and searching and manipulating data based upon these quantum numbers.

– In principle, HAOS-DIPER can handle conditions from LTE to coronal-like conditions, in a manner controlled by one system variable !REGIME.

– There is some capability for estimating data for which no accurate parameters are available, and for accounting for the effects of missing atomic levels.

Access to the package is through the HAO website::

        http://www.hao.ucar.edu/modeling/haos-diper/

and the author may be contacted at

                judge@ucar.edu

---

[2]Lindler's database system is available as part of the IDL Astronomy Library: (http://idlastro.gsfc.nasa.gov/), and is a part of the SolarSoft IDL system (SSW: http://www.lmsal.com/solarsoft/)

1   Should you consider using `HAOS-DIPER`?

The following table can be browsed by a potential user to see if `HAOS-DIPER` might be useful to her or him.
The various points are elaborated on below.

Table 1: Should you use `HAOS-DIPER`? A Summary

Targeted problems	
	tenuous plasmas, "low energy" regime
	LTE to optically thin plasmas
	compilation of needed rate coefficients
	teaching/learning spectroscopy
	simple statistical equilibrium calculations
	- including escape probabilities
	simple non-equilibrium calculations
	- evolution of atomic systems
	provide "building blocks" of data and code to permit the user
	to make more sophisticated calculations, e.g.
	- detailed radiative transfer or radiation hydrodynamics
Limitations	
	elements lighter than Zn (nuclear charge 30)
	principal quantum numbers < 10
	incomplete databases
	photoionization data are summed over final states,
	and are split approximately over fine structure
	no impact line broadening
	no hyperfine structure
	no configuration mixing
Cannot handle	
	non-Maxwellian particle distributions
	inner shell excitations (high energy phenomena)
	atomic and spectral polarization
	molecules
	accurate radiative transfer
	. . .

1.1   Things `HAOS-DIPER` **might be good for**

`HAOS-DIPER` may be useful if

– you are an IDL user and need/wish to study atomic data and processes, in tenuous plasmas. By "tenuous" it is meant that atoms and ions do not experience very large perturbations to the atomic Hamiltonian from the plasma itself, and that to a good approximation the ions can be considered as isolated but weakly perturbed (see section 2.1).

– you wish to manipulate atomic data, for example, to study how changing a given atomic parameter affects the interpretation of some spectral data,

– you wish to compute atomic level populations in plasmas under conditions from local thermodynamic equilibrium (LTE) to optically thin non-LTE coronal conditions, in or out of statistical equilibrium. The HAOS-DIPER encompasses sufficiently wide conditions to be useful throughout stellar atmospheres and their more tenuous envelopes (e.g., their coronae),

– you wish to see how radiative transfer may influence the populations and emergent spectra, in a crude way (using escape probabilities, detailed radiative transfer is not treated),

– you wish to manipulate atomic data, and write the data in a form to be used by another program, for example for detailed radiative transfer or radiation (magneto-) hydrodynamic calculations,

– you wish to manipulate atomic data easily based upon quantum numbers,

– you wish to use real atomic data to teach students about quantum mechanics and spectroscopy.

– you wish to try to identify spectral lines in a simple way, and mark up spectra of atoms and atomic ions from XUV to IR wavelengths.

1.2 Limitations

A potential HAOS-DIPER user should be aware of the following limitations, which may provide additional discouragement.

– The data within HAOS-DIPER currently do not extend to elements heavier than zinc (nuclear charge of 30). Although in principle it is possible to include heavier elements, such data are less complete, the elements are not very abundant in the universe, and the energy level structure is complex and less likely to conform to the configuration/ parent/ outer orbital/ term structure which has been adopted in HAOS-DIPER (sections 4.4.2 and 4.4.3). The adoption of this structure is needed for the computation of the "good quantum numbers" for each level, the transition probabilities etc. The HAOS-DIPER uses these quantum numbers extensively. This means that while the complex spectra of heavier elements are in principle straightforward to include, the quantum numbers are not likely to be good ones, requiring

a higher level of sophistication than is encoded in the `HAOS-DIPER`. Indeed, there are many levels (particularly of neutral species where the central field is weakest and electron-electron correlations largest) for lighter elements which do not conform to the assumed simple coupling schemes (which include LS, JJ and pair coupling). These levels are omitted from the database. Again, these restrictions apply mostly to neutral atoms of heavy atomic species.

– Because of the way the `HAOS-DIPER` encodes quantum numbers (see sections 4.4.2 and 4.4.3), levels containing any orbital angular momentum greater than 9 cannot be included in the database. Likewise, those configurations with more than 9 equivalent electrons cannot be handled. (This restriction is not usually as serious as it may appear, just a handful of levels were omitted from the current version of the database).

– For the same reasons, neither hyperfine structure nor configuration mixing are currently handled, the `HAOS-DIPER` expects the levels to conform to the leading single configuration and fine structure conventions outlined in sections 4.4.2 and 4.4.3.

– There is occasionally an ambiguity in assigning a transition type (magnetic dipole vs. electric quadrupole) for a very few transitions for which the selection rules allow both. If the multipole order is important then such cases should be checked. They are flagged with `trn.type='M1E2'`, see section 4.4.4)

– If *completeness* in the levels and spectra of atomic species is required, it's best therefore to go to the NIST database for atomic spectroscopy[3]. The `HAOS-DIPER` attempts to be as complete as existing energy level databases allow. It includes all levels with the same principal quantum number as the ground levels, and also includes many cases of significantly higher principal quantum numbers. This is sufficient to account for many of the strongest ad diagnostic lines from emission line sources, and many cases of absorption lines (photospheric lines for example).

– Another limitation is imposed by the adoption of photoionization data from the `OPACITY` project. While these data represent the best and most complete set of data needed to compute opacities, their application to non-LTE problems requiring photoionization and recombinations must be handled with care owing to subtleties concerning dielectronic recombination (see section A.3), and because they are for LS-coupled terms (not the individual levels). The `HAOS-DIPER` treats the latter only approximately to preserve the total transition probabilities for ionization and recombination. Furthermore, the `OPACITY` project data consist of *total* cross sections, and are not specific to the "final state" (the state in which the photoionized ion finds itself after photoionization, it could be the ground state or excited states.

---

[3]`http://physics.nist.gov/Pubs/AtSpec/index.html`

See e.g. Nahar and Pradhan 1991 for some examples). Thus, in cases where photoionization and or recombination directly influence level populations of excited levels of interest, the results cannot be trusted.

– Data for line broadening by particle impact are not included in the database, although there is provision to store certain data in the `trn` structure (see section 4.4.4).

1.3   When to use something else

Like some other projects concerned with the radiation emitted by optically thin plasmas, `HAOS-DIPER` is basically intended for "low energy" cases. The "low energy" limit refers to the small typical energies of plasma particles and photons relative to the energies needed to ionize and/or excite levels of atomic ions. The threshold energies for ionization of an ion of core charge[4] z is $I \sim 10z^2$ eV. The low energy limit of $k_B T_e < I$ commonly applies to quiescent stellar atmospheres from photosphere to corona, and in many photoionized astrophysical plasmas. At low temperatures, Coulomb cross sections are large, and the assumption that the electron distribution functions are thermalized may be quite reasonable, even at very low densities found in planetary nebulae, for example. Currently, `HAOS-DIPER` assumes that many-electron excitations are unimportant and that the plasma particles are indeed thermalized. This "low energy" condition therefore means that `HAOS-DIPER` cannot handle some important cases of potential interest:

– Non-Maxwellian electron distribution functions. While some of the atomic data are given as cross sections as functions of energy (the electron impact ionization data compiled by Arnaud and colleagues used in `HAOS-DIPER`, see section 4.2), many others, such as bound-bound collisional data, are given as Maxwellian-averaged collision strengths.

– Cases where excited levels of high principal quantum number are important subjects of interest, such as those states involving dielectronic recombination and autoionization. `HAOS-DIPER` does treat these processes, but only in a crude sense: these highly excited levels are assumed to be integrated over in order to derive rate coefficients for recombination for example, and the states involved are not treated separately.

– Atomic polarization caused by anisotropic photon scattering. Atomic polarization, resulting from different magnetic substate populations of a given level, is required

---

[4]The core charge is the net charge seen by the outermost electron(s) in a given ion, $z = 1$ for neutral atoms for example.

for the Hanle effect, for example (Landi degl'Innocenti and Landolfi 2004). Magnetic substates are not handled by `HAOS-DIPER`, but `HAOS-DIPER` models can be used in resonance scattering calculations using special computer codes (Casini and Judge 1999 with erratum in Casini and Judge 2000, Judge et al. 2006).

– Atomic polarization caused by anisotropic collisions (particle beams). The particle distribution functions are assumed to be thermal and hence isotropic.

– Cases where many electrons are excited in atomic shells, such as may occur in transiently excited, heated or irradiated plasmas (e.g., impulsive phases of flares, beam-foil experiments).

For some of these cases, a far more extensive and physically complete database and accompanying software is available in `ADAS` developed by H. Summers and collaborators (Summers 2003). Another recently released code, applicable to high energy conditions, is `FLYCHK`[5] developed by a team at `NIST`.

Lastly, if you are interested in molecules and molecular ions, `HAOS-DIPER` is not for you. No data are stored for these systems, and the quantum numbers in any case assume that atomic, not molecular, structure is present.

1.4   How `HAOS-DIPER` works, in a nutshell

Atomic data are stored in database files, which are compiled and provided by the author and which should not be changed. The user instructs the `HAOS-DIPER` to read these data. `HAOS-DIPER` then stores them in data structures to be used in IDL. It is these structures which the user works with. The structures are assembled and checked by the `HAOS-DIPER`, the user can manipulate these structures and, for example, make simple calculations of interest, remove levels and transitions, and refine the data for use in another CPU-intensive program, for example.

The philosophy behind this is that `HAOS-DIPER` provides a simple foundation for working with data of atoms and atomic ions. The user can develop their own tools to work with these data. Several procedures are provided in `HAOS-DIPER` to allow the user to become familiar with the building blocks developed. Some of these "building block" procedures (`sesolv, tsolv, isostr`) will be discussed below

---

[5]`http://nlte.nist.gov/FLY/`

2 Physical assumptions

2.1 Physical vs. chemical picture

A fundamental assumption of `HAOS-DIPER` (in common with the vast majority of work in stellar atmospheres, see Mihalas 1978) is that the physics of a multi-electron, multi-ion atomic system can, because of different energy regimes, different time scales, be treated separately from the physics of the plasma taken as a whole. Thus, while the multi-electron atomic ions are embedded in a plasma consisting of electrons and ions, all in motion, leading to a very difficult many-body system in its full generality, one can make many meaningful approximations. This is possible because many plasmas of interest are physically tenuous. This assumption is often an excellent one when a researcher is trying to understand the radiation emerging from a plasma, because radiation does not directly escape from the deep, dense interiors of massive astrophysical objects (stars, their degenerate remains) and so the radiation which can be observed necessarily emerges from the outermost, least dense layers. As a consequence, the atomic and ionic energy levels are not drastically "blurred" by the influence of neighboring particles, as happens in the solid or liquid states, for example, because the collisional processes usually make only small and infrequent perturbations to the atomic Hamiltonian. The electron-ion and electron-atom collisions are of a very short duration compared with the natural radiative relaxation times of atomic states- this permits one to treat radiative and collisional processes separately (the "impact approximation" of Lamb and ter Haar 1971, see eq. 11 below). Thus, one can treat the atoms and ions as if they are isolated to zeroth order, embedded in a plasma with accompanying radiation. The motions of the charges and particles in the plasma, and the radiation field, are then treated as perturbations to the atomic ions.

The equations describing the evolution of the atomic systems are cast in the form of the evolution of the population densities of the eigenstates of the unperturbed atomic Hamiltonian, and the evolution of the embedded radiation can then be set up in terms of the usual "rate" equations[6]. Reviewed in Appendix A, these equations describe the transfer of population from one atomic level to another, using rate coefficients for the important processes. This is sometimes known as a "chemical" picture of the system, as opposed to a "physical" description, because of the assumed clean separation of the physical system into the atomic part and the plasma part. An example of differences of these pictures is given, in stellar interior research, by the `OPACITY` project (chemical picture) and `OPAL` project (physical picture) whose goals were to re-determine stellar opacities (e.g., see Seaton 1987, Hummer and Mihalas 1988, Daeppen et al. 1990).

The `HAOS-DIPER` is an attempt to collect the data needed to solve such equa-

---

[6]The general problem solves for the density matrix of the radiating atomic system, of which the population densities are just the diagonal part of the atomic component (e.g., Landi degl'Innocenti and Landolfi 2004). The off-diagonal components, the coherences, are needed under circumstances which include the Hanle effect, for example.

tions, solve some simple cases, and to allow researchers to "play" with atomic data to investigate how certain atomic parameters might affect the interpretation of real spectra, without necessarily being limited to specific regimes other than the general ones listed above.

2.2   Physical assumptions and related system variables

HAOS-DIPER uses several new IDL "system variables", linked to underlying physical assumptions, designed to make the use of the package more flexible, useful and straightforward. These system variables control the behavior of the package and the output, and are related to some basic physical assumptions:

!REGIME	0: "coronal", 1: "nLTE", 2: LTE
!APPROX	integer between 0 and 31: the "bits" in base 2 are switches, 0 or 1

These system variables should be set using, for example

IDL> diper,regime=1	; set to nLTE case, default=0
IDL> diper,approx=1	; set to add approximate data, default=0

Both !REGIME and !APPROX affect the way in which data are handled because of several underlying physical assumptions[7]. !REGIME is the more fundamental parameter. If it is set to 2, only energy level and radiative rate data are read. No collisional data are needed. This is useful, for example, if you simply want to search for wavelengths in a certain range from the atomic ions stored as a structure, as well as for LTE calculations themselves.

If !REGIME is set to 0, the "coronal" regime, HAOS-DIPER does several things corresponding to physical assumptions. (1) It sets the lvl.meta[8] variable to 0 except for levels belonging to the ground terms of each ionization stage, where it is set to 1. lvl.meta determines if a given level must be treated as "metastable" or not. If metastable, HAOS-DIPER will add the ionization and recombination data from the text files ar85ci.dat, ar85ct.dat, shull82.dat (see section 4.2) to these levels only, and (2) no photo-ionization data are extracted from the atom_bf database, recombination being treated solely via rate coefficients.

Note that the "coronal" regime in HAOS-DIPER does not assume all populations are zero except for the ground level of all ions- a common definition of a coronal regime. Instead, all levels of the ground *terms* are set to be metastable levels, levels for which ionization and recombination coefficients are non-zero. Furthermore, when the rate

---

[7]Note that, if !REGIME is changed, you *must* re-load the atomic data using diprd or atomrd for the changes to take place.   It is also advisable to do this when !APPROX is changed to ensure all changes are carried out.

[8]This variable lvl.meta introduced here is the "tag" meta of the IDL structure lvl defined in section 4.4.2. The lvl structure is one of the four major structures used to store and manipulate atomic data in HAOS-DIPER, see section 4.4.

equations are solved, the full equations are solved with no assumptions concerning population densities of excited levels.

If `!REGIME` is set to 1, the most general "nLTE" regime, `HAOS-DIPER` sets `lvl.meta` for levels of the entire ground configuration to 1, and it will include photoionization cross sections from the `atom_bf` database file. Recombination is then computed via the photoionization cross sections instead of rate coefficients, and any incident radiation prescribed by the user is included as photoionization.

Levels labeled as "non-metastable" are those identified by the particular value of `!REGIME` which have rapid decays to lower levels via electric dipole (E1) transitions. These levels are given rate coefficients for direct collisional ionization by electron impact using the semi-empirical formula of Seaton (Allen 1973) for neutral atoms, and the formula of Burgess and Chidichimo (1983) for ionized species.

2.3   Concerning doubly-excited states

Outside of these physical approximations determined by `!REGIME`, an important basic assumption made is that multi-electron excited atoms and atomic ions can be treated as having either purely "bound" states or "free" states. In this way the transition probabilities are split by `HAOS-DIPER` physically into "bound-bound" and "bound-free" transitions. However, there is a very important class of states involving "doubly excited states"– those levels qualitatively described as having two excited electrons– which strictly speaking can have both "bound" and "free" character. More importantly, such levels can, under non-LTE conditions, have critical influences on the atomic and ionic populations of interest. The reciprocal phenomena of dielectronic recombination and autoionization describe the processes involving doubly excited states which generally have large influences, and which must be treated (Burgess 1964, Storey 1981, see section A.3).

In `HAOS-DIPER`, autoionization and dielectronic recombination is treated as described in the Appendix (section A.3). Briefly, when `!REGIME=0`, coefficients for electron impact ionization (autoionization included) and recombination are adopted which take account of the summed effects of such levels, following Arnaud and Rothenflug (1985) and references therein. However, in the case of `!REGIME=1`, when photoionization cross section data are included, special care is needed since the photoionization cross sections contain resonance structure from the doubly excited autoionizing levels, and these data may or may not be consistent with the treatments used for dielectronic recombination and autoionization. Most of the relevant issues are nicely discussed by Nahar and Pradhan (1992). See section A.3 for more details. There is also a need to account for plasma microfields in the dielectronic recombination process, and this is addressed in section A.4. `!REGIME=2` is the LTE case for which, of course, no rates are needed.

2.4   Multiple ionization stages

Multiple ionization stages are handled by `HAOS-DIPER`. Several different ionization stages are read as follows

```
IDL> diprd,'c',[2,4]                    ; store C II, C III, C IV, ground level of C V
```

data are available in the database for all these ions, as can be seen in the term diagram of figure 1, created using

```
IDL> td,/main,/perm,wmax=1600,$         ; plot a term diagram of the levels,
                                              showing only the main, permitted lines

     /fix,/contlong,title='C II-IV'
```

The additional keywords to `td` can be accessed using the usual `doc_library` procedure.
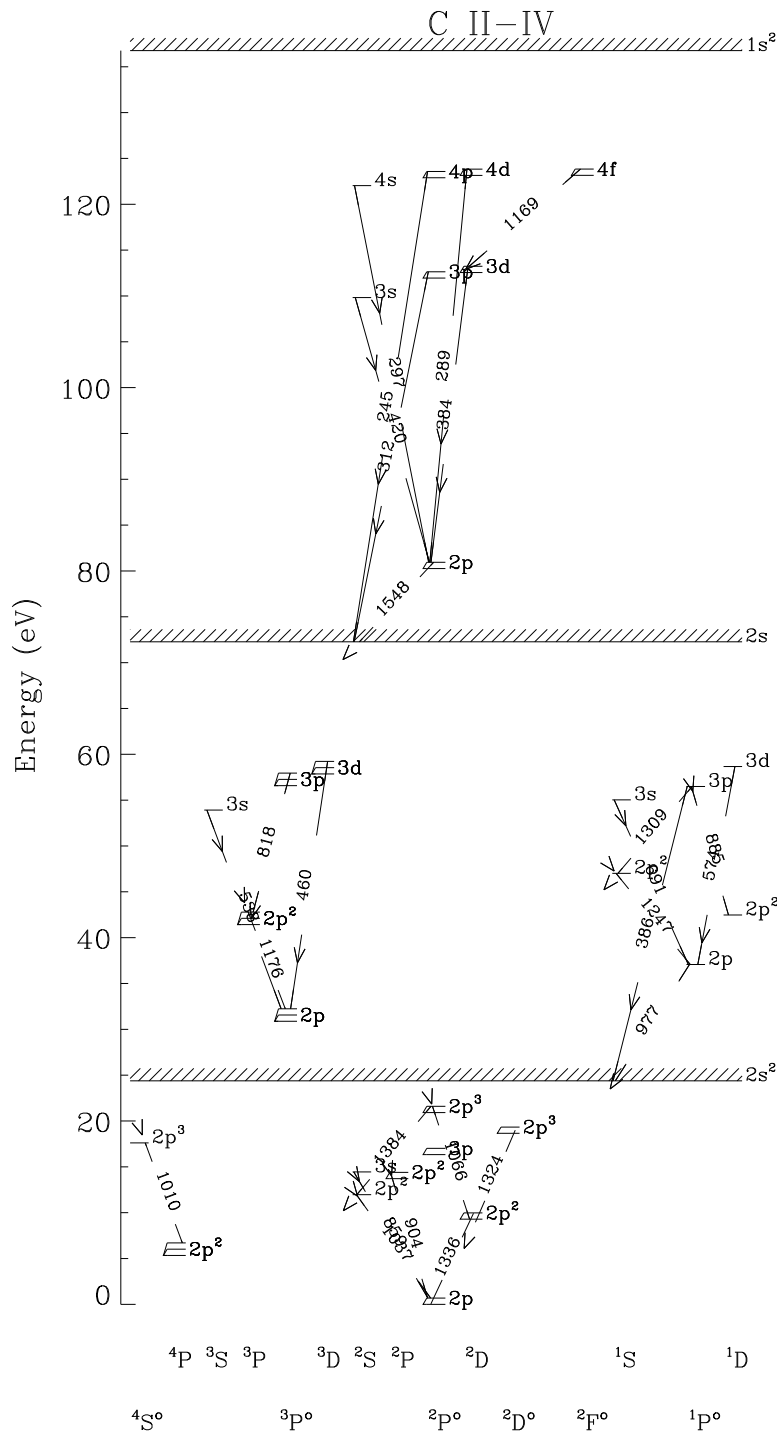
Figure 1: *A (rather messy) term diagram of the levels of ions of C II-IV, showing just the main, permitted lines of each multiplet, and all the levels in the database. A call to* `doc_library` *will describe the use of other keywords which can be used to refine the figure.*

The procedure `diprd` (discussed further in section 3) automatically deals with consistently handling the data from many different ionization stages. The question arises, what happens when you ask for data for ions for which no level data exist in the database? In this case, `HAOS-DIPER` will simply add in the ground level for that ion into the data stored, and there will be just one level for this particular ion.

