SYNSPEC — A User's Guide

Version 43

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I.Hubeny and T. Lanz, NASA/GSFC, Code 681, Greenbelt, MD 20771

1 General characteristics

Unlike stellar atmospheric program TLUSTY (Hubeny 1988), this program does not have any comprehensive published description. A brief description of the program was given by Hubeny et al. (1985). Program SYNSPEC is a general spectrum synthesis program. It assumes that the model atmosphere (or an accretion disk model – vertical structure of one ring) is given; either calculated by TLUSTY (or TLUSDISK), or taken from the literature, as for instance from the Kurucz (1979; 1994 CDROMs) grid of models. Program reads a general line list (typically that of Kurucz 1991), and dynamically selects lines which contribute to the total opacity, based on physical parameters of the actual model atmosphere. SYNSPEC then solves the radiative transfer equation, wavelength by wavelength, in a specified wavelength range, and with a specified wavelength resolution. The wavelength points generally are not equidistant. Instead, they are calculated by the program in such a way that there is always a wavelength point at a line center, and in the midpoint between two neighboring lines. The program then adds a certain number of points, equidistantly spaced between these two, such that the interval between the points does not exceed some prespecified value (SPACE – usually about half of a typical Doppler width of a typical metal line). This procedure assures that neither any line center nor any continuum window is omitted.

The adopted continuum as well as line opacity is fully specified by the user. In principle, the line and continuum opacity sources used in calculating a model stellar atmosphere and in calculating the detailed spectrum should be identical. However, it is a common practice that model atmospheres, particularly those allowing for some departures from LTE, are calculated with fewer opacity sources (lines and continua) than a subsequent calculation of a synthetic spectrum. The rationale for this approach is that the atmospheric structure (*i.e.* the run of temperature and number densities) is predominantly influenced by the strongest opacity sources, while the emergent spectrum has to be computed in detail.

1.1 Improvements over version 42

The most significant change with respect to the version 42 is an inclusion of molecular lines. Also, the internal definition of the solar abundance was modified from the previous old "solar" abundances to more recent ones from Grevese (19xx). Besides, there is a number of small modifications, transparent to the user.

1.2 Basic modes of operation

1.2.1 Standard mode – IMODE=0

In the basic mode the program proceeds first by selecting lines which may potentially contribute to the total opacity. This is done by selecting the "characteristic depth" in the atmosphere (IDSTD – see description of input file 55), which is roughly given as a depth of formation of the continuum. The program reads the line list, calculates the opacity in the line center at the characteristic depth, and rejects all lines whose central opacity is less than a selected fraction of the continuum opacity (parameter RELOP; typically 0.0001 to 0.001). The parameters for all selected lines are stored in (relatively big) arrays in the program.

Note: in the prehistoric versions of SYNSPEC the line list was read over and over again, to avoid large arrays which contain data for all selected lines. However, this procedure, albeit very memory efficient, was extremely time consuming. Since the memory seemed to be no longer an issue in most computers and workstations, SYNSPEC version 24 changed this strategy by storing data for *all* selected lines in several big arrays. However, since the number of lines may be enormous, we have recently adopted a hybrid strategy: the maximum dimension of array is specified (typically 10000 to 100000, depending on the available computer memory). If this number is reached before the end of the intended wavelength interval is reached, SYNSPEC computes a spectrum for a corresponding interval covered with selected lines, and then reads the line list again. This strategy thus combines advantages of those used previously: avoiding an excessive number of I/O operations, and avoiding an excessive memory consumption.

The program then proceeds by calculating many small intervals of spectrum, called "sets". One set is defined as an optional number of wavelength points (MFREQ; typical value is 120) set up by the program as outlined above; the pure continuum opacity is calculated at the endpoints of the interval and linearly interpolated in between. The first two points of the set apply for the pure continuum radiation field, and the remaining (MFREQ−2) points describe the spectrum including all lines. The wavelength interval of the individual sets varies because the wavelength points are set by the program, depending on the number of contributing lines and on RELOP; it is typically (for the optical and UV region) about 0.5 - 2 Å. For each set, the program sets up a subset of lines which contribute in the corresponding interval, both those lines which are located in the interval, as well as those which are "close" and may therefore contribute through their wings. The program provides an output of the parameters for all selected lines (Unit 12 and, if required, also the standard output on Unit 6). This provides an internal identification of computed lines.

To make the identification easier, the program also calculates an approximate equivalent widths of all selected lines, using the ratio of line-center opacity to the continuum opacity and the broadening parameter at the standard depth. The equivalent widths are calculated by means of the classical theory (see e.g. Mihalas 1978, Chapter 10.). It should be kept in mind that *these equivalent widths are meant for the identification purposes only*, and do not represent the actual predicted equivalent widths. It is impractical to calculate automatically the actual equivalent widths for all lines because virtually all predicted features are blends of several lines. Therefore, the program only calculates the total equivalent width for each set (output onto Unit 16).