If, on the other hand, one wishes to examine, say, line ratios within one particular ionization stage, the following syntax can read in the data needed to achieve this:

```
IDL> diprd,'Al',10,/nofill      ; read levels for Al X without storing data for the next
                                   ionization stage Al XI
```

The above example illustrates a convenient and shorthand way of doing the same thing but using the data structures to be described below:

```
IDL> diprd,'Al',10              ; read levels for Al X including the next ionization stage
                                   Al XI
IDL> i=where(lvl.ion gt 10)     ; find indices of level(s) to delete
IDL> level, del=i               ; remove those levels
IDL> level                      ; list the remaining levels
IDL> td,/main                   ; plot a term diagram of the levels
```

 The variables and syntax will be made clearer by running the demos and by reading the next section. The output of the procedure to draw a term diagram showing only the main lines of each multiplet, `td,/main`, is shown in figure 2
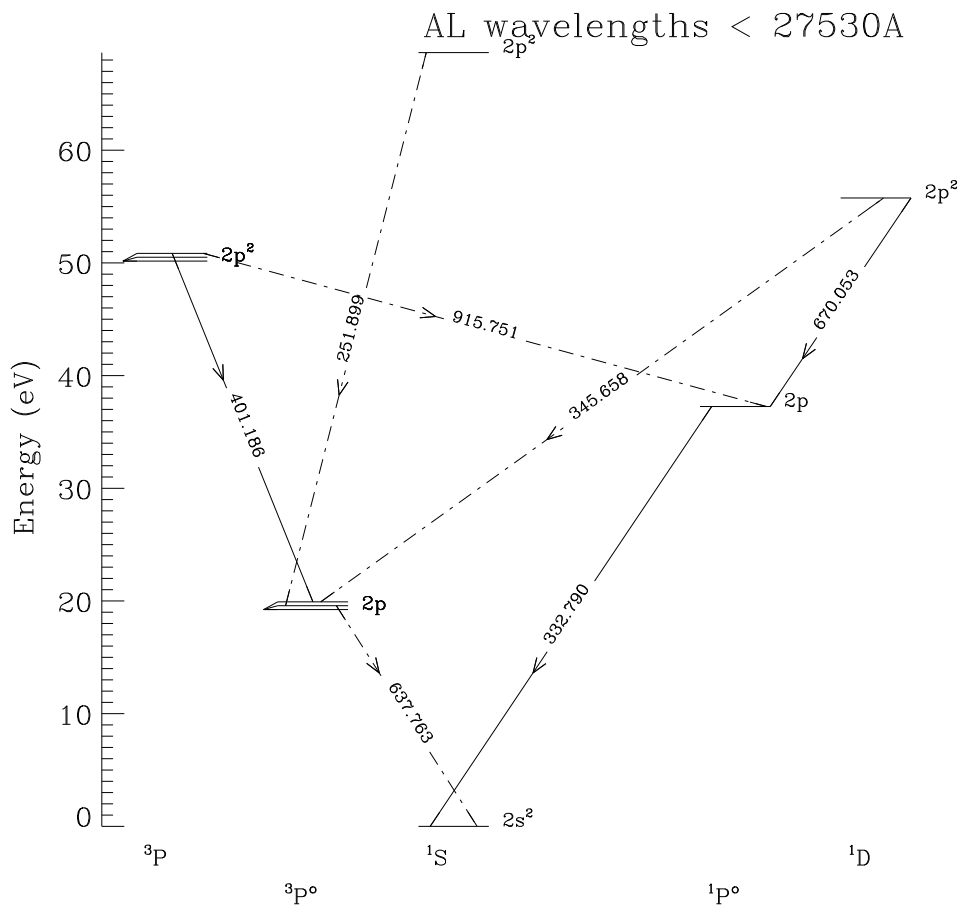
Figure 2: *A term diagram of the levels of Al X, of the beryllium isoelectronic sequence. Just the main lines of each multiplet are marked.*

2.5   A note on transition probabilities

A few words of explanation of transition probabilities are warranted. Einstein A and B coefficients as well as oscillator strengths are stored by the HAOS-DIPER (in structure trn, see section 4.4.4), but only the oscillator strengths are stored in the database files. This parameter choice was made because the vast majority of transitions in the database are E1 transitions for which oscillator strengths have a clear physical meaning, being directly related to quantum mechanical quantities (specifically, the "line strength" S_{ij} between levels i and j), and the strength of a "classical" oscillator (e.e., Cowan 1981). In contrast, the Einstein coefficients contain extra dependencies of wavelength, making their values less directly related to the quantum mechanics and highly dependent on ionic charge, for example. Thus, the behavior of oscillator strengths along series of terms or along isoelectronic sequences, enables one to gain some understanding of particular quantum processes in a simple fashion (e.g., Dufton and Kingston 1981).

Customarily, however, oscillator strengths are reserved for permitted transitions, and A coefficients are used for forbidden transitions (e.g., see the NIST online monograph on atomic spectroscopy[9]). In HAOS-DIPER, the Einstein A coefficient is related to the absorption oscillator strength, for *all* transitions, via

$$A_{ji} = \frac{6.6702 \times 10^{15}}{\lambda_{ij}^2} \frac{g_i f_{ij}}{g_j} \tag{1}$$

with λ_{ij} the wavelength of the transition in Å. For forbidden transitions (both magnetic dipole M1 and electric quadrupole E2), the A coefficients from the original sources are used to compute oscillator strengths via eq. (1), which are stored in the database. These oscillator strengths no longer have the same physical meaning (the "strength of a classical oscillator") as they do for E1 transitions, indeed they are simply dimensionless parameters parameterizing the transition probability via eq. (1). This is made clear by considering multipolar transitions of order n, $n = 1$: dipole, $n = 2$: quadrupole. The A-coefficient is proportional to $S_{ij}\lambda_{ij}^{-(2n+1)}$. Thus, only when $n = 1$ is f_{ij} simply related to quantum mechanical quantities.

The oscillator strengths f_{ij} remain useful, even for the forbidden transitions, because the thermodynamic relationships between the Einstein coefficients,

$$B_{ji} = \frac{2hc}{\lambda_{ji}^3} A_{ji} \tag{2}$$

$$g_i B_{ij} = g_j B_{ji}, \tag{3}$$

hold universally, irrespective of whether a transition is permitted or forbidden. Thus, use of f_{ij} via equations (1), (2), and (3) for all transitions guarantees that opacities and radiative rates, induced and spontaneous, are correct.

---

[9]http://physics.nist.gov/Pubs/AtSpec/index.html

3   Getting started

Access to the package is through the HAO website:

    http://www.hao.ucar.edu/modeling/haos-diper/

The files are stored in a compressed `tar` file whose directory structure is as follows

```
diper/
diper/AAAREADME
diper/data/
diper/doc/
diper/idl/
diper/setup/
diper/SUMMARY
diper/VERSION
diper/zdbase/
```

Installation instructions are in the `AAAREADME` text file in the main `diper` directory. This reference guide you are reading is found in the `doc` subdirectory. Text data files are found in the `data` subdirectory, and the Lindler database files are in `zdbase` (refer to sections 4.2 and 4.3). `setup` contains some files which make the package compatible with the SSW. `idl` contains the `HAOS-DIPER` IDL procedures.

Before running the `HAOS-DIPER`. it is necessary to set up system variables and initialize other variables, this is done using

IDL> diper	; better to put this in IDL_STARTUP file.
IDL> @cdiper	; this too, it gives you access to diper structures

Upon the first call, `diper` will open an XTEXT window displaying messages from the `HAOS-DIPER` as it is running[10]. If the messages pass too quickly to see, they are also logged in a file in the working directory or folded called `diplog.xxx` where `xxx` is a string specifying the system time. This file is continually updated during runtime, and can be examined at any time. As noted above, it's best to place the first `diper` command into your IDL_STARTUP file. Perhaps you always want to work with a certain regime or certain approximations, in which case the keywords `regime` and `approx` can be specified in IDL_STARTUP (see section 2.2).

The main procedure for loading data into `HAOS-DIPER` for further manipulation/ calculations is

IDL> diprd,element,[ions]	; `element` is an integer atomic number or a shorthand element name, such as 'He'. `ions` [recommended but optional] is an integer or a two element integer array. See text

---

[10]An XTEXT window is used provided X windows can be displayed and provided that the `IDL` system variable `!d.name` equals 'X'. If this is not the case, then the messages are sent to the command screen. This is not usually helpful because `HAOS-DIPER` produces quite verbose messages.

diprd does quite a lot more than just load data. For example, when the optional input parameter `ions` is omitted, HAOS-DIPER reads all data for all ion stages of the element (that would be 27 for iron!). The `ions` parameter can be used to limit which ion stages to read in, for example both of the following cases are acceptable:

```
IDL> diprd,'fe',9              ; store Fe IX and the ground level of Fe X
IDL> diprd,'fe',[9,14]         ; store Fe IX, X, XI, XII, XIII, XIV and the ground level of
                                 Fe XV
```

When `diprd` tries to read data for an ion for which no data exist in the database, it will "fill in" the missing ion's ground level (unless the `nofill` keyword is used in `diprd`). To get a feel for how `diprd` works, it is recommended that the new user run several "demos", to get familiar with the data structures and running some programs. This is done using

```
IDL> diper,demo=nn             ; nn is an integer between 1 and 5,
```

and the new user should start with `nn=1` and go through the demos in sequence. This document is a reference guide, and the demos can serve as a user guide.

The following procedures should be sufficient to begin work with the HAOS-DIPER:

```
IDL> diper                     ; basic control and information of diper behavior
IDL> diprd                     ; read data into IDL variables
IDL> level                     ; list, remove atomic levels
IDL> trans                     ; list, remove radiative transitions
IDL> col                       ; list, remove collisional transitions
IDL> td                        ; plot term (Grotrian) diagrams
IDL> ltep                      ; get LTE population densities
IDL> sesolv                    ; solve statistical equilibrium equations
IDL> timeser                   ; solve time evolution of atomic levels
IDL> idspec                    ; identify features on a plotted spectrum
```

All of these procedures have keywords and inputs which can be found using the IDL routine `doc_library` and the SSW IDL procedure `chkarg`.

Note that, if atomic levels with indices `index` are removed using

```
IDL> level, del=index                        ; remove levels from atomic model
```

then there is no need to remove associated collisional or transition data using `col` and `trans`, this is automatically taken care of.

The data can also be manipulated directly (for examples, see section 4.5) once the data are read and made available using

```
IDL> @cdiper                   ; make the basic structures atom, lvl, trn, col
                                 available
IDL> diprd,'he'                ; read data for all helium ions
IDL> help,/structure,lvl       ; look at the structure called lvl, for example
```

```
** Structure LVL, 18 tags, length=100, data length=96:
   EV                 DOUBLE            0.0000000
   LABEL              STRING      ' 1S2 1SE 0                              '
   ION                INT               1
   G                  FLOAT             1.00000
   COUPLING           STRING      'LS'
   GLANDE             FLOAT             1.00000
   N                  INT               1
   EFF                FLOAT             0.743728
   SMALLL             INT               0
   ACTIVE             INT               2
   TSP1               INT               1
   BIGL               INT               0
   PARITY             STRING      'E'
   TJP1               INT               1
   TERM               INT         Array[3]
   ORB                INT         Array[3]
   META               INT               1
   REF                STRING      'Fuhr et al.  1999  NIST Atomic Spectra Dat'...
```

IDL> print,level(0:2).label   ; look at the labels of the first three levels, for example.

```
 1S2 1SE 0                              1S 2S 3SE 1
 1S 2S 1SE 0
IDL> print,trn(0:2).alamb
      625.56270       601.40413       591.41198
```

IDL> print,trn(0:2).alamb   ; look at the wavelengths labels of the first three
                                 transitions, for example.

```
        625.56270       601.40413       591.41198
```

The HAOS-DIPER structures are described below.

4   Data in `HAOS-DIPER`

Atomic data are stored as files using D. Lindler's database system, and in some plain text files. The plain text files contain data needed to evaluate "bound-free" collisional process of electron impact ionization, ionization and recombination by charge transfer, and data for radiative and dielectronic recombination. The database files contain energy level data, data for "bound-bound" processes (oscillator and collision strengths), and bound-free processes (photoionization cross sections).

4.1   Data sources

The source for any particular datum is contained in the `xxx.ref` where `xxx` is one of the data structures (`lvl`, `trn` or `col`) discussed below. The data in `HAOS-DIPER` have been adopted from several sources.

– For charged ions and neutral H and He, the vast majority of energy level data, bound-bound radiative and electron impact transition probabilities are taken, by kind permission, from version 5.2 of the `CHIANTI project` (Landi et al. (2006))[11].

– For neutral atomic species (except H and He), data have been taken from the NIST spectroscopy database (Ralchenko et al. 2005, Ralchenko 2005), including only those levels for which transition probability data exist[12].

– For neutrals, measurements for electron impact excitation are generally available for only certain transitions (e.g., Rountree 1977), and calculations present special challenges (Seaton 1962b) which mean that, unlike charged ions, theoretical cross sections are generally unavailable for most neutral atomic species. The current version of `HAOS-DIPER` can be used (with `!APPROX`) to adopt the semi-empirical approximation from Van Regemorter (1962) and the "impact approximation" of Seaton (1962a), with priority given to the latter (where it is arguably more accurate).

– Photoionization cross sections are entirely from the `OPACITY` project (Seaton 1987), re-sampled so that just 75 wavelengths points are stored. The sampling has been done to preserve the integrals over the cross sections including the resonance structure. Thus, much of the resonance structure is lost. The detailed frequency dependent cross sections in `HAOS-DIPER` are inaccurate, it is only in a crude wavelength-integrated sense that these data can be used. This is acceptable in the following senses: First, the `OPACITY` project photoionization cross sections have not only uncertainties in magnitude but also in the positions of resonances, i.e. these data

---

[11]The levels above the first ionization potentials (contained in `CHIANTI`'s "dielectronic" datasets, `fe_10d.elvlc` for example), were omitted.

[12]In this way an attempt has been made to provide a dataset for which meaningful rates can be computed, similar to the philosophy behind the `CHIANTI` project

contain uncertainties both in wavelength as well as cross sections. Second, because recombination involves integration over functions smooth compared with autoionizing resonance widths (see equation 19), the effects of resonances on recombination are accounted for by HAOS-DIPER, and this is why the sampling was done (see figure 13). The OPACITY project computed cross-sections for LS-coupled terms, and so HAOS-DIPER distributes the cross sections between the different levels in a manner which conserves the total probability of photo-ionization and recombination[13]. The way the HAOS-DIPER cross sections are derived is illustrated in the typical example shown in Figure 3.

---

[13]This approximation should be removed, but it will not affect results provided that recombination rates are much smaller than other collisional rates for the individual levels involved. This is usually the case, except for photoionized plasmas or transient, recombining plasmas, for levels in multi-electron configurations.
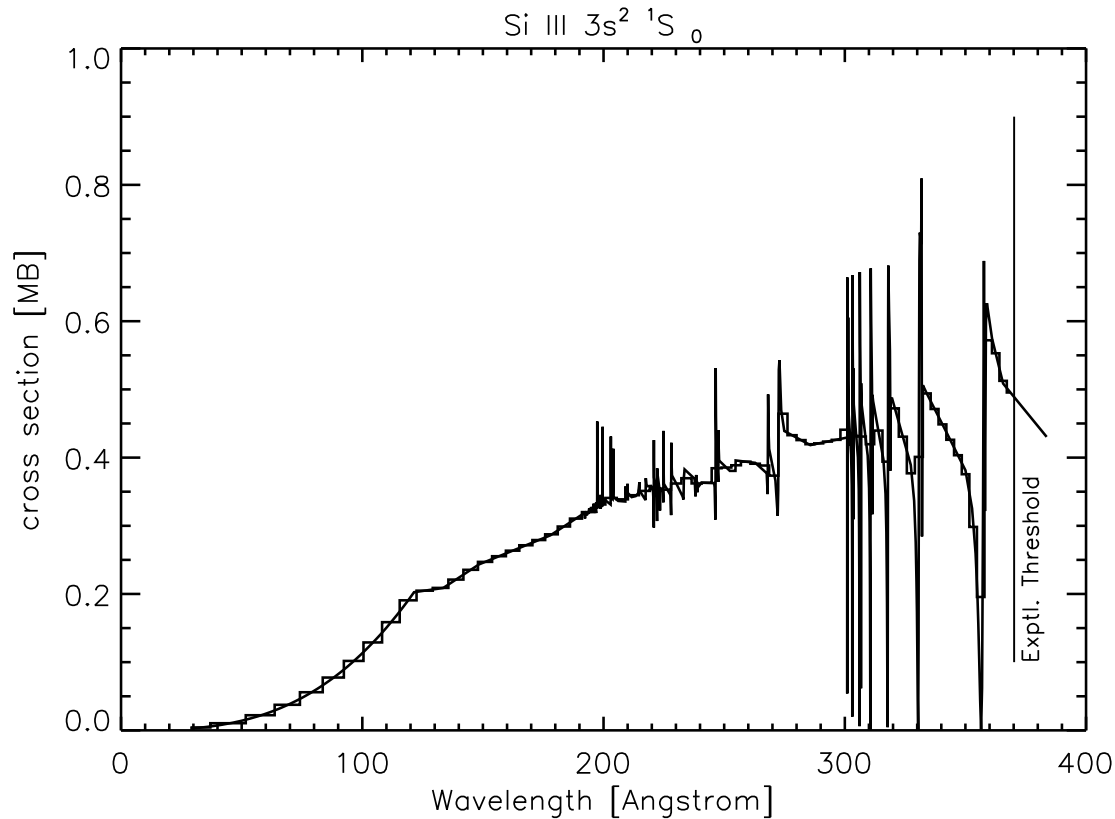
Figure 3: *The photoionization cross section of the ground level of Si III ($3s^2$ $^1S_0$) is shown in MB (1MB $\equiv 10^{-18}$ cm^{-2}) as a function of wavelength in Å. The* OPACITY *project data are shown as lines, the* HAOS-DIPER *data, derived from the* OPACITY *project data, as histograms. The histograms were determined such that the total area underneath each block of the histogram equals the total area of the original data computed between the same limits. The bin widths for the* HAOS-DIPER *data were determined such that there is a larger number of points near threshold than at higher energies.*

– Cross sections and rate coefficients for bound-free collisional ionization by electron impact from levels in ground terms are taken from the compilations[14] of Arnaud and Rothenflug (1985) and Arnaud and Raymond (1992). Maxwellian-averaged electron impact ionization rates for excited levels are computed using general approximations listed in section 2.2.

– Charge transfer with atoms and ions of the abundant species H, H^+, He, He^+, He^{2+} is treated as in Arnaud and Rothenflug (1985).

– Recombination data, when the use of rate coefficients is required (`!REGIME=0`, or when no photoionization data exist) are from the compilation of Shull and Steenberg (1982), corrected for some errors, and based on earlier work of Aldrovandi and Pequignot (1973).

The `CHIANTI` project has done an enormous amount of work compiling, checking, and making generally available data for many charged ions of astrophysical interest (Dere et al. 1997, Landi et al. 2006). Their database consists of a critically assessed set of data for each ion, combining observed energy levels, some measured and/or computed radiative transition probabilities, and a largely theoretical set of electron and proton impact excitation rates. The `CHIANTI` energy level data are largely from the NIST compilation of spectral data (Ralchenko et al. 2005). Data for proton collisions between bound levels are currently not included in `HAOS-DIPER`, but some important charge transfer collisions involving protons are.

4.2   Text files: particle impact ionization and recombination

In the `data` subdirectory of the main `HAOS-DIPER` installation directory, several text data files exist

`ar85ci.dat`	data for electron impact ionization
`ar85ct.dat`	data for charge transfer rates of ionization and recombination

The user will rarely have to be concerned with these data as they are handled in a straightforward way by `HAOS-DIPER`, using `diprd` (and `atomrd`). The files `ar85ci.dat` and `ar85ct.dat` contain data compiled by Arnaud and Rothenflug (1985), with data for iron ions updated by Arnaud and Raymond (1992), for "direct" electron impact ionization, and for charge transfer processes for collisions of atomic ions with atoms and ions of H and He. By "direct" ionization, it is implied that no doubly excited states are included in the process of ionization, in contrast with autoionization (see below). When these data are read from the files, using `diprd` or `atomrd`, the structure `col` is modified to include these ionization and recombination processes. These data can

---

[14]These cross sections can also be used when non-Maxwellian electron distribution functions are present.

be examined by looking at the `col.key` variable (see below), where entries such as `AR85CI` and `AR85CT` will be present.

Ionization by autoionization following excitation is treated in the manner described by Arnaud and Rothenflug (1985), and appears as entries with `col.key` values of `AR85CEA`. Evaluation of the rate coefficients for this process is hard-coded into the relevant routine (`crat.pro`), being dependent on the charge and isoelectronic sequence of the target ion or atom.

Recombination rate coefficients are taken from data from Shull and Steenberg (1982), corrected for several errors, and these are read from the database file `shull82`. Recombination using rate coefficients must be handled carefully, the scheme used by `HAOS-DIPER` is outlined in the Appendix. `HAOS-DIPER` includes approximate corrections to dielectronic recombination due to finite density effects, by using trial-and-error fits to the behavior seen in the calculations of Summers (1974a). Some details of the way `HAOS-DIPER` handles this are described in the Appendix, refer to section A.4. This treatment is far from ideal, but significant improvements involve large scale atomic calculations beyond the scope of the `HAOS-DIPER` (see the calculations made by Summers 1974b, Summers 1974a, Badnell et al. 2003, for example).

4.3   Database files: energy levels, bound-bound transitions

The database files are in the `zdbase` subdirectory of the main `HAOS-DIPER` installation directory. Lindler's software provides interface routines to these data. For example,

```
IDL> dbhelp                         ; list available database files
```

The `HAOS-DIPER` database files mostly begin with `atom_`, but include `abund` and `shull82`:

```
abund            atom_bb          atom_bf          atom_bib
atom_cbb         atom_ip          atom_lvl         shull82 ...
```

Depending on the task at hand, the user will not need to work with the routines supplied by Lindler, such as `dbopen`, `dbclose`, `dblist`, `dbext`, although the user can certainly do so. Usually, the data should be extracted using `diprd` and then the stored data in structures `atom`, `lvl`, `trn` and `col` can be manipulated as desired, and used for calculations. An IDL procedure `isostr.pro` is used to extract data for different ions along isoelectronic sequences **The user should not set the Lindler system variable** `!PRIV` **to anything other than zero**, because then the database data are protected.

To list the variables stored in individual database files, use `dbhelp,1` after opening the database:

```
IDL> dbopen,'atom_bb,atom_bib'              ; open bound-bound transition and
                                              bibliographic database files. atom_bib is
                                              linked to atom_bb
```

```
IDL> dbhelp,1                                    ; use 1 for more information
IDL> dbclose                                     ; close database files
```

This gives as output:

```
----- ATOM_BB  HAOS-DIPER:  Bound-bound transition data
    ITEM                TYPE              DESCRIPTION
ENTRY               int*4    Entry or Record Number
F                   real*4   Absorption Oscillator Strength
WL                  real*8   Wavelength of transition (\AA{} in vacuo).
F_LAB_J             int*2    Index of upper level in atom_lvl.
F_LAB_I             int*2    Index of lower level in atom_lvl.
TYPE                char*4   Type ('E1','M1','E2','M1E2','F')
F_ACC               int*2    Accuracy:  %(*100)
ATOM                int*2    Atom Name/Number (i.e. 6 for carbon)
ION                 int*2    Ion Spectrum Number (i.e. 2 for C II)
ISOS                int*2    Isosequence (= ATOM-ION+1)
BB_REF              int*2    Data Reference in atom_bib.dbd file
TIME                char*13  Data input date and time.


----- ATOM_BIB  HAOS-DIPER:  Bibliography
    ITEM                TYPE              DESCRIPTION
ENTRY               int*4    Entry or Record Number
BIB_REF             char*480 Short-handed Reference


-------  Indexed Items ------
F                       WL                      ATOM
ION                     BB_REF                  BIB_REF


----- Pointer Information ----
ATOM_BB.BB_REF ---> ATOM_BIB (presently opened)


data base contains      45826 entries
```

Any of the available database files can be examined in this way, including of course the HAOS-DIPER database files atom_bb, atom_bf, atom_cbb, atom_ip, shull82.

   It should be noted that the atom_cbb and atom_bf files contain "compressed" forms of Maxwellian-averaged collision strengths and photoionization cross sections respectively, which are respectively "de-coded" using IDL procedure ups_bt (from the CHIANTI project) and IDL function picom.

To list a summary of the data stored in the HAOS-DIPER database files, type

```
IDL> diper,/summary          ; list available level and transition data
```

Which lists the names of the atomic ions for which data are available, the number of

bound levels in each ion, the maximum principal quantum number for each ion, the number of radiative transitions and the number of collisional rate coefficients. The first few entries of this table may look like

```
Summary of data in HAOS-DIPER
NK=number of levels
MAX QN=maximum principal quantum number
NLINE=number of line transitions
NCOL=number of collisional transitions
NBF=number of bound-free radiative transitions (photoionization cross secns)
ION            NK   MAX QN   NLINE    NCOL     NBF
H I            25     5        75       54      55
HE I           49     5       187      268      43
HE II          25     5        68       45      15
C I           173     8      1298        0     220
C II           18     3        46       75      30
C III          20     3        49      184      50
C IV           15     4        18       14      14
C V            47     5       158      133      23
C VI           25     5        68       47      15
N I            26     3        72      115     149
N II           23     3        86      245     111
etc...
```

4.4   The way `HAOS-DIPER` **handles data**

The data are extracted from the database and text files, and are stored as IDL structures. These structures are called `atom`, `lvl`, `trn` and `col` and are accessible in IDL by typing

```
IDL> @cdiper              ; make the basic structures atom, lvl, trn, col
                               available
IDL> help, /structure,atom    ; look at the structure called atom, for example
IDL> print,atom.atomid        ; look at the atomid variable, as another example
```

Note that data are stored in these structures by `diprd` *one atomic species at a time*, but the structures may contain many different stages of ionization.

Users of the non-LTE radiative transfer program `MULTI` Carlsson (1986) will recognize that the `HAOS-DIPER` inherited variables from this program, and added some more.

4.4.1   The `atom` **structure**

The `atom` structure is a scalar having just 6 "tags". It is defined through

```
IDL> atom={atom,atomid:'',abnd:0.0,awgt:0.0,nk:0l,nline:0l,nrad:0l}
```

`atom.atomid` contains the symbol for the element stored, for example, 'Ne' for neon.
`atom.abnd` contains a number used for the elemental abundance (logarithmic scale,
H=12). To change it simply set `IDL> atom.abnd=xxx` *after* running `diprd` or `atomrd`.
`atom.awgt` contains the atomic weight in units where C=12. `atom.nk`, `atom.nline`
and `atom.nrad` are integers containing the number of atomic levels stored, the num-
ber of bound-bound transitions stored, and the total number (bound-bound plus bound-
free) transitions stored.

4.4.2   The `lvl` structure

The `lvl` structure is an array of `atom.nk` elements with 19 tags, defined through

```
IDL> lvl = {lvl,ev:0.d0,label:'',ion:0,g:0.0,coupling:'',glande:0.,$
        n:0, eff:0.0, smalll:0, active:0, tsp1:0, bigl:0, $
        parity:'', tjp1:0, term:intarr(3), orb:intarr(3), meta:0, ref:''}
```

   The following table describes these variable types and meanings:

`lvl.ev`	REAL*8 level energy in eV
`lvl.label`	CHARACTER*35 entire label of the energy level
`lvl.ion`	INTEGER core charge (=1 for neutrals, 2 for singly charged ions..)
`lvl.g`	REAL*4 level degeneracy
`lvl.coupling`	CHARACTER*2 ('LS', 'JJ' or 'PA') is the coupling scheme used in describing the quantum numbers in the level's label
`lvl.glande`	REAL*4 for LS coupled levels, the Landé g-factor of the level in the LS coupling approximation, otherwise zero for other levels
`lvl.n`	INTEGER principal quantum number of the outermost electron(s)
`lvl.eff`	REAL*4 effective quantum number of the level
`lvl.smalll`	INTEGER angular momentum quantum number for the electrons in the outermost sub-shell (e.g., 1 for a "p-electron")
`lvl.active`	the number of electrons in this sub-shell
`lvl.tsp1`	INTEGER $2S+1$ LS coupled quantum number of the atomic term $^{2S+1}L_J$
`lvl.bigl`	INTEGER L LS coupled quantum number of the atomic term $^{2S+1}L_J$
`lvl.parity`	CHARACTER parity of the level
`lvl.tjp1`	INTEGER $2J+1$, J is total angular momentum quantum number

`lvl.term`	INTEGER translating spectroscopic term = (2S+1)*100+(2L+1)*10+P, P=0 (even) =1 (odd) parity
`lvl.orb`	INTEGER translating orbitals = 100*n+10*l+a, n=principal qn, l=ang. mom. qn, a= number of electrons
`lvl.meta`	INTEGER (values 0 or 1) describe a whether the level is deemed "metastable" as determined by the value of `!REGIME`
`lvl.ref`	CHARACTER variable containing bibliographic references

The `label` tag is expected to use the following format, (this is taken from the header of the `lab2int.pro` procedure):

```
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
For LS coupling the label is usually of the form:
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;

 ... 3P4 (3P) 3D  4DE 7/2'
     ___ ____ __  ___ [_]
 1   n-4 n-3  n-2 n-1  n
where the underlined regions are treated as "words"
Word:
anything else other than closed sub-shells/shells
n-4               parent's outermost orbital
n-3               (if present, with "(" or ")")  parent term
n-2               outermost orbital
n-1               TERM
n                 J
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
    For jj coupling (non-equivalent electrons)
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
  3S2 3P (2PO) 6P (1/2,3/2)E 1
___ __ _____ __ _____ [_]
 ...              n-1         n
here, the j=1/2 2PO term of Si II and j=3/2 of the 6p electron
(contained in the (1/2,3/2) string) are coupled to give a
total ang mom J=1
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
    For pair coupling
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;

 2S2 2P (2PO) 4F 2[5/2]E 3
 ___ __ _____ __ _____ [_]
  ...              n-1       n
```

```
 here, the J1=5/2 level of the (2PO) term of C II couples with a
 4f electron (s2=1/2) to produce J=3.  This is encoded in the string
 (2*s2+1)[J1]
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
Lastly, the label can also take the form:
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;

 3P6 3D6 (3F) 4S 4P (3PO) 3FO 4

 in which the two ``parent'' terms (3F) (3PO) couple to form
 the final 3FO term. This type of coupling is common in the
 iron group.
```

   If the label tag is one of these formats, then it will be consistent with the quantum numbers stored in the database[15] In fact the procedure `qn.pro` would be able to compute new values of the quantum numbers from these labels. Using `qn` is neither needed nor recommended when using `diprd`, but `qn` is called by `atomrd`.

4.4.3   Encoding of quantum numbers

The encoding of quantum numbers into integers follows the example set by the `OPACITY` project, and is done by the `lab2int.pro` procedure). To illustrate the meaning of the `term` and `orb` tags, as an example, consider the level described by the label `'3P4 (3P) 3D 4DE 7/2'`, which in standard notation is $3p^4$ (^3P) $3d$ $^4D_{7/2}$. Then the mapping of the label to the quantum numbers is as follows:

```
    3P4        (3P)        3D        4DE        7/2
    orb(1)     term(1)     orb(0)    term(0)    tjp1
    314        310         321       420        8
```

Note that for the terms, the encoded integers are of the form $(2S + 1)LP$, where the parity P is zero (even) or 1 (odd). This is the convention used by the `OPACITY` project. For the orbitals, the encoding is nLa where n is the principal quantum number, L the total orbital angular momentum, and a is the number of equivalent electrons. Thus, for this case, we have `lvl.term(0)=420`, `lvl.term(1)=310`, `lvl.orb(0)=321`, `lvl.orb(1)=314`. The integers `lvl.term(2)` `lvl.orb(2)` are both zero because only two terms and orbitals are listed in the label. These third components are set to zero, with the assumption that beneath these outer electron shells there are only closed sub-shells. This closed shell assumption is related to the basic "low-energy" approximation built into the `HAOS-DIPER` (see section 1.3).

---

[15]There is just one exception: in the database the parentheses "(" and ")", and square brackets "[" "]" are replaced by "{", "}", "|" and "!" respectively, because the parentheses and square brackets have special meanings in Lindler's software. The procedure `labcnv` converts from the database format to that given above, and vice versa. `labcnv` is called by `diprd.pro, atomrd.pro` .

It is clear that if any of the quantum numbers are greater than 9, then this scheme fails. For example, a $3f^{11}$ orbital would be encoded as 341 (=3*100+3*10+1*11), which would incorrectly be decoded as a $3g$ orbital. Hence the restriction on quantum numbers mentioned in section 1.2.

4.4.4   The `trn` structure

The `trn` structure is an array of `atom.nrad` elements with 20 tags, defined through

```
IDL> trn={trn,irad:0,jrad:0,alamb:0.d0,f:0.0,qmax:0,q0:0.,nq:0,$
     q:fltarr(mq),wq:fltarr(mq),frq:fltarr(mq),alfac:fltarr(mq),$
     ga:0.,gw:0.,gq:0.,a:0.,bij:0.,bji:0.,$
     type:'',multnum:0,ref:''}
```

The parameter `mq`, which sets the maximum number of frequencies in any transition which can be stored, is set upon startup `diper.pro` to 60 (parameter `mcol` is likewise set to 40), and is stored in a common block accessible at any time using

```
IDL> @cdiper                    ; make common block variables accessible
```

To change this value to store more frequency points one should edit `dipdef.pro`, exit IDL and restart. The data stored here refer both to line (bound-bound) and continuum (bound-free) transitions. Note that *all wavelengths are stored* in vacuo, *even though it is traditional to use wavelengths in air for wavelengths in excess of 2000* Å. The procedures `airtovac` and `vactoair` convert between these two standards. Where wavelengths are plotted or printed, they are by default in vacuo below 2000 Å, and in air above this. For the *bound-bound* or "line" transitions

`trn.irad`	INTEGER index (in `lvl` structure) of the lower level
`trn.jrad`	INTEGER index (in `lvl` structure) of the upper level
`trn.alamb`	REAL*4 vacuum wavelength of the line transition in Å
`trn.f`	REAL*4 absorption oscillator strength
`trn.ga`	REAL*4 radiative damping line broadening parameter
`trn.gw`	REAL*4 Van der Waals damping line broadening parameter
`trn.gq`	REAL*4 Stark damping line broadening parameter
`trn.a`	REAL*4 Einstein A coefficient
`trn.bij`	REAL*4 Einstein absorption B coefficient (transition from `irad` to `jrad`)
`trn.bji`	REAL*4 Einstein emission B coefficient (`jrad-irad`)
`trn.type`	CHARACTER transition type: one of `'E1'`, `'M1'`, `'E2'`, `'M1E2'`,`'BF'`
`trn.ref`	CHARACTER variable containing bibliographic references
`trn.qmax`	not defined (for lines)
`trn.q0`	not defined (for lines)

`trn.nq`	not defined (for lines)
`trn.q`	not defined (for lines)
`trn.wq`	not defined (for lines)
`trn.frq`	not defined (for lines)
`trn.alfac`	not defined (for lines)

The `trn.q` tags are concerned with frequency integrations needed to evaluate radiative rates using the scheme of `MULTI` Carlsson (1986), but are not currently used for lines in `HAOS-DIPER`. (The radiative rate coefficients are evaluated in `HAOS-DIPER` using the frequency-independent Einstein A and B coefficients- see the Appendix). The tag `trn.type` identifies the transition as electric dipole (`'E1'`), magnetic dipole (`'M1'`), electric quadrupole (`'E2'`), either `M1` or `E2` (`'M1E2'` - type either `M1` or `E2` but unspecified in the data, just a total transition rate is given), for lines. It is set to `'BF'` for continua. For the *bound-free* or "continuum" transitions, the tags `ga,gw,gq,a,bij,bji` have no meaning, `ilo`, `ihi`, `type`, `ref` have the same meanings as above, but the following tags are different:

`trn.alamb`	REAL*4 vacuum wavelength of the continuum edge in Å
`trn.f`	REAL*4 cross section at the edge in cm^2
`trn.qmax`	REAL*4 if > 0, cross section varies as ν^{-3}
`trn.q0`	not used
`trn.nq`	INTEGER number of frequency or wavelength points given
`trn.q`	REAL*4 array of `trn.nq+1` wavelengths (Å) at which the cross sections are given, beginning at the edge
`trn.wq`	REAL*4 array of `trn.nq` weights for integration of mean intensities and cross sections
`trn.frq`	REAL*4 array of `trn.nq+1` frequencies (Hz) at which the cross sections are given, beginning at the edge
`trn.alfac`	REAL*4 array of `trn.nq+1` cross sections (cm^2), first entry is the cross section at the edge

At present, line broadening parameters by particle collisions (`trn.gw, trn.gq`) are not included in the database.