The other basic modes of SYNSPEC are similar.

1.2.2 A few-lines option – IMODE=1

This mode is almost identical to the basic mode; the only difference is that the wavelengths are selected equidistantly. Also, the program works well even if the line list contains just one line, which it is not possible in the basic mode IMODE=0 since the program is not able to select the

wavelength points properly.

1.2.3 A continuum option – IMODE=2

In this mode the line opacity is set to zero. The program thus calculates the opacity (and consequently emergent flux) in the continuum. However, by default, the hydrogen lines are also taken into account. If the parameter IFHE2 (see Sect. 3) is set to 1, the He II lines are also included in this mode.

1.3 Molecular option – IMODE≥10

In this mode the molecules are included. They change the situation with respect to the previous modes in essentially two ways:
(i) The presence of molecules changes the state equation, sinc some atomic species are being depleted by a molecular formation; and
(ii) there is an additional opacity due to molecular lines. In the present version the molecular continua, i.e. an absorption of photons due to radiative dissociation, is neglected.

The meaning of IMODE in this case is that IMODE−10 has the analogous meaning to the previous IMODE; i.e., IMODE=10 corresponds to the standard molecular option, IMODE=11 the option with few lines, and IMODE=12 the "continuum" mode, in which molecules are allowed to contribute in the state equation, but the molecular opacity is neglected.

1.3.1 Identification mode – IMODE=−1

(IMODE=−1) proceeds similarly as the basic mode, only does not perform the most time-consuming step – solving the radiative transfer equation and producing the synthetic spectrum. The program only produces the identification table, which may be useful for a number of purposes.

1.3.2 Iron curtain mode – IMODE=−2

It calculates a monochromatic opacity for a homogeneous slab of given temperature and density. The input model atmosphere therefore consists of one single line of input which contains the parameters of the slab.

1.4 Continuum opacity

The continuum opacity is calculated exactly the same way as in TLUSTY, and its evaluation is controlled by the data provided from Unit 5, plus possibly other files as specified by the standard input. The program considers the following default continuum opacity sources: i) photoionizations from all explicit levels (possibly including pseudo-continua due to dissolution of Rydberg states as described by Hubeny, Hummer and Lanz 1994); ii) free-free opacity for all explicit ions; and iii) electron scattering. The optional continuum opacity sources, included in the program and switched on by setting a corresponding flag, are the Rayleigh scattering, the H^- bound-free and free-free opacity, and the H_2^+ opacity. If SYNSPEC is used for calculating spectra for a model previously calculated by TLUSTY, the necessary data are already available from the previous runs of TLUSTY. For the use of SYNSPEC for calculating synthetic spectra for Kurucz models, the user has to set up the data set him/herself, or can use a TLUSTY data set for a model with similar basic parameters. We stress that in the latter case, the 'explicit' levels, which are originally meant to be the 'NLTE' levels, are set to LTE anyway; the only reason for them being considered as explicit is that the photoionizations from them are selected as the contributing continuum opacity sources.

1.5 Atomic line opacity

If the input model atmosphere was calculated assuming LTE, then the source functions for all the lines and continua also have their LTE values (i.e. are given by the Planck function). If the input model specifies that some atomic energy levels depart from LTE, then the lines originating between these NLTE levels are calculated by a corresponding NLTE source function. (They do not have to be, though; the user may force LTE). If only a few levels of an ion were taken in NLTE in the model construction, the program takes the NLTE value for those, and LTE values for the remaining levels. Finally, for the lines originating between levels for which no precalculated NLTE population are available one may still use an approximate NLTE treatment, based on the second-order escape probability theory, as described by Hubeny et al. (1986). The NLTE treatment of lines is described in detail in Sect. 5.

The intrinsic line profiles have the form of a Voigt function and take into account the effects of natural, Stark, Van der Waals, and thermal Doppler broadening. The line broadening data are either given in the line list (see Sect. 3.3), or, if no broadening parameters are given, are assumed to be given by the classical expressions (see, e.g., Kurucz 1979). The user may also choose to take the Stark broadening data from Griem (1974); in this case the line list has to contain an additional record (see Sect. 3.3).

For hydrogen and helium, the user may choose from several options, ranging from approximate profiles to the use of detailed tables. For hydrogen, the best option is to use tables calculated by Vidal, Cooper, and Smith (1973) for the first four members of the Lyman and Balmer series, supplemented and upgraded recently by Schöning and Butler (private communication) up to H_{10}. For higher members of the spectral series (together with an occupation probability treatment of high level dissolution), the approach described by Hubeny, Hummer and Lanz (1994) is used as default. For He I, detailed line broadening tables for the λ 4471 line are from Barnard, Cooper and Smith (1974), those for $\lambda\lambda$ 4026, 4387, and 4922 are from Shamey (1969), and those for all other lines, from Dimitrijevic and Sahal-Brechot (1984). For He II, the tables calculated by Schöning and Butler (1989) and Schöning (1995) may be used.