4.4.5   The `col` structure

The `col` structure is an array with 10 tags, defined through

```
IDL> col={col,nt:0,temp:fltarr(mcol),key:'',ihi:0,ilo:0, $
        lab:'',type:0,approx:0,data:fltarr(mcol),ref:''}
```

The data contain the information needed to determine collisional rates between two levels, with indices `lvl.ihi` and `lvl.ilo`. The data apply to both bound-bound and

bound-free transitions, and the following table describes these variable types and meanings:

`col.nt`	INTEGER number of data points for this transition
`col.temp`	REAL*4 array of `col.nt` elements containing either electron temperatures or equivalent independent variables needed to determine the collisional rate
`col.key`	CHARACTER a keyword describing the type of data stored
`col.data`	REAL*4 array of `col.nt` elements containing, for example, Maxwellian-averaged collision strengths as a function of temperature, or an equivalent parameter
`col.ihi`	INTEGER index (in `lvl` structure) of the upper level
`col.ilo`	INTEGER index (in `lvl` structure) of the lower level
`col.lab`	CHARACTER label containing additional notes
`col.type`	INTEGER transition type (not used in version 1)
`col.ref`	CHARACTER variable containing bibliographic references

4.4.6   The `misstrn` structure

The `misstrn` structure is an array of a number of elements with 20 tags, defined exactly as `trn`. The difference is that `misstrn` contains those transitions belonging to multiplets in the structure `trn`, but whose individual transitions are missing, according to the multipolar selection rules for the total angular momentum J. `misstrn` is computed in `multchk`. Only the tags `alamb`, `type`, `multnum`, `irad`, `jrad` and `ref` are set to non-zero, non-blank values. These transitions are those which are listed in the XTEXT output and in the logfile as in the following example:

```
missing E1 trans.  1S2 4D 2DE 5/2 - 1S2 3P 2PO 3/2
missing E1 trans.  1S2 3D 2DE 3/2 - 1S2 3P 2PO 1/2
```

`misstrn` can be useful if one requires a complete list of lines for each multiplet even though the transition database `atom_bb` is not complete. Thus, while one must be careful with calculations using, e.g., `sesolv` , the following example shows how one might list, or plot in a term diagram, transitions in each multiplet:

```
IDL> diprd,6,1              ; read data
IDL> trnok=trn              ; save original trn
IDL> trn=[trn,trnmiss]      ; build new trn structure
IDL> s=sort(trn.alamb)      ; sort index
IDL> trn=trn(s)             ; sort according to wavelength
IDL> trans                  ; list transitions including missing levels
IDL> trn=trnok              ; restore original trn
```

Note that the `tran.ref` variables listed by `trans` for missing transitions contain the word "missing".

4.5   Modifying, editing the atomic data

Several procedures are provided which enable the user to "edit" the data stored in the basic `HAOS-DIPER` data structures (but not, of course, the database files). An example is that sometimes one wishes to remove levels of no real interest. This can be done using `level,del=i` where `i` is an integer array listing those levels to be removed. As an example, we can remove all levels with a multiplicity > 3 from a given model, as follows:

```
IDL> i=where(lvl.tsp1 gt 3)     ; find indices of levels to delete
IDL> level, del=i               ; remove those levels
IDL> level                      ; list the remaining levels
```

This illustrates one of the strengths of `HAOS-DIPER`: the ability to manipulate the atomic data using the quantum numbers stored in structure `lvl`. The same manipulations can be made using the structure `trn`. For example:

```
IDL> i=where(trn.alamb gt 912); find indices of transitions with wavelength greater than
                                         912 Angstroms
IDL> trans, del=i               ; remove those transitions
IDL> trans                      ; list the remaining transitions
```

Or,

```
IDL> i=where(trn.type ne 'E1'); indices of non electric dipole transitions
IDL> trans, del=i               ; remove those transitions
IDL> trans                      ; list the remaining transitions
```

 These data, once edited, can of course be saved:

```
IDL> save,file='atom.save',$   ; save the edited data
    atom,lvl,trn,col
```

There are two procedures which can be used to write the data to a text file for editing, and to read the data:

```
IDL> atomwr,'atom.text'          ; write the data to text file
unix> emacs atom.text            # edit the file with a favorite editor
IDL> atomrd,'atom.text'          ; read the data from the text file
```

The business of *adding* atomic data is best done by editing the text files written by `atomwr`, for example. It is not recommended that one should add data directly into the database- Lindler's system is a simple not relational database- thus there are no checks that added transitions/levels/ collisional data are going to be fully consistent with the rest of the data.

5   Working with `HAOS-DIPER`

5.1   Statistical equilibrium calculations

Given a set of plasma parameters as input (at least electron densities and temperatures are required), `sesolv` solves statistical equilibrium equations for a given set of atomic levels, read with `diprd`. In the general (nonLTE) case, the statistical equilibrium equations are strongly coupled to those of radiative transfer, but the `HAOS-DIPER` does not include any detailed transfer algorithms- instead this should be handled using other codes for which the data from `HAOS-DIPER` can be used. While there is a capability to examine the effects of transfer very crudely in `sesolv` using escape probabilities (use the keyword `depth` in `sesolv`, if radiative transfer is important it should be solved properly. Refer to section A.2 in the Appendix for more details.

The populations q computed by `sesolv` for each ion are normalized such that the total number density of populations for each element is set to $N_H \mathcal{A}$, where N_H is the population density of hydrogen nuclei (protons and H atoms), and $\mathcal{A}$ is the elemental abundance. N_H is given by the function `hion` which gives the neutral and ionized hydrogen ionization fractions, and by N_e the electron density:

$$N_H = 0.8 N_e / h(1), \tag{4}$$

where $h(1)$ is the second element of the array returned by `hion` (the ionized fraction, $h(0)$ is the neutral fraction). The factor 0.8 ensures that the correct limit is obtained for fully ionized plasmas of astrophysical abundance ($h(1) \to 1$, Allen 1973). Note that $N_H \gg N_e$ at low temperatures where hydrogen is not fully ionized.

`sesolv` is one of the basic procedures which might be called in more detailed calculations by a user. As an example of a calculation which looks into the various approximations concerning some of the more uncertain processes involving, for example, doubly excited states, a typical use of `sesolv` might be

```
IDL> diper,regime=0            ; coronal regime
IDL> diprd,'c',[2,5]           ; store C II- C V and ground level of C VI
IDL> t=4.0+findgen(21)/20.     ; define log10 temperature
IDL> ed=1.e15/10.^ t           ; define electron density
IDL> sesolv,10.^ t,ed,q,elc    ; solve SE equations, return q=population densities, elc
                                   = emission line coefficients
IDL> ionp,t,q,f                ; compute and plot ion fractions
```

This calculation might be repeated using `!APPROX=8`, which sets dielectronic recombination rates to their very low-density values. A comparison of these two cases, for ions of carbon, is shown in the upper panel of Figure 4, where an electron density of $N_e = 10^9$ cm^{-3} was used for the finite density corrections (see sections 5.3 and A.4). This could also be repeated using detailed recombination calculations (`!regime=1`),

for example, to see the differences in the resulting ionization fractions. This comparison for carbon ions is shown in the lower panel of Figure 4. In this case one might also set `approx=2` to see the effects of the missing high-n levels on the ion fractions. The procedure `ionp` returns ion fractions and the results over-plotted (use `doc_library,'ionp'` to see the calling sequence or `chkarg,'ionp'`).
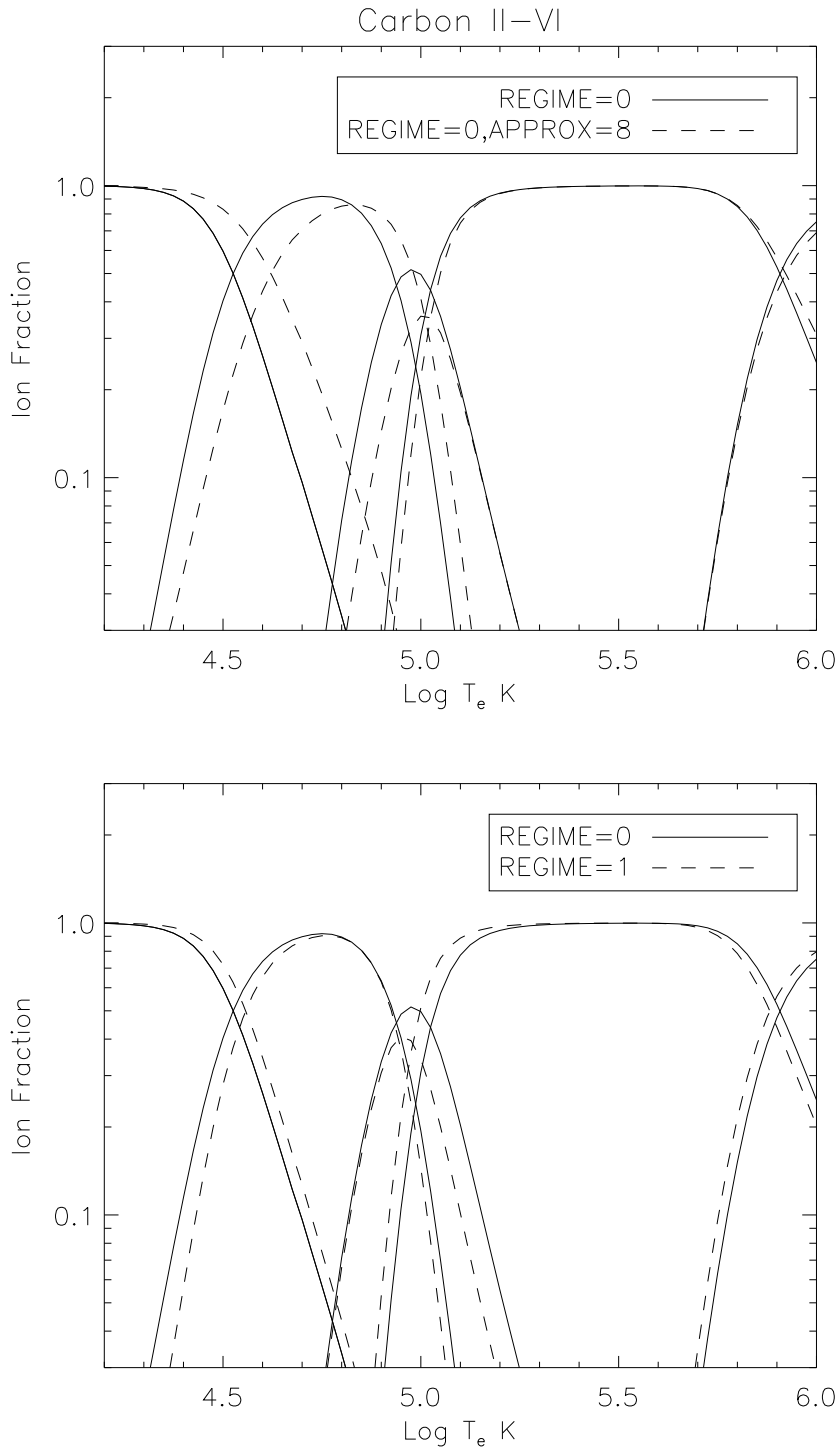
Figure 4: *Ionization fractions are plotted versus electron temperature for ions of Carbon (C II through C VI). The upper panel compares those computed using corrections for density dependent dielectronic recombination (solid line) and those without (dashed line). The lower panel compares those computed using rate coefficients for radiative recombination (solid lines) and those computed in detail using the photoionization cross sections (dashed lines).*

The variables `elc` return the emission line coefficients in units of erg $\mathrm{cm}^{-3}\,\mathrm{sr}^{-1}\,\mathrm{s}^{-1}$. Under optically thin conditions,

$$\texttt{elc} = \frac{h\nu_{ji}}{4\pi}q_j A_{ji} \ \ \mathrm{erg\ cm}^{-3}\,\mathrm{s}^{-1}\,\mathrm{sr}^{-1}. \tag{5}$$

(The equivalent expression, multiplied by 4π, for optically thick lines using the mean escape probability approximation, is given in equation 23). Here, q_j is the population density of level j, h Planck's constant, and ν_{ji} and A_{ji} are the frequency and Einstein A-coefficient of the transition between bound levels j and i.

The emission coefficients `elc` are starting points for a variety of diagnostic procedures commonly applied to optically thin emission lines. This is because integration of `elc` along a given line-of-sight will yield frequency-integrated emergent line intensities from the emitting optically thin plasma. In the simplest diagnostic schemes, ratios of `elc` for different lines as functions of electron temperature and/or electron density are used as well-known "thermometers" (temperature-sensitive line pairs) and "barometers" (density-sensitive line pairs) respectively. Figure 5 shows a term diagram of O IV with four transitions marked: two spin-forbidden transitions whose emission coefficient ratios are sensitive primarily to electron density, and two permitted transitions sensitive primarily sensitive to electron temperature. The emission ratios computed by HAOS-DIPER are shown in figure 6, generated with the the following IDL code:

```
IDL>; density sensitive line pair
IDL> diprd,'o',4,/nofill            ; read data
IDL> ed=10.^(8.0+findgen(40)/9.)  & ; define arrays
   te=ed*0+2.e5
IDL> sesolv,te,ed,pops,elc          ; solve equations
IDL> plot_oi,ed,elc(2,*)/elc(1,*)   ; plot (labels omitted here)
IDL>; temperature sensitive line pair
IDL> te=10.^(4.8+findgen(20)/10.)  &
   ed=10.^11+te*0.
IDL> sesolv,te,ed,pops,elc
IDL> k=where(trn.type eq 'E1')
IDL> plot_oo,te,elc(k(0),*)/elc(k(6),*)
```

It would be an instructive exercise for the student to try to understand why, in simple terms, the chosen ratios would behave qualitatively in the fashion shown in these figures, on the basis of the atomic parameters. Some difficulties in using such line ratios are discussed in Judge et al. (1997) and, for the particular case of O IV, by McIntosh et al. (1998).
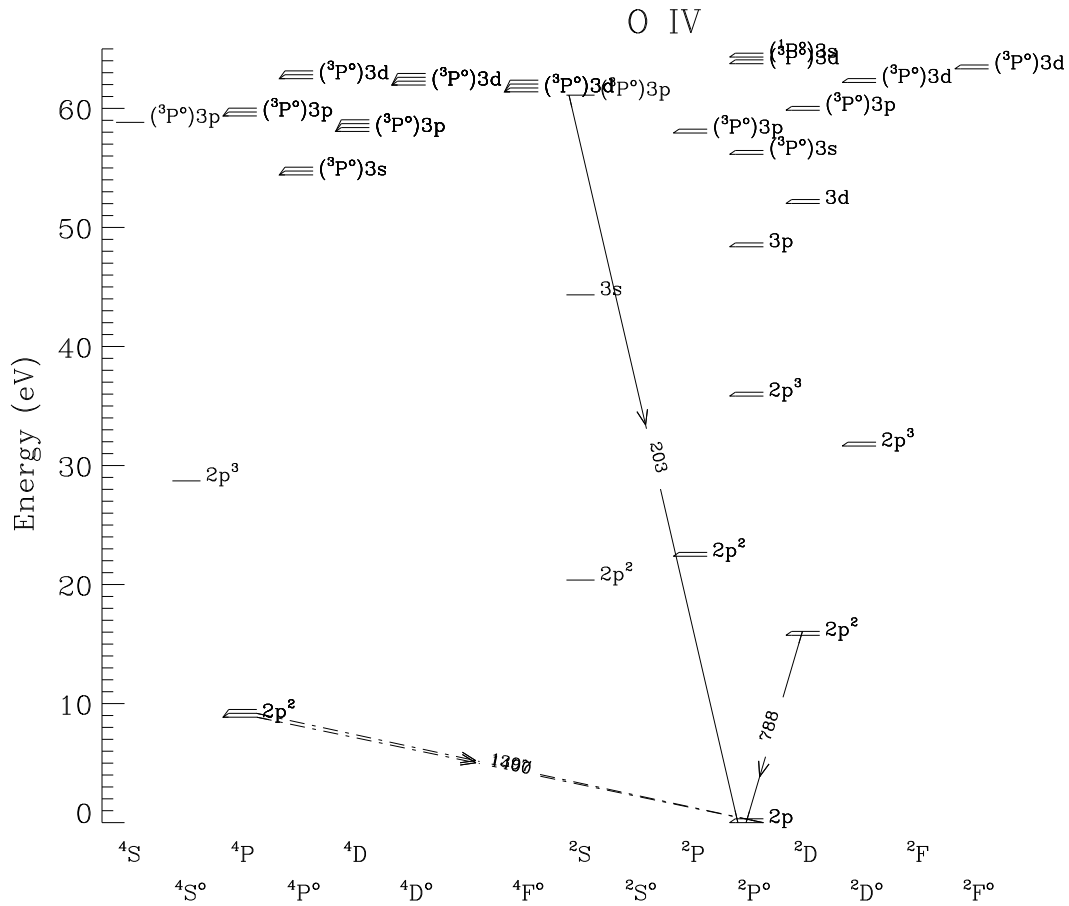
Figure 5: *A term diagram of O IV showing pairs of transitions with emission coefficients sensitive primarily to electron density (spin forbidden transitions, dot-dashed lines) and electron temperature (permitted transitions solid lines), under conditions applicable to the Solar transition region.*
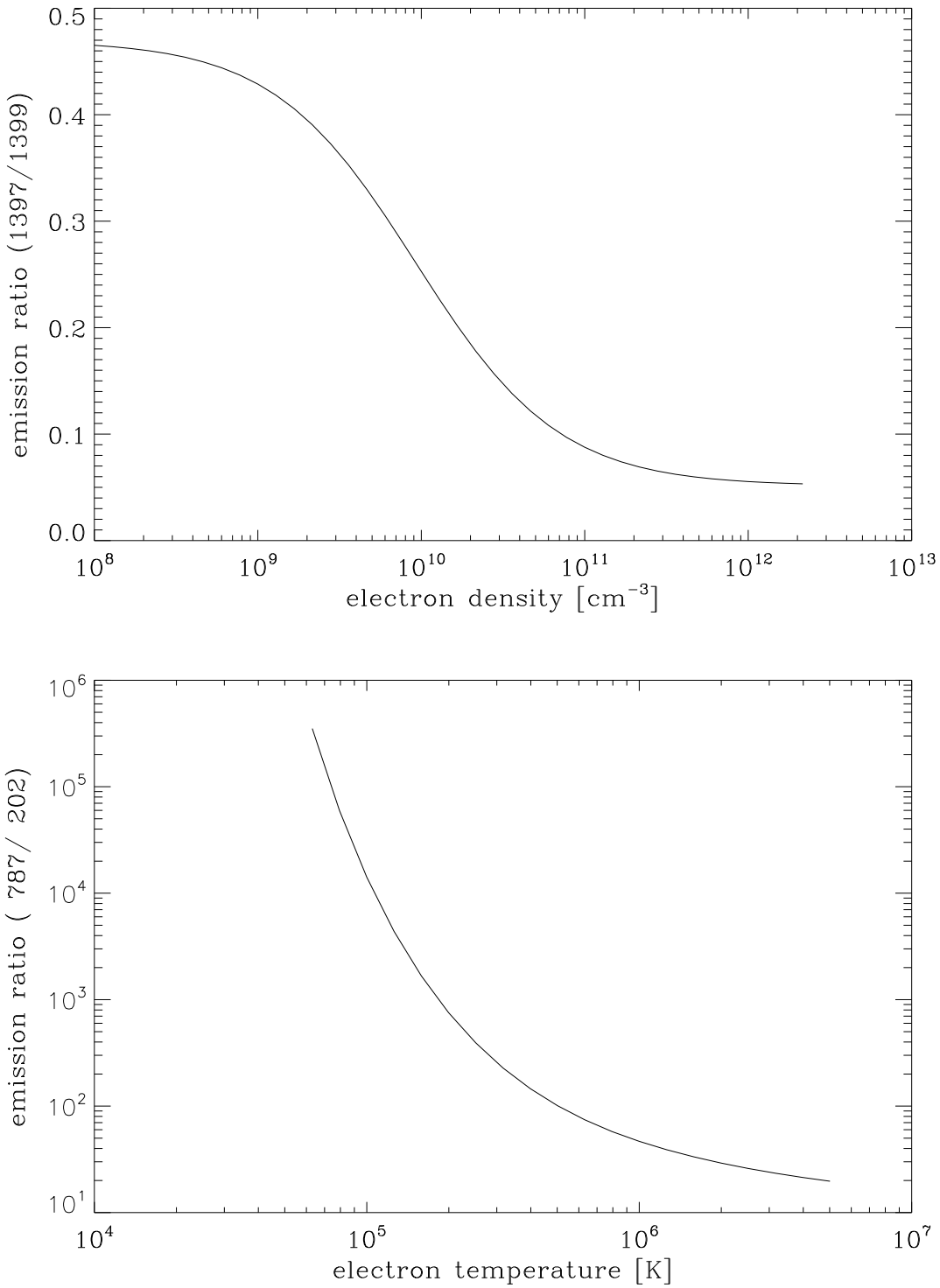
Figure 6: *Results of* `sesolv` *calculations for pairs of lines in O IV whose emission coefficients are sensitive primarily to electron density (spin forbidden transitions, upper panel) and electron temperature (permitted transitions, lower panel), computed under conditions applicable to the Sun. The line ratios are labeled with the line wavelengths in Å units.*

When the `elc` values are multiplied by 4π and summed over all transitions of all abundant elements, this yields the total emission line radiative losses, which when divided by $N_H N_e$ gives the line contributions to the well-known radiative loss function $\Phi(T_e)$ in erg cm^{+3} s^{-1}. The bound-free contributions can be neglected, being a percent or so of these values, which are uncertain to $\pm 10\%$ or more.

With the simple addition of the component due to Bremsstrahlung radiation:

$$\Phi_{Bremss}(T_e) = 1.96 \times 10^{-27} T_e^{1/2} \quad \text{erg cm}^{+3}\text{ s}^{-1},$$

(see e.g. Cox and Tucker 1969, Cook et al. 1989), important above $T_e \sim 10^7$ K, this yields an accurate approximation to the total radiative loss function for equilibrium plasmas.

The use of `elc` for emission measure analysis should be clear to the reader- `elc` is the "kernel" of the integral equation for which the emission measure function is the desired quantity to be obtained by "inverting" the integral equation (see, e.g., Craig and Brown 1976, Craig and Brown 1986 or Pietarila and Judge 2004). The reader may or may not be aware of some of the limitations of emission measure analysis and line ratio spectroscopy. Papers by Judge et al. (1995) and Pietarila and Judge (2004) discuss different problems with solar emission measure analyses, and Judge et al. (1997) and a review by Judge and McIntosh (2000) discuss some more general issues. Lastly, McIntosh et al. (1998) have discussed the formal equivalence of emission measure and line ratio techniques.

5.2   Time dependent calculations

The procedure `tsolv` solves for the time dependence of atomic energy level populations, given an initial state and prescribed thermal parameters as a function of time. The procedure works strictly on optically thin plasmas. Again, refer to the header information (using `doc_library`). `timeser` is a wrapper for `tsolv` in which one can specify the evolution of thermal parameters as a function of time, for example during a flare. The populations q are normalized to maintain the total population of the initial conditions for all later times.

As an example of `tsolv`, figure 7, taken directly from Judge (2005), shows $q_j(t)A_{ji}$, proportional to the radiated power for three transitions of Fe IX, studied in the context a "burst picture" of heating (sudden onset of energy deposition) by Feldman (1992). It includes the 241.7 and 244.9 Å spin-forbidden transitions and the 171.1 Å resonance line. This calculation is for a plasma with fixed $N_e = 3 \times 10^{10}$ cm^{-3}, evolving from an initial state at 7×10^5 K to a final state at 7×10^6 K. The system does not evolve according to Feldman's intuition (being based upon a 2-level atom concept), and curiously the line ratios behave in a manner opposite to those expected by Feldman. Refer to Judge (2005) for details.
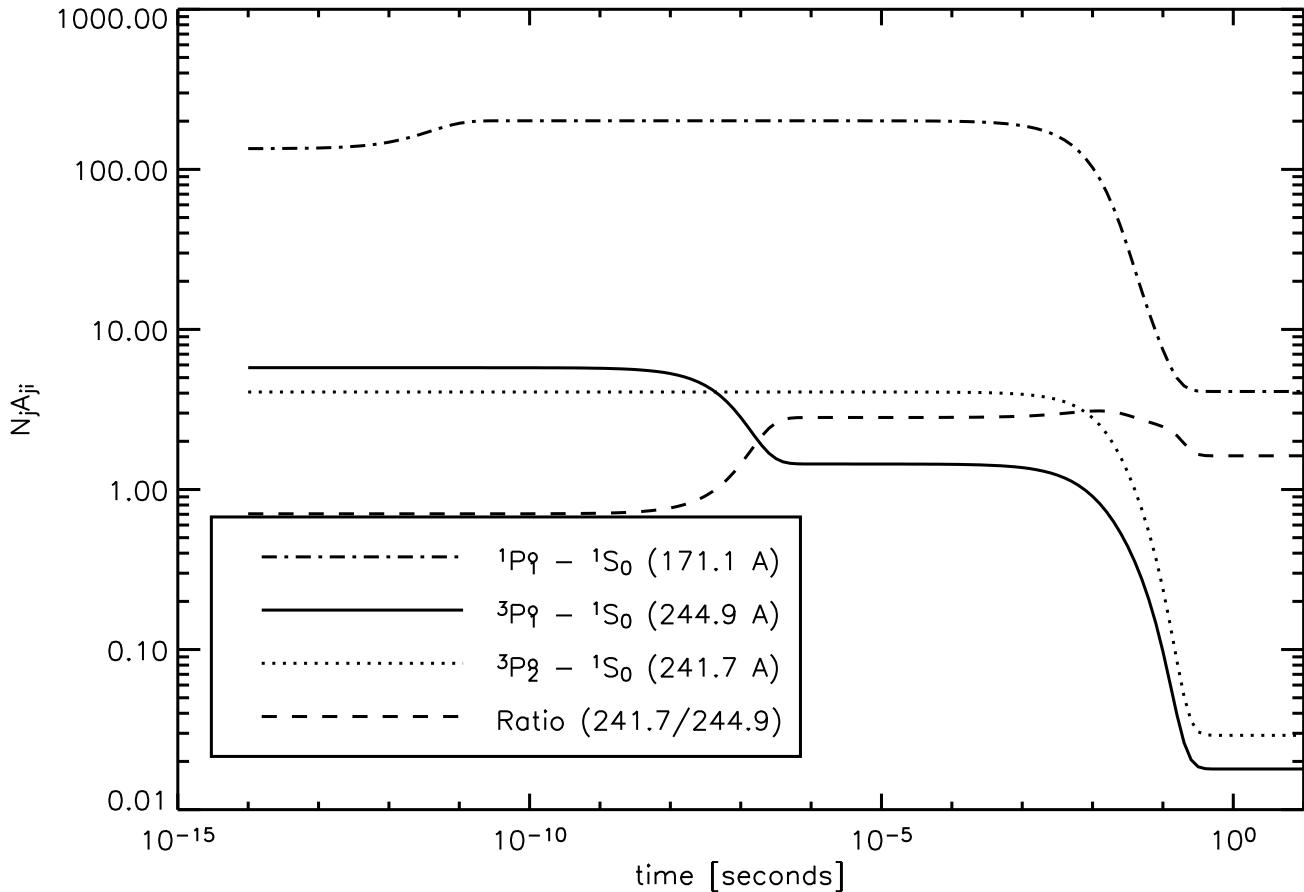
Figure 7: *Results of* `tsolv` *calculations for lines in Fe IX whose ratios may be indicative of impulsive heating, taken from Judge (2005). The figure shows the time evolution of Fe IX level populations, scaled with Einstein A-values of some transitions discussed in the text. The initial statistical equilibrium state has $T_e = 7 \times 10^5$ K, the final state has $T_e = 7 \times 10^6$ K, both for an electron density of 3×10^{10} cm^{-3}. The calculation approximates the behavior of Fe IX ions during a "burst" of heating postulated during flares Feldman (1992).*

The time evolution of atomic systems is discussed in general terms by Judge (2005).

5.3 Treatment of "missing data": use of `!APPROX`

Sometimes it feels like there is never "enough" atomic data. Measurements of energy levels and their properties exist only up to certain values of the principal quantum number, yet an isolated atom has an infinity of bound atomic levels. Data for transition probabilities, bound-bound collisional cross sections and bound-free cross sections become increasingly scarce with increasing quantum numbers. Yet meaningful calculations can still be made in plasmas and other situations, in spite of the apparently "infinite amount of missing data". The reasons for this are that physical processes reduce the infinities to finite numbers, and that there are many cases of interest where processes involving high-n levels produce small, calculable perturbations on the lower-n levels usually of more direct interest[16].

While an unperturbed atom has an infinite number of bound states, ionization energies are reduced to account for the energy released on embedding an electron-ion pair into a plasma, effectively reducing the number of bound states to a finite number. The last bound state has principal quantum number n_D, where

$$n_D \approx \sqrt{\frac{z^2 \rho_0}{2a_0}} \approx 1140z \, (T_4/N_{10})^{1/4} \, , \tag{6}$$

and where z is again the core charge, ρ_0 is the Debye radius, a_0 the Bohr radius, $T_4 = T_e/10^4$ K and $N_{10} = N_e/10^{10}$ cm^{-3} (Griem 1964). The HAOS-DIPER reduces each ion's ionization potential by $\mathcal{R}z^2/n_D^2$ erg, where $\mathcal{R}$ is the Rydberg, for the purpose of computing LTE populations which are used in evaluating collisional rate coefficients. In the HAOS-DIPER database files, energy level data are available for principal quantum numbers n typically between 2 and 18, depending on the particular ion. Data for radiative and collisional processes tend to be available only for levels with small n, $n < 6$ or so, and data for certain atoms and ions which may be particularly awkward to work with (e.g., sulfur) may be largely theoretical. There is therefore, for many plasmas of astrophysical interest, a vast number of levels absent in the models which are potentially of interest.

Out of LTE (`!REGIME =0 or 1`), the HAOS-DIPER can be used to estimate the influence of some of the missing data on the levels of interest[17]. The missing data are of two kinds: missing data for levels which exist in the database, and missing levels themselves.

---

[16]The missing high-n levels have calculable properties, given that their wavefunctions can approach "hydrogenic" functions or that they are amenable to the powerful "quantum defect" technique, see for example Cowan 1981, Seaton 1983.

[17]If the user wishes to work with transitions involving the missing levels, he or she will have to add these levels. The HAOS-DIPER simply tries to estimate the influence of the missing higher levels on the rate matrices for levels already existing in the database.

Table 2: The meaning of the value of `!APPROX`

bit	action if the bit is set
1	Estimate missing collisional rate coefficients, store and flag them in structure `col`
2	Add effects of recombination to levels between n_{max}, the maximum principal quantum number for a given ion and n_{lte} to the rate matrix
3	Add bound-bound collisions in $n \to n+1$ transitions in the highest n levels to the rate matrix
4	switch off density dependent effects in dielectronic recombination
5	not used (yet)

These effects are controlled by the system variable `!APPROX`, whose value in base 10 is first converted to base 2 and the various bits, either 0 or 1, are examined to see if `HAOS-DIPER` should include a certain effect. The meanings of the various bits are listed in table 2.

If no bits are set `!APPROX=0` which is ...00000 in base 2, subsequent calculations will proceed with no corrections for missing data, but will include density dependent corrections to dielectronic recombination rates.

If the first bit is set (`!APPROX =...xxxx1` in base 2, where x is 0 or 1), then `HAOS-DIPER` will attempt to make some reasonable guesses for missing collisional rates between bound levels stored in the `lvl` structure. The approximated data are stored in the IDL structure `col` but of course they do not enter the database files. The variable `col.approx` can be examined to see if it has been approximated (1) or is a "reliable" value read from the database (0).

The second and third bits are meant to account for missing levels with relatively high quantum numbers, and they depend on the relative values of quantum numbers n_D, n_{max} and n_{lte}. The `HAOS-DIPER` makes corrections only when n_{lte} (defined below) is "large enough", practically speaking $> 3 + n_G$ where n_G is the principal quantum number of the ground levels, because the corrections make use of hydrogenic approximations. n_{lte} is the principal quantum number n above which $n \to n+1$ collision rates dominate over radiative rates. This happens because the integrated bound-bound radiative decay rates decrease rapidly with increasing n (like n^{-5}, see e.g., section 14-17 Cowan 1981), whereas collision rates increase rapidly as the orbital dimensions and accompanying cross sections increase with n. Thus, when incident radiation is unimportant (i.e. the radiation temperature does not greatly exceed the plasma electron temperature), the value of n_{lte} is roughly (Griem 1964):

$$n_{lte} \approx 8.4 \left(N_{10}\right)^{-2/17} \left(\frac{k_B T_e}{z^2 \mathcal{R}}\right)^{1/17} z^{14/17}. \tag{7}$$

For values of $n > n_{lte}$, the levels are dominated by collisional processes in a stepwise fashion all the way to n_D. These levels are therefore expected to have LTE populations

relative to the continuum state upon which they converge. The relative values of n_{max} and n_{lte} for a given situation then suggest the use of two approximations:

- If the second bit is set (`!APPROX =xxx1x` in base 2), then if $n_{max} < n_{lte}$, recombination is added to the rate matrix using hydrogenic formulae for all the levels in this range, and the recombination is (somewhat arbitrarily) added to levels with $n = n_{max}$ in proportion to each individual level's degeneracy. In this way, missing recombination is approximately added to the relevant components of each ion's rate matrix.

- If the third bit is set (`!APPROX =xx1xx` in base 2), then if $n_{max} > n_{lte}$, the effects of the stepwise upward collisions are included approximately in the rate matrix by adding a hydrogenic $n_{max} \rightarrow n_{max} + 1$ collisional rate to the $n_{max} \rightarrow$ continuum level(s) κ rate coefficients $C_{n_{max}\kappa}$. The downward collision rates are computed from $C_{\kappa n_{max}} = C_{n_{max}\kappa}q^*_{n_{max}}/q^*_{\kappa}$, where q^* represent LTE populations. In this way, missing collisional coupling between levels with $n = n_{max}$ and the continuum is approximately added to the relevant components of each ion's rate matrix.

If the fourth bit is set (`!APPROX =x1xxx` in base 2), then density dependent modifications to dielectronic recombination rates are switched off.

It is stressed that these are strictly *approximate* corrections for missing levels. It is recommended that the user run and compare the output from two calculations with one another to judge the magnitude of potential effects.

5.4   Working with isoelectronic sequences

`HAOS-DIPER` can easily and quickly work with data along isoelectronic sequences, which are simply sequences of ions having the same number of electrons. This can be very useful for finding data outliers for example, or for teaching/ learning purposes. Because of the increasing dominance of the central, Coulomb force (over the force between electrons) with increasing core charge z, atomic parameters should vary slowly with z along isoelectronic sequences.

While there are many ways that isoelectronic behavior this might be studied, `HAOS-DIPER` has a simple procedure `isostr.pro` to extract data along isoelectronic sequences. Just as, for example, the `lvl` structure contains data for levels for a particular element, it is convenient to use the same kind of structures to store data along an isoelectronic sequence. It works as in the following example:

```
IDL> diprd,'c',2,/nofill          ; store data for B-like C II
IDL> iso=isostr(l=1)              ; match and read data for the same level
                                     along the isoelectronic sequence (the
                                     first level is number 0)
IDL> tl= getwrd(lvl(1).label,2,50) ; get a plot title, removing first two words
                                     from label "C II"
```

```
IDL> plot,iso.ion,iso.ev,ps=1,title=tl    ; plot the energy of this level as a function
                                             of the charge seen by the outermost
                                             electron
```
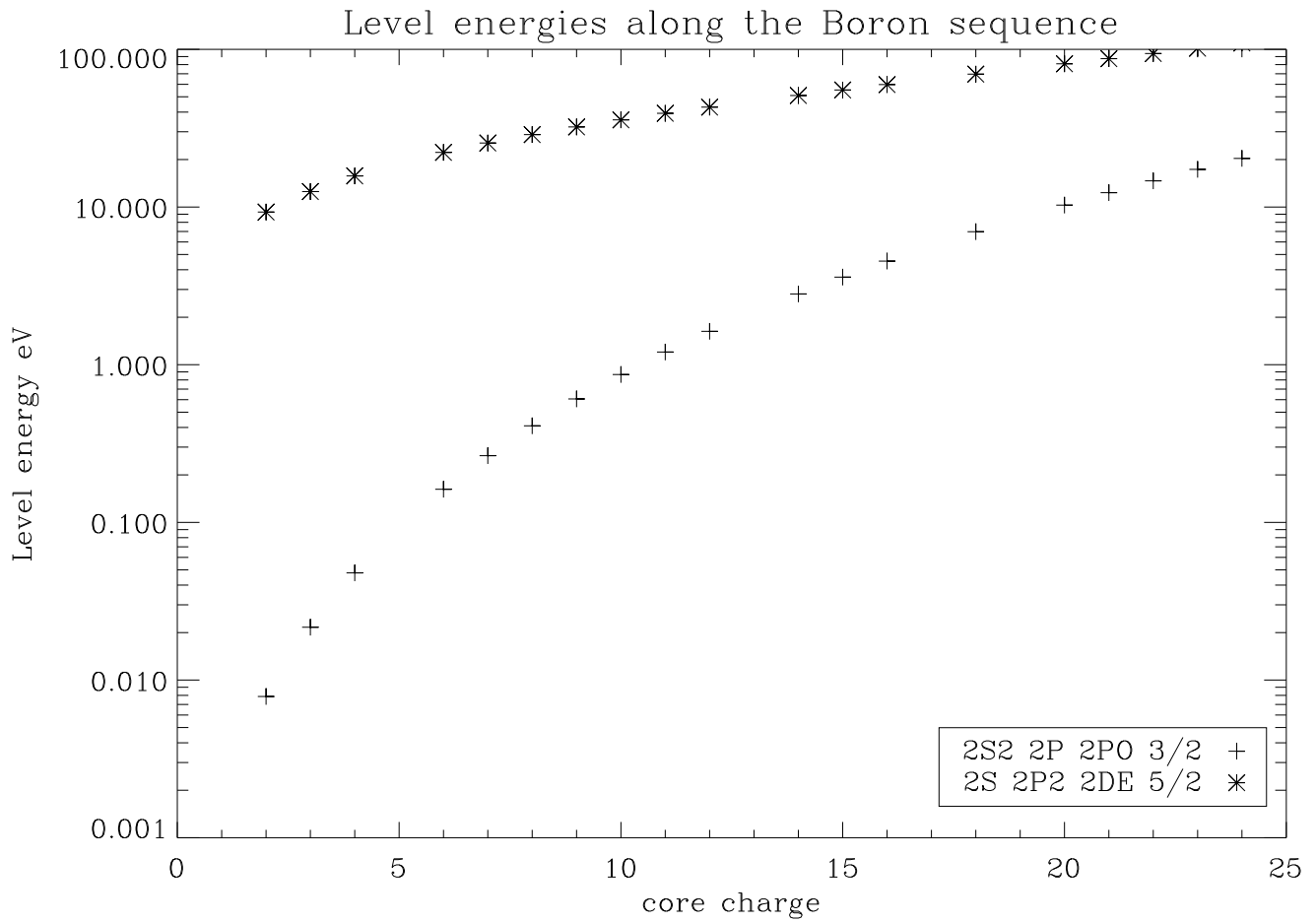
Figure 8: *Energies (eV) of the $2s^2 2p\ ^2P^o_{3/2}$ level (plus symbols) and of the $2s2p^2\ ^2D_{5/2}$ level (star symbols), relative to the ground level, across the boron isoelectronic sequence, plotted as a function of the core charge z.*

Here, the `l=1` keyword instructs the procedure to extract level information corresponding to the index 1 of the currently stored `lvl` structure. Figure 8 shows the result of the above plot, but including the same syntax to extract the isoelectronic behavior of a level belonging to a different configuration. Such plots are useful as ways to understand the relative sizes of terms in atomic Hamiltonians (e.g., Dufton and Kingston 1981).

The same can be done using the structures `trn` and `col`, to examine transition and collisional data along isoelectronic sequences, using `t=nn` as input for transitions, and `c=mm` for collisional data.

```
IDL> diprd,'c',2                        ; store data for B-like C II
IDL> trans, list=indgen(5)              ; list the first 5 elements of the trn
                                           structure
IDL> iso=isostr(t=3,elem,ion)           ; match and read data for the same
                                           transition along the isoelectronic
                                           sequence, the atomic number returned
                                           in variable elem, ion charge+1 in
                                           variable ion
IDL> i=trn(5).irad & j=trn(5).jrad      ; indices of lower, upper levels
IDL> tl=getwrd(lvl(j).label,2,50)$      ; get a plot title
 +' - '+getwrd(lvl(i).label,2,50)
IDL> plot,ion,iso.alamb,ps=1,title=tl   ; plot the wavelength of this transition as a
                                           function of the charge seen by the
                                           jumping electron
IDL> plot,ion,iso.f,ps=1                ; plot the oscillator strength of this
                                           transition
```

Figure 9 shows this particular plot.
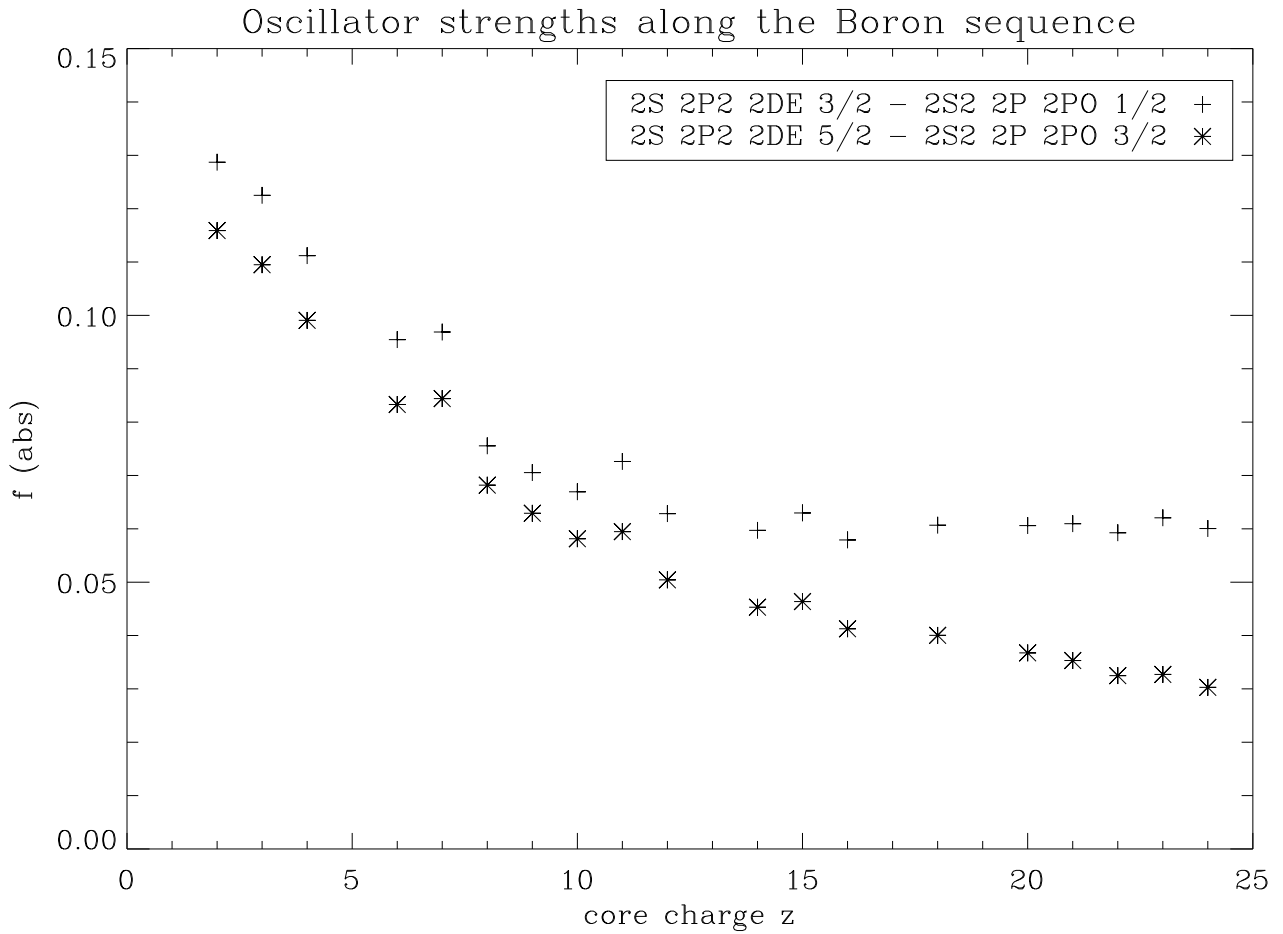
Figure 9: *Absorption oscillator strengths of the* $2s2p^2\ ^2P_{1/2} - 2s^22p\ ^2P^o_{1/2}$ *transition along the boron isoelectronic sequence, plotted as a function of the core charge* z.

The keyword parameters `elem, ion` are needed above, because `isostr` always returns as output a structure which inherits the same structure asked for at input. In the last example, the `trn` structure is inherited by `iso`, and this structure does not include the `atom` or `ion` tags (see `dipdef.pro`). Note that for `col`, the stored parameters often need to be transformed before they can be plotted as simply as in the above example. `isostr` can be used to returning the Maxwellian-averaged collision strength at a temperature $T_e = 10^4 \mathrm{ion}^2$ K:

```
IDL> diprd,'c',2                          ; store data for B-like C II
IDL> col, list=indgen(5)                  ; list the first 5 elements of the col
                                            structure
IDL> iso=isostr(c=2,el,ion,om=om)         ; match and read data for the same
                                            collisional transition along the
                                            isoelectronic sequence, return collision
                                            strength in om
IDL> i=col(2).ilo & j=col(2).ihi          ; indices of lower, upper levels
IDL> tl=getwrd(lvl(j).label,2,50)$        ; get a plot title
 +' - '+getwrd(lvl(i).label,2,50)
IDL> plot,ion,om,ps=1,title=tl            ; plot the collision strength as a function of
                                            the charge seen by the jumping electron
```

Figure 10 shows this particular plot.
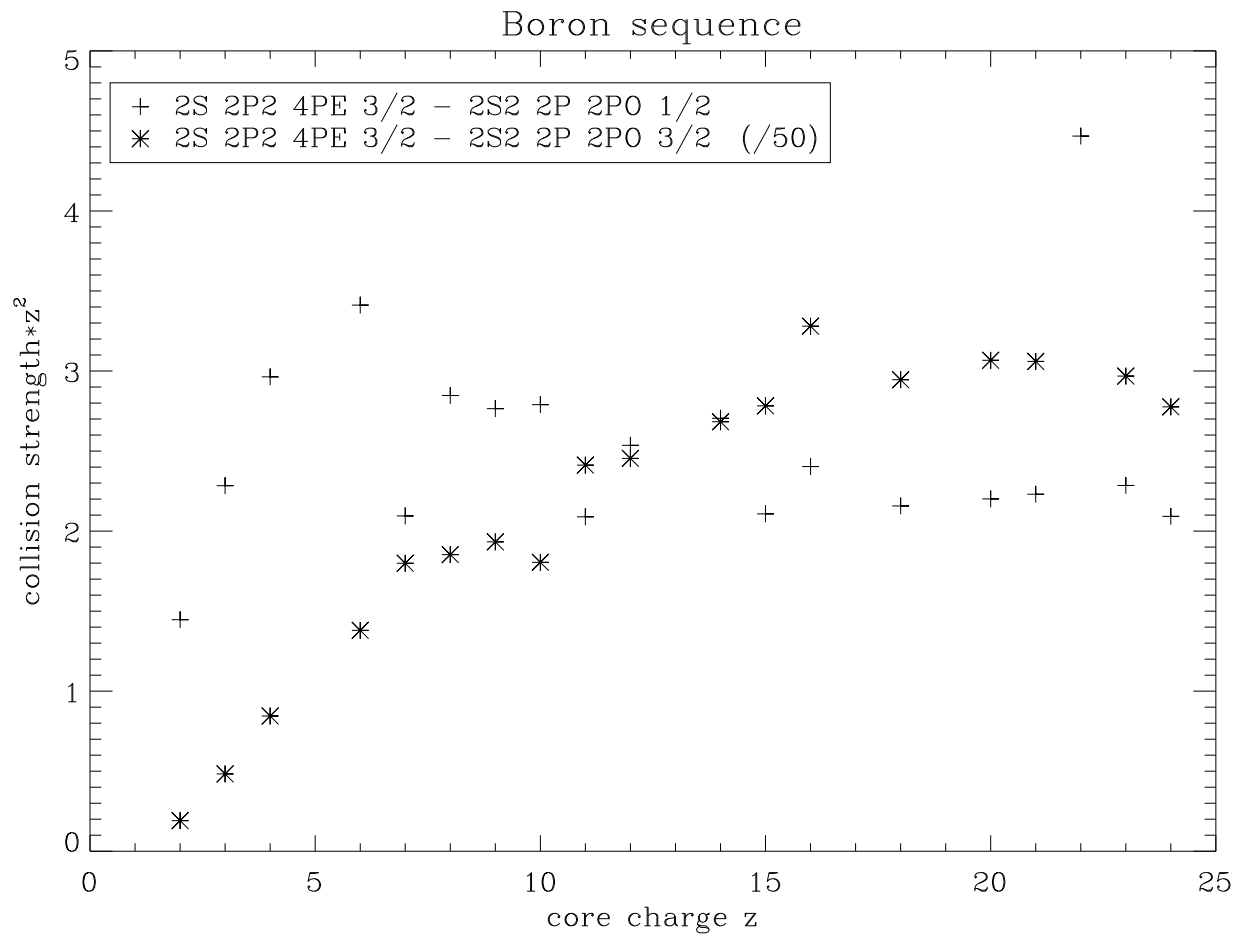
Figure 10: *Collision strengths of the $2s2p^2\ ^4P_{3/2} - 2s^22p\ ^2P^o_{1/2}$ collisional transition (plus signs) and $2s2p^2\ ^4P_{3/2} - 2s^22p\ ^2P^o_{3/2}$ transition (star symbols, the plotted data are divided by 50) along the boron isoelectronic sequence. The collision strengths were multiplied by z^2 and plotted as a function of the core charge z. The collision strengths were interpolated to the temperature $T_e = 10^4z^2$ K for each ion. There appears to be an erroneous data point for $z = 22$ for the 3/2-1/2 transition (Fe XXIII).*

The choice of $T_e = 10^4 \text{ion}^2$ K is arbitrary, it roughly corresponds to a temperature of maximum ion abundance when "coronal ionization equilibrium" holds (far from LTE, just 2-body collisional processes dominate, e.g. Woolley and Allen 1948). This scaling of T_e with ion^2 means that the ratio of mean thermal energy to excitation energy is roughly constant, for transitions involving changes of principal quantum number.

5.5 Directly accessing the database files

The user may have a need to access the data in `HAOS-DIPER` using the interface provided by Lindler The database files have been built in order to enable rapid searches on certain variables (see the entries under #index in the database definition files – those with extension .dbd– in the `zdbase` subdirectory). Here are some examples. The user should refer to the database manual (`http://idlastro.gsfc.nasa.gov-/ftp/text/database.tex`) for the syntax used here.

   Suppose the user wishes to find all spectral lines between 1300 and 1310 Å, the following will achieve this:

```
IDL> dbopen,'atom_bb'                          ; open the bound-bound radiative
                                                  transition database
IDL> all=dbfind('1300.<wl<1310.')              ; wavelengths must be given in Å units
IDL> dbprint,all,'wl,atom,ion,isos'            ; print out the wavelength, atomic number,
                                                  ion number, number of electrons
```

 Note that the operators $> <$ mean "greater than or equal to" and "less than or equal to" respectively. The output is:

```
 HAOS-DIPER:  Bound-bound transition data
 -----------------------------
   Wavelength   Atom Ion  Isos


 -----------------------------
     1308.644   26    6    21
     1309.910   26    6    21
... (total of 50 entries)
```

If one wants to refine the search, it can be done as follows. Suppose we wish to look for permitted transitions of ions with charge 3 or less, and for atoms heavier than carbon. Then we would follow the above commands immediately with

```
IDL> e1=dbfind('ion<4,atom>7,type=E1',all) ; find E1 transitions
                                           ; among those just found
                                           ; all is included in argument
                                           ; list to speed up the search
IDL> dbprint,e1,'wl,f,type,atom,ion,isos'
IDL> dbclose
```

The output is now

```
        HAOS-DIPER:  Bound-bound transition data
        ---------------------------------------------
          Wavelength          F        Type Atom Ion  Isos


        ---------------------------------------------
              1302.336 7.600E-02 E1        16     1    16
              1302.862 4.100E-02 E1        16     1    16
              1303.110 5.600E-02 E1        16     1    16
              1303.430 2.900E-02 E1        16     1    16
              1305.884 1.800E-01 E1        16     1    16
              1304.369 8.399E-02 E1        14     2    13
              1309.274 8.399E-02 E1        14     2    13
              1301.148 1.920E-01 E1        14     3    12
              1303.322 1.444E-01 E1        14     3    12
              1302.168 5.200E-02 E1         8     1     8
              1304.858 5.180E-02 E1         8     1     8
              1306.029 5.190E-02 E1         8     1     8
```

The same syntax can be used in the procedure for marking spectral line identifications, `idspec`, through the `subset` keyword

```
IDL> ps,'idspec_ex.eps',/enc
IDL> plot,lambda,int,xtitle = 'Wavelength [A]',$
   ytitle = 'Intensity erg cm!u-2!nsr!u-1!ns!u-1!n',$
   xran = [1300,1310],title = 'HRTS quiet sun' ; plot a spectrum
IDL> subset='ion<4,atom>7,type=E1' ; find E1 transitions in the
                                    ; desired range of ions
IDL> idspec,subset=subset          ; mark lines on the spectrum
IDL> psclose
```

`idspec` uses the plotted x range as the limits for the wavelength search. The resulting plot is shown in figure 11. `idspec` can be called many consecutive times, to plot individual ions/elements/ multiplets if desired. If this is done the keyword `ystart` is useful to determine where to place the annotated transitions with respect to the others.
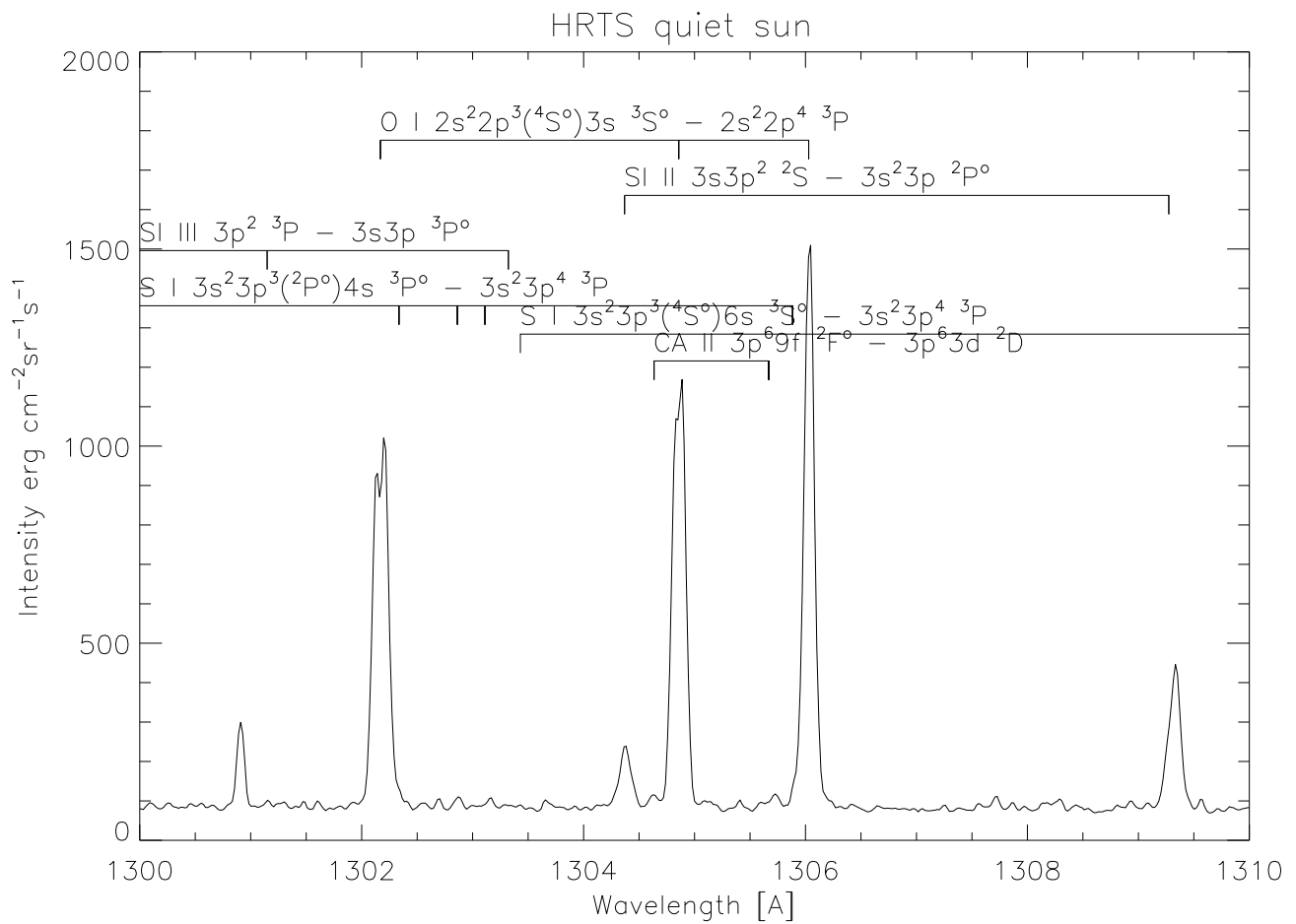
Figure 11: *An example of how* `idspec` *marks transitions on a spectrum. Note that the transitions are not identifications – no algorithm is implemented to do that – but are simply marked on the spectrum, according to the user inputs as specified using keyword* `subset` *– for example, there are no obvious lines of S I or Si III in the spectrum, although the wavelengths of possible lines are marked.*

idspec by default uses vacuum wavelengths below 2000Å, and air above. The keyword vac can be used to enforce vacuum wavelengths for all wavelengths.

Lastly, an example of using just id_atom is shown in figure 12. In this case the transitions shown are missing from the atom_bb database, but they were identified as missing by HAOS-DIPER, and placed in the misstrn structure. Concatenating the trn and misstrn structures, and converting the trn.alamb values from vacuum to air wavelengths, the id_atom was then used to make figure 12, as follows:

```
fil = concat_dir(getenv('DIPER'),'data')
fil= concat_dir(fil,'spectra')
fil= concat_dir(fil,'sp.xdr')
restore,fil
diper,reg = 2
diprd,26,1
trn = [trn,misstrn]
ww = trn.alamb
vactoair,ww
trn.alamb = ww
;
plot,w,f,xtitle = 'Wavelength [A]',ytitle = 'Relative Intensity',$
   xran = [6301,6303]+[-0,+0],xsty = 1,yran = [0.,1.1],ysty = 1
id_atom,/mult,xshift = 0.1
```

Note that the "nice" labels for the atomic levels were constructed by id_atom by calling int2lab. (Contrast this with, say, figure 10).
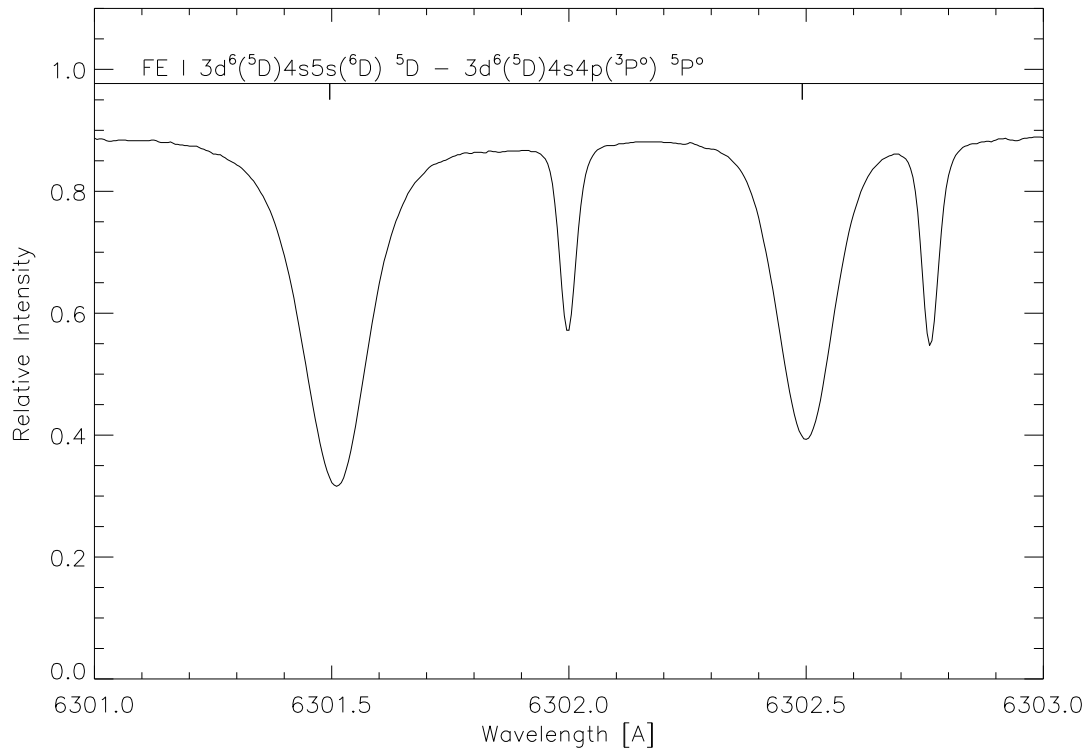
Figure 12: *Solar intensity spectrum from the Sacramento Peak atlas, near 6302 Å, showing the two main lines used for spectropolarimetry by the Advanced Stokes Polarimeter at the Dunn Solar Telescope, and on the spectropolarimeter on board the HINODE satellite. In this case the lines are missing from the* atom_bb *database, based on the NIST database, but were found by* HAOS-DIPER *and stored in the* misstrn *structure. The procedure* id_atom *was used after reading the Fe I data with* diprd,26,1. *The other transitions are not present in the database. This case illustrates one of the limitations of the present version of* HAOS-DIPER.

6   Future plans

Currently, collisional data for neutral atomic species are not as abundant as for ions. This is due, in part, to some significant differences associated with computation of electron collisional cross sections for neutrals compared with charged ions. It is hoped that this situation will be remedied in time, and `HAOS-DIPER` will attempt to include data as they become available. Summers and Kato (2000) have shown how the treatment of collision strengths (bound-bound collisions) for ions developed by Burgess and Tully (1992), and used by `HAOS-DIPER` and `CHIANTI` for example, can be extended to neutrals, once cross sections become available.

It is possible that collisional data might be treated using energy-dependent collision cross sections, allowing the study of the effects of non-Maxwellian distribution functions on the populations of levels in atoms and ions. This would involve building a new database file, and defining a new regime (`!REGIME=3`, perhaps).

State-to-state photoionization data would be worthwhile including in the database, going beyond the currently used cross sections from the `OPACITY` project which are summed over final states. The transition from LS coupled terms to the individual levels should be implemented properly (in `bfrd`). At present, if photoionization and recombination can compete with bound-bound processes, such as in photoionized plasmas like planetary nebulae, the relative populations of the individual levels within each term are incorrect.

It would certainly be of interest to incorporate line broadening by particle impact, for stellar photospheres and other relatively high density plasmas, for example. Whether this would involve the existing data structures or more sophisticated structures requiring additional database files remains to be seen.

In principle the `HAOS-DIPER` could be easily used to *interpolate* data along isoelectronic sequences, this is yet to be implemented. Such a scheme might also be useful as a way to find and correct certain types of errors in the existing database- to remove outliers for example.

Suggestions for improvements of any kind, or donations of contributed useful code should be sent to `judge@ucar.edu`.

A   Rate equations

Consider an atomic model consisting of N levels. A transition from one level i to another j (by spontaneous radiative decay, for example) occurs statistically such that an ensemble of such atoms obeys the exponential decay law, with a characteristic lifetime of τ_{ij} sec. The transition probability (or "transition rate") is $P_{ij} = 1/\tau_{ij}$ sec^{-1}. For a large ensemble of such atoms, the population densities $q_i(\vec{r}, t)$ (units of cm^{-3}), $i = 1, N$, given an initial level, obey the set of N equations:

$$\frac{D}{Dt} q_i(\vec{r}, t) = \sum_{j \neq i}^{N} q_j(\vec{r}, t) P_{ji}(\vec{r}, t) - q_i(\vec{r}, t) \sum_{j \neq i}^{N} P_{ij}(\vec{r}, t). \tag{8}$$

In eq. (8), $q_i(\vec{r}, t)$ are functions of spatial coordinates $\vec{r}$ and time t. The LHS is the Lagrangian time derivative. The general properties of the rate matrices of the above kind have been described in an eigenfunction expansion by Judge (2005).

Under *statistical equilibrium* conditions, it is assumed that the dynamical time scales, given by the v $\cdot \nabla$ part of the $\frac{D}{Dt}$ operator, are much longer than the "atomic" time scales - those at which the RHS of eq. (8) evolve, so that we may write

$$\sum_{j \neq i}^{N} q_j P_{ji} - q_i \sum_{j \neq i}^{N} P_{ij} = 0. \tag{9}$$

Here and henceforth, for notational brevity, we drop the coordinates $\vec{r}$ and t. In setting the RHS of this equation to zero, the assumption is that the all the atoms have plenty of time to "relax" such that this condition (of statistical equilibrium) is true (see Judge 2005 for the relaxation processes). Since the above equation is homogeneous in q, it is traditional to replace one of the equations of eq. (9) by the particle conservation equation (Mihalas 1978):

$$\sum_{j}^{N} q_j = q_{\text{tot}}, \tag{10}$$

where q_{tot} is fixed in some prescribed manner (from hydrostatic equilibrium and a fixed abundance, for example).

P_{ji} is the total transition probability for an ion in level j to make a transition to level i, in units of s^{-1}. The rates P_{ji} are, under the "impact approximation" (section 2.1), split into the sum of collisional C_{ji} and radiative R_{ji} transition probabilities:

$$P_{ji} = C_{ji} + R_{ji}. \tag{11}$$

A.1   Collisional processes

C_{ji} is the total transition probability for an ion in level j to make a transition to level i induced by particle collisions. Assuming that the colliding particles are thermalized

at a temperature T, these rate coefficients are functions of the colliding particle densities N and T. The downward and upward rate coefficients are related by the detailed balance relation

$$q_j^* C_{ji} = q_i^* C_{ij} \tag{12}$$

where the variables q^* are LTE population densities. For levels j and i which are both bound levels, the Boltzmann formula applies:

$$\frac{q_j^*}{q_i^*} = \frac{g_j}{g_i} exp \left\{ -\frac{(E_j - E_i)}{k_B T} \right\}, \tag{13}$$

which, when j is a free state, is modified to the Saha-Boltzmann formula:

$$\frac{q_j^*}{q_i^*} = N_e^{-1} \left(\frac{2\pi m_e k_B T_e}{h^2} \right)^{3/2} 2\frac{g_j}{g_i} exp \left\{ -\frac{(E_j - E_i)}{k_B T} \right\}. \tag{14}$$

For bound-bound transitions induced by electron impact,

$$C_{ji} = 8.63 \times 10^{-6} \frac{\Upsilon_{ji}(T_e)}{g_j} T_e^{-1/2} N_e \ \sec^{-1}, \tag{15}$$

so that

$$C_{ij} = 8.63 \times 10^{-6} \frac{\Upsilon_{ji}(T_e)}{g_i} T_e^{-1/2} exp \left\{ -\frac{(E_j - E_i)}{k_B T} \right\} N_e \ \sec^{-1}. \tag{16}$$

Here, $\Upsilon_{ji}(T_e)$ is the "Maxwellian-averaged collision strength" at electron temperature T_e (Burgess and Tully 1992, and references therein). $\Upsilon_{ji}(T_e) = \Upsilon_{ij}(T_e)$ is a weak function of T_e for many types of transitions. The CHIANTI project (Landi et al. 2006, and references therein) has studied, critically assessed and compiled data for $\Upsilon_{ji}(T_e)$ over many years, and much of the HAOS-DIPER bound-bound collisional data has been taken from that valuable resource (keywords SPLUPS and SPLUPS9 in col.key).

For bound-free transitions, the functional dependences of C_{ij} on T_e vary, depending on the various quantum numbers via different contribution of different partial waves and other factors to the cross sections. These have been discussed at some length (e.g., Arnaud and Rothenflug 1985). As a simple example, Seaton's "semi-empirical formula", obtained by integrating Thomson's classical cross section for the energy exchanged during electron collisions and assuming that all collisions with energies imparted to the target electron lead to ionization, is

$$C_{ij} = 2.0 \times 10^{-8} T_e^{+1/2} \sum_i \xi_i (\epsilon_j - \epsilon_i)^{-2} exp \left\{ -\frac{e(\epsilon_j - \epsilon_i)}{k_B T_e} \right\} N_e \ \sec^{-1}. \tag{17}$$

where ξ_i is the number of equivalent electrons in the shell with energy $E_i = e\epsilon_i$ (ϵ is the level energy in eV). It is a surprisingly good approximation near threshold energies, or when $(E_j - E_i)/k_B T \gg 1$ as occurs in many astrophysical plasmas of interest. The HAOS-DIPER adopts the more elaborate and accurate formulae from

Arnaud and Rothenflug (1985) and Arnaud and Raymond (1992) for metastable levels, where available. The above general formula is adopted for the non-metastable levels neutral atoms, and another general formula by Burgess and Chidichimo (1983) is adopted for ionized species.

As a result of the different forms of equations (13) and (14), the "downward" collisional rates ($j \rightarrow i$) for bound-bound and bound-free collisions have quite different behaviors: for bound-bound transitions C_{ji}/C_{ij} is independent of N_e, but for bound free transitions $C_{ji}/C_{ij} \propto N_e$. The process described by coefficient C_{ji} is called "three body recombination (initial state: two free electrons plus an ion of charge Z; final state: one free electron and an ion of charge $Z - 1$, the reciprocal process of electron impact excitation) becomes important only at high densities N_e. At lower densities two-body collisions dominate (in this case radiative and/or dielectronic recombination). This was first realized by Biermann, and Woolley and Allen in 1947 (Woolley and Allen 1948, Biermann's work is summarized in Van de Hulst 1953). Thus, under the low density conditions present in the chromospheres and coronae of stars, the three body process does not balance its reciprocal process, thus ionization balance is far from thermal equilibrium, $q_j/q_i \neq q_j^*/q_i^*$. "Detailed balance" is invalid. Curiously, the "two-body" processes are usually studied as radiative processes, to which we now turn.

A.2 Radiative processes

In general, R_{ji} depends on the radiation field through integrals over frequency of the radiative cross sections and the mean intensity J_ν. J_ν depends implicitly on the vector $\mathbf{q} = (q_1, q_2, \ldots, q_N)^T$, throughout the plasma, and boundary conditions, through the radiative transfer equation. Consider transitions between two levels i and j, where j (a bound or continuum level) lies energetically higher than level i. Then (see p. 131 of Mihalas 1978)

$$R_{ij} = 4\pi \int_0^\infty \alpha_{ij}(\nu)\,(h\nu)^{-1}\, J_\nu\, d\nu, \text{ and} \tag{18}$$

$$R_{ji} = 4\pi \frac{q_i^*}{q_j^*} \int_0^\infty \alpha_{ij}(\nu)\,(h\nu)^{-1} \Big(\frac{2h\nu^3}{c^2} + J_\nu\Big)\, e^{-h\nu/k_B T}\, d\nu. \tag{19}$$

Here the cross sections $\alpha_{ij}(\nu)$ are simple photo-ionization cross sections when j is a continuum level. When j is a bound level, the $\alpha_{ij}(\nu)$ are given in terms of the Einstein coefficients by $\alpha_{ij}(\nu) = \frac{h\nu}{4\pi} B_{ij}\phi(\nu)$, $g_i B_{ij} = g_j B_{ji}$, and $A_{ji} = (2h\nu^3/c^2)B_{ji}$. ϕ_ν is the line profile function at frequency ν, where $\int_0^\infty \phi(\nu) = 1$, and by writing the equations in this form, complete redistribution of the scattered radiation in the line has been assumed (see Mihalas 1978). The implicit dependence of R_{ji} and R_{ij} on $\mathbf{q}$ noted above arises from the formal solution to the transfer equation:

$$J_\nu = \Lambda\{S_\nu\}, \tag{20}$$

$$S_\nu = S_L = S_{ij} q_j A_{ji}/(q_i B_{ij} - q_j B_{ji}), \tag{21}$$

where Λ is an integral operator, integrating over the entire plasma and incorporating appropriate boundary conditions, and S_ν is the source function. In writing eq. (21), complete redistribution and no background source of emission has been assumed for simplicity.

In `HAOS-DIPER`, no detailed radiative transfer is treated in the evaluation of the radiative rates R_{ij} and R_{ji}. The accurate treatment of boundary conditions and the need to make the radiation fields consistent with the atomic populations is beyond the scope of the `HAOS-DIPER`, but is treated, for example, in special programs such as `MULTI`[18] (Carlsson 1986). The main purpose of the `HAOS-DIPER` is instead to work with the atomic data with the aim of understanding those factors determining the atomic populations and the emergent spectra. Since radiative transfer is clearly important under many conditions, one idea behind the `HAOS-DIPER` is to provide atomic data needed as input to other programs. The procedure `atomwr` writes data to ascii files which can be read with `MULTI`, in fact.

To this end, `HAOS-DIPER` solves the above equations in the optically thin limit with a prescribed, fixed radiation field[19]. In `HAOS-DIPER`, the radiation field is determined by keyword `incident='myradiation'` passed to `sesolv`, in which `myradiation.pro` is a function returning the radiation field as a function of wavelength (`jval81.pro`, an approximation to the mean intensities from observed intensities given by Vernazza et al. 1981, is an example). Given this radiation field J_ν, which can be (and by default is) zero, the above equations are integrated over frequency[20] for continua (for lines they are replaced by one "mean" frequency point) and the equations solved.

The procedure `sesolv` also provides a simple, very approximate way of examining the magnitude of the effects of radiative transfer via the "mean escape probability" approximation. This is automatically used- it becomes important if the plasma is optically thick. `sesolv` deals with this using keyword `depth=depth`, which is the length scale (cm) from which optical depths are computed given the statistical equilibrium and abundance values. (By default, `depth` is set to a zero guaranteeing all transitions are optically thin). In this approximation, all frequency information in lines and continua are replaced by one frequency, a dramatic simplification, and the radiative transfer problem is drastically reduced to the simultaneous solution of escape probabilities $p(\tau)$, modified incident mean intensities $\overline{J}$, and population densities $\mathbf{q}$, all at one point. From a starting solution, the equations are iterated using a Newton-Raphson scheme to convergence. In the converged solution the effects of the radiative transfer for an emission line are that the net radiative rates between levels i and j

---

[18]`http://www.astro.uio.no/~matsc/mul22/index.html`

[19]While this may seem overly restrictive, there are situations when such calculations are what might be needed. For example, Judge (1998) computed the influence of solar radiation on the statistical equilibrium of coronal ions in a search for forbidden coronal lines which may find use in coronal magnetometry.

[20]At low electron temperatures, the integrations can be poorly sampled. The `HAOS-DIPER` interpolates the threshold frequencies and cross sections to ensure an accurate integration.

and power $\mathcal{P}_{ji}$ radiated in line ij are

$$
\begin{align}
q_j A_{ji} p_{ji} &= q_j(A_{ji} + B_{ji}\overline{J}) - q_j B_{ij}\overline{J} \tag{22} \\
\mathcal{P}_{ji} &= q_j A_{ji} p_{ij} h\nu_{ji} \text{ erg cm}^{-3}\text{ s}^{-1}, \tag{23}
\end{align}
$$

where the influence of any incident radition has been omitted for simplicity. Equation (22) means that the rate equation between levels i and j becomes

$$
q_j(C_{ji} + A_{ji} p_{ji}) = q_i C_{ij} \tag{24}
$$

Note that, when optically thin ($\tau \ll 1$ for all transitions), $p = 1$, and the equations reduce to the well-known optically thin limit, as required. Note that *the use of this approximation is not recommended - if radiation transfer is important it should be solved correctly.* Instead the idea is to provide an idea of when radiative transfer is likely to be important and what magnitude the effects might be.

A.3 Bound-free transitions: collisional? radiative?

The bound-free rates in eq. (19) need further comment. When $J_\nu \ll 2h\nu^3/c^2$, one has "spontaneous" recombination. This limit is met for most bound-free transitions, the exception being those for high-n (principal quantum number) levels where collisions tend to dominate P_{ji} anyway, because of large orbital dimensions. Thus, for practical purposes, the recombination rates P_{ji} do not depend much on the radiation field J_ν. As noted in section A.1, these can be considered "two body" collisions (initial state, free electron+ion of charge Z, final state, ion of charge $Z - 1$). This is the reason why recombination can be treated as a collisional process as it is in the absence of a significant radiation field (e.g., Arnaud and Rothenflug 1985), and why HAOS-DIPER, under !REGIME=0 (coronal regime), has adopted such approximations from earlier work.

However, this presents a problem, when *both* collisional rate coefficients for recombination *and* photoionization data are present in the atomic models, because one can count the recombination process twice. In the HAOS-DIPER package, this means potential problems when !REGIME=1. It is yet more complex because of the role of autoionization resonance structure and a somewhat artificial separation of recombination into two components: "radiative" and "dielectronic".

When photoionization cross sections contain no auto-ionization resonances, one has simple "radiative recombination". This occurs in hydrogen-like ions and can occur near threshold in recombination to ions with closed shells (e.g. $C^{4+}+e \to C^{3+}$), because in the first case only one electron is involved and in the second, doubly excited states lie at energies significantly higher than threshold energies.

When autoionization resonances are present in the cross sections, the enhanced recombination resulting from the resonance peaks constitute "dielectronic recombination". In the general formalism of Burgess (1964), the recombination occurs as the innermost "core" electron of a doubly excited state decays leaving the outermost

high-n ($n \gtrsim 200$, say) electron in a bound or "recombined" state (e.g., $3p\,nl$, $n \gg 3$, autoionizing, decays to $2s\,nl$, a bound level). HAOS-DIPER, by adopting the rate coefficients of Aldrovandi and Pequignot (1973) and Shull and Steenberg (1982), includes the summed effects of the high-n levels following Burgess (1964). Autoionization resonances associated with smaller values of n can, however, be very important. Of these, those lying energetically close to the threshold of the resonance continuum (with energy $\lesssim k_B T_e$) can have an abnormally large influence on dielectronic recombination rates (Storey 1981). This process is termed "low temperature dielectronic recombination". It can be important when doubly excited states with *small* principal quantum numbers (close to those of the ground levels of the ions involved), relax via emission of a photon, thereby leading to recombination.

The HAOS-DIPER attempts to deal with dielectronic recombination in an approximate, but physically resonable way. First, if !REGIME=0, no photoionization data are used and all recombination is treated using the coefficients of Aldrovandi and Pequignot (1973) and Shull and Steenberg (1982). No "low temperature" component is presently included in this case. If !REGIME=1, and when photoionization data from the OPACITY project are present, the radiative recombination coefficients of Aldrovandi and Pequignot (1973) and Shull and Steenberg (1982) are set to zero. The dielectronic recombination coefficients computed by these authors are kept, however, and modified by default for the effects of plasma microfields as discussed in section A.4. The rationale is that the bulk of the contributions to the dielectronic recombination as envisaged by Burgess (1964) involve very high-n (say 200) doubly excited states, which are absent from the OPACITY project's photoionization data. To the extent that the OPACITY project has accurately computed and included doubly excited states of small and intermediate n, the HAOS-DIPER will accurately compute recombination rates using these cross sections, in principle including the "low temperature" component identified by Storey (1981).

This hybrid approach is not really defensible, but is perhaps the best compromise which can be applied in a general way. Nahar and Pradhan (1992) provide a clear explanation of some of the subtleties concerning dielectronic recombination. Figure 13 compares their results with HAOS-DIPER calculations using the OPACITY project data, for $O^{3+}+e \to O^{2+}$ and $Ne^{5+}+e \to Ne^{4+}$. Also included in the figure are the radiative and dielectronic coefficients from Shull and Steenberg (1982). Large and significant differences are apparent between these cases, where the "high-n" or "Burgess" dielectronic components are significant at higher electron temperatures. At lower temperatures, the HAOS-DIPER calculations using the OPACITY project data and the full treatment by Nahar and Pradhan (1992) are in far better agreement, although differences still exist. At very low particle densities, the calculations of Nahar & Pradhan are the most accurate. The detailed HAOS-DIPER calculations should be next most accurate, and the "radiative" components of the rate coefficients of Shull and Steenberg (1982), the least reliable.
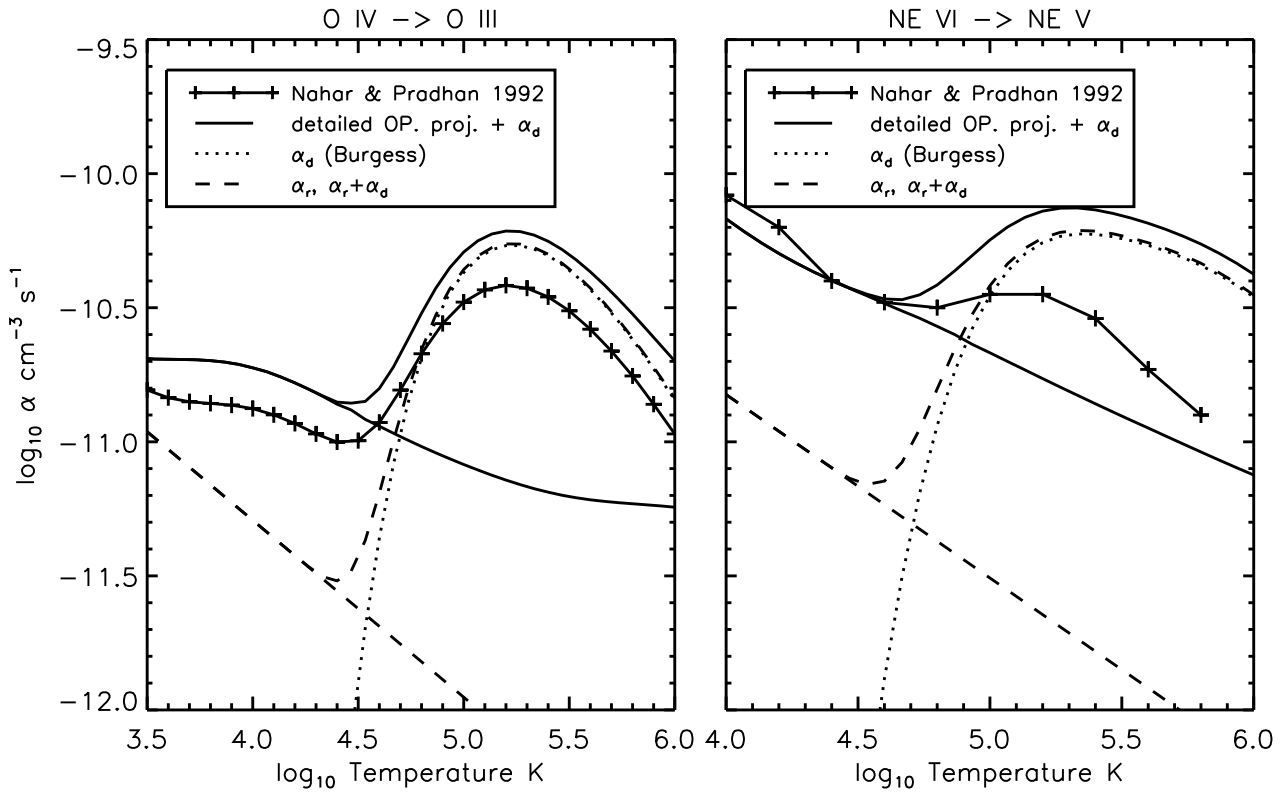
Figure 13: Recombination rate coefficients are shown as computed from the `HAOS-DIPER` (solid lines), with and without the dielectronic recombination rate of Shull and Steenberg (1982), and the detailed calculations of Nahar and Pradhan (1992) (solid lines with crosses). Radiative and dielectronic rates from Shull and Steenberg (1982), based on data without photoionization resonances near threshold (Aldrovandi and Pequignot 1973), are shown as dashed and dotted lines respectively. None of these calculations includes corrections for microfields associated with finite electron densities discussed in section A.4.

These problems again relate to the "chemical" picture instead of the "physical" picture which was adopted from the outset (section 2.1).

A.4   Fits to density dependent dielectronic recombination corrections

An attempt has been made to fit the density-dependent behavior exhibited by the calculations of Summers (1974a), in his evaluation of temperature and density dependent dielectronic recombination rates. The resulting "fit" to the behavior seen in Summers' tables 1-19, based upon trial and error, has just a few parameters, and is given as follows.

Let z be the charge on the recombining ion, of the element with atomic number A. If N_e is the electron density in cm^{-3}, define

$$\rho = N_e/z^7 \tag{25}$$

and let $y = A - z + 1$ (y is the number of electrons in the recombined ion, the element corresponding to its isoelectronic sequence). Then determine the row and column of the isosequence y in the periodic table, r_y, c_y. Then

$$x = (z/2 + (c_y - 1))\, r_y/3, \tag{26}$$
$$\beta = -0.2/ln(x + e), \tag{27}$$
$$\rho_0 = 30 + 50x, \tag{28}$$
$$\delta = (1 + \rho/\rho_0)^\beta. \tag{29}$$

Here, e is the base of the natural logarithms. The dielectronic components of the rate coefficients of Shull and Steenberg (1982) are multiplied by δ. $\delta = 1$ recovers the usual "low density" case.

The accuracy of this procedure is not known, and it is not vouched for. Nevertheless, the corrections δ are included because omitting them is arguably worse (e.g., Jordan 1969).

References

Aldrovandi, S. M. V. and Pequignot, D.: 1973, "Radiative and Dielectronic Recombination Coefficients for Complex Ions", *Astron. Astrophys.* **25**, 137

Allen, C. W.: 1973, *Astrophysical Quantities*, Athlone Press, Univ. London

Arnaud, M. and Raymond, J.: 1992, "Iron ionization and recombination rates and ionization equilibrium", *Astrophys. J.* **398**, 394

Arnaud, M. and Rothenflug, R.: 1985, "An updated evaluation of recombination and ionization rates", *Astron. Astrophys. Suppl. Ser.* **60**, 425

Badnell, N. R., O'Mullane, M. G., Summers, H. P., Altun, Z., Bautista, M. A., Colgan, J., Gorczyca, T. W., Mitnik, D. M., Pindzola, M. S., and Zatsarinny, O.: 2003, "Dielectronic recombination data for dynamic finite-density plasmas. I. Goals and methodology", *Astron. Astrophys.* **406**, 1151–1165

Burgess, A.: 1964, "Dielectronic recombination and the temperature of the solar corona", *Astrophys. J.* **139**, 776

Burgess, A. and Chidichimo, M. C.: 1983, "Electron impact ionization of complex ions", *Mon. Not. R. Astron. Soc.* **203**, 1269

Burgess, A. and Tully, J. A.: 1992, "On the Analysis of Collisions Strengths and Rate Coefficients", *Astron. Astrophys.* **254**, 436–453

Carlsson, M.: 1986, *A Computer Program for Solving Multi-Level Non-LTE Radiative Transfer Problems in Moving or Static Atmospheres*, Report No. 33, Uppsala Astronomical Observatory

Casini, R. and Judge, P. G.: 1999, "Spectral Lines for Polarization Measurements of The Coronal Magnetic Field. II. Consistent Theory of The Stokes Vector for Magnetic Dipole Transitions", *Astrophys. J.* **522**, 524–539

Casini, R. and Judge, P. G.: 2000, "Erratum: Spectral Lines for Polarization Measurements of The Coronal Magnetic Field. II. Consistent Theory of The Stokes Vector for Magnetic Dipole Transitions", *Astrophys. J.* **533**, 574–574

Cook, J. W., Cheng, C. C., Jacobs, V. L., and Antiochos, S. K.: 1989, "Effect of Coronal Elemental Abundances on the Radiative Loss Function", *Astrophys. J.* **338**, 1176–1183

Cowan, R. D.: 1981, *The Theory of Atomic Structure and Spectra*, University of California Press, Berkeley CA

Cox, D. P. and Tucker, W. H.: 1969, "Ionization Equilibrium and Radiative Cooling of a Low-Density Plasma", *Astrophys. J.* **157**, 1157–1167

Craig, I. J. D. and Brown, J. C.: 1976, "Fundamental Limitations of X-Ray Spectra as Diagnostics of Plasma Temperature Structure", *Astron. Astrophys.* **49**, 239–250

Craig, I. J. D. and Brown, J. C.: 1986, *Inverse problems in astronomy*, Hilger, Bristol

Daeppen, W., Lebreton, Y., and Rogers, F.: 1990, "The equation of state of the solar interior - A comparison of results from two competing formalisms", *Solar Phys.* **128**, 35–47

Dere, K. P., Landi, E., Mason, H. E., Monsignori Fossi, B. C., and Young, P. R.: 1997,

"CHIANTI - an atomic database for emission lines", *Astron. Astrophys. Suppl. Ser.* **125**, 149–173

Dufton, P. L. and Kingston, A. E.: 1981, "Atomic Processes in the Sun", *Adv. At. Molec. Phys.* **17**, 355–418

Feldman, U.: 1992, "Transitions from metastable levels emitted during short-duration bursts - How valid are their calculated intensities?", *Astrophys. J.* **385**, 758–762

Griem, H.: 1964, *Plasma Spectroscopy*, McGraw-Hill.

Hummer, D. G. and Mihalas, D.: 1988, "The equation of state for stellar envelopes. I - an occupation probability formalism for the truncation of internal partition functions", *Astrophys. J.* **331**, 794–814

Jordan, C.: 1969, "The ionization equilibrium of elements between carbon and nickel", *Mon. Not. R. Astron. Soc.* **142**, 501–521

Judge, P. G.: 1998, "Spectral Lines for Polarization Measurements of The Coronal Magnetic Field. I. Theoretical Intensities", *Astrophys. J.* **500**, 1009–1022

Judge, P. G.: 2005, "Understanding the evolution of atomic number densities with time in astrophysical plasmas", *J. Quant. Spectrosc. Radiat. Transfer* **92(4)**, 479–510

Judge, P. G., Hubeny, V., and Brown, J. C.: 1997, "Fundamental Limitations of Emission Line Spectra as Diagnostics of Plasma Temperature and Density Structure", *Astrophys. J.* **475**, 275–290

Judge, P. G., Low, B. C., and Casini, R.: 2006, "Spectral Lines for Polarization Measurements of The Coronal Magnetic Field. IV. Stokes signals in current-carrying fields", *Astrophys. J.* **651**, 1229

Judge, P. G. and McIntosh, S.: 2000, "Non-Uniqueness of Atmospheric Modeling", *Solar Phys.* **190**, 331–350

Judge, P. G. and Meisner, R.: 1994, "The HAO Spectral Diagnostics Package (HAOS-DIAPER)", in J. J. Hunt (Ed.), *The Third Soho Workshop, Solar Dynamic Phenomena and Solar Wind Consequences*, ESA SP-373, ESTEC, Noordwijk, the Netherlands, 67–71

Judge, P. G., Woods, T. N., Brekke, P., and Rottman, G. J.: 1995, "On the Failure of Standard Emission Measure Analysis for Solar EUV and UV Irradiance Spectra", *Astrophys. J. Lett.* **455**, L85–L89

Lamb, F. K. and ter Haar, D.: 1971, "The interaction of atoms with polarised light", *Phys. Rep.* **2**, 253

Landi, E., Del Zanna, G., Young, P. R., Dere, K. P., Mason, H. E., and Landini, M.: 2006, "CHIANTI-An Atomic Database for Emission Lines. VII. New Data for X-Rays and Other Improvements", *Astrophys. J. Suppl. Ser.* **162**, 261–280

Landi degl'Innocenti, E. L. and Landolfi, M.: 2004, *Polarization in Spectral Lines*, Vol. 307 of *Astrophysics and Space Library*, Kluwer Academic Publishers, Dordrecht

McIntosh, S., Brown, J. C., and Judge, P. G.: 1998, "The relation between line ratio and emission measure analyses", *Astron. Astrophys.* **333**, 333–337

McIntosh, S. W., Diver, D. A., Judge, P. G., Charbonneau, P., Ireland, J., and Brown, J. C.: 1998, "Spectral decomposition by genetic forward modelling", *Astron. Astrophys. Suppl. Ser.* **132**, 145–153

Mihalas, D.: 1978, *Stellar Atmospheres*, W. H. Freeman and Co., San Francisco (second edition)

Nahar, S. and Pradhan, A. K.: 1991, "Photoionization and electron-ion recombination: The carbon sequence", *Phys. Rev. A* **44**, 2935–2948

Nahar, S. and Pradhan, A. K.: 1992, " Electron-ion recombination in the Close-Coupling Approximation", *Phys. Rev. Lett.* **68**, 1488–1491

Pietarila, A. and Judge, P. G.: 2004, "On the formation of the resonance lines of helium in the Sun", *Astrophys. J.* **606**, 1239–1257

Ralchenko, Y.: 2005, "NIST atomic spectra database .", *Memorie della Societa Astronomica Italiana Supplement* **8**, 96

Ralchenko, Y., Jou, F.-C., Kelleher, D., Kramida, A., Musgrove, A., Reader, J., Wiese, W., and K., O.: 2005, *Atomic Spectra Database version 3.0*, NIST `http://physics.nist.gov/PhysRefData/ASD/index.html`

Rountree, S. P.: 1977, "Electron-impact excitation of atomic oxygen: $^3P - 3s^5S^o$ and $^3P - 3s^3S^o$", *J. Phys. B* **10**, 2719

Seaton, M. J.: 1962a, "The Impact Parameter Method for Electron Excitation of Optically Allowed Atomic Transitions", *Proc. Phys. Soc.* **79**, 1105

Seaton, M. J.: 1962b, "The Theory of Excitation and Ionization by Electron Impact", in D. R. Bates (Ed.), *Atomic and Molecular Processes*, Academic Press, New York, 11

Seaton, M. J.: 1983, "Quantum defect theory", *Reports of Progress in Physics* **46**, 167–257

Seaton, M. J.: 1987, "Atomic data for opacity calculations: I. General description", *J. Phys. B: At. Mol. Phys.* **20**, 6363–6378

Shull, J. M. and Steenberg, M. V.: 1982, "The ionization equilibrium of astrophysically abundant elements", *Astrophys. J. Suppl. Ser.* **48**, 95

Storey, P. J.: 1981, "Dielectronic recombination at nebular temperatures", *Mon. Not. R. Astron. Soc.* **195**, 27P–31P

Summers, H. P.: 1974a, *Collisional dielectronic recombination and ionisation coefficients and ionisation equilibria of H-like to Ar-like ions of elements*, Technical Report 367, Culham Laboratory

Summers, H. P.: 1974b, "The ionization equilibrium of hydrogen-like to argon-like ions of elements", *Mon. Not. R. Astron. Soc.* **169**, 663–680

Summers, H. P.: 2003, *The ADAS User Manual*, `http://adas.phys.strath.ac.uk`

Summers, H. P. and Kato, T.: 2000, "Extension of the Burgess-Tully method to fit neutral atom and molecule cross-sections", *Astron. Astrophys.* **144**, 501–507

Van de Hulst, H. C.: 1953, "The chromosphere and the corona", in G. P. Kuiper (Ed.), *The Sun*, Chicago University Press, Chicago, 207–321

Van Regemorter, H.: 1962, "Rate of Collisional Excitation in Stellar Atmospheres", *Astrophys. J.* **136**, 906

Vernazza, J., Avrett, E., and Loeser, R.: 1981, "Structure of the solar chromosphere. III - Models of the EUV brightness components of the quiet-sun", *Astrophys. J. Suppl. Ser.* **45**, 635

Woolley, R. D. V. R. and Allen, C. W.: 1948, "The Coronal Emission Spectrum", *Mon. Not. R. Astron. Soc.* **108**, 292–305

Index