1.6 Molecular line opacity

The molecular lines are treated analogously to atomic lines. In the present version, molecular lines are *always* in LTE. The line data are stored in a separate file from the atomic lines. The molecular line data were taken from Kurucz CDROM 15.

2 Compiling and linking

The program is distributed as several files. The largest is `SYNSPECnn`, `nn` represents the current version number. Communication between subprograms is principally carried out through labeled common blocks, and to allow for the program to be scaled easily, arrays are dimensioned by parameter constants. The arrays and parameters are defined using INCLUDE files `PARAMS.FOR, LINDAT.FOR, MODELP.FOR, SYNTHP.FOR` The parameters defining array dimensions appear in `PARAMS.FOR` and `LINDAT.FOR`. The crucial number `MLINO`, which specifies the total number of selected lines, is in file `LINDAT.FOR`.

The compilation and linking is done, in UNIX, as follows:

```
f77 [-N160] [-O4] synspec42.f
```

where the option "-Nl60" is sometimes needed for older SPARCstations to increases the allowed number of continuation lines to 60. The optimization (the option -O4) is a default at most workstations. If not, the optimization should be switched on since it improves the performance of the code considerably.
The INCLUDE file names must appear in capital letters.

3 Input data

The following input files may be required by SYNSPEC; the corresponding subroutines in which they are accessed are shown in parentheses:

1. Basic input
   - Unit 1 — Same file as used for TLUSTY - indicator of the input format
   - Unit 5 — Same file as used for TLUSTY - basic input file
   - non-standard flag file — Same file as used for TLUSTY; its actual name is specified in Unit 5
   - Unit 55 — Basic parameters for the synthetic spectrum (`START, INIBLO`)
   - Unit 8 — Model atmosphere (`INPMOD, INKUR`)
   - Unit 19 — Linelist (`INILIN`)
2. Additional – optional – input
   - Unit 20 — Molecular line list (`INMOLI`)
   - Unit 56 — Change of chemical composition with respect to the input model atmosphere (`STATE0`)
   - Unit IHYDPR — Detailed Balmer line profiles (`HYDINI`)
   - Unit IHE1PR — Detailed HeI 4026, 4388, 4471, and 4922 line profiles (`HE1INI`)
   - Unit IHE2PR — Detailed HeII line profiles calculated by Schoening and Butler (`HE2INI`)
   - Unit 13 — list of ions with superlevels and limiting energies for superlevels, used for detailed bound-free cross-sections (`NLTSET`)
   - Unit 54 — detailed non-explicit superlevel photoionization cross-sections (`SIGAVS`) – see Sect.6
   - Unit 57 — detailed photoionization cross-section (`READPH`) – see Section 6
   - Auxiliary molecular files — This is the only case where the program uses hird-wired file names. There are three auxiliary molecular files that are distributed together with the source program:
     - `tsuji.atoms` — basic data for atoms needed for the molecular state equation routine
     - `tsuji.molec` — data for the individual molecules
     - `irwin.dat` — low-T atomic partition function data (after Irwin 1981)
   - Other — there may be other input files for detailed bound-free cross-sections; the unit numbers are specified in Units 54, 57, as well as 5 (`SIGAVS, READPH`) – see Sect. 6

Note: Unit numbers IHYDPR, IHE1PR, IHE2PR are not hard-wired in the code; instead they are specified by the user in the input file on unit 55.

Units 1 and 5

These files are deliberately kept in exactly the same form as for TLUSTY. Although not all parameters needed for TLUSTY are required for a run of SYNSPEC, this arrangement is very convenient from the point of view of the user, since it eliminates a need to create another standard input file.

The reader is referred to the TLUSTY User's Guide for a detailed description of the Unit 5 input.

The data needed for the run of SYNSPEC are basically the numbering of explicit atoms, ions, and levels, and the way that the continuum opacity is calculated.

Unit 55: Basic parameters for the synthetic spectrum

The file contains fundamental parameters for evaluating the synthetic spectrum. There are 6 or 7 lines in the file.

1. The first line of input contains the following parameters:

   IMODE – basic mode of SYNSPEC:
   $= 0$ – normal synthetic spectrum
   $= 1$ – detailed profiles of a few individual lines
   $= 2$ – emergent flux in the continuum (without the contribution of lines)
   ≥ 10 – molecular option. The meaning of IMODE in this case is that IMODE-10 has the analogous meaning to the previous IMODE; i.e.,
   $= 10$ – standard molecular option
   $= 11$ – the molecular option with few lines
   $= 12$ the "continuum" mode, in which molecules are allowed to contribute in the state equation, but the molecular opacity is neglected.
   $= -1$ – identification table, ie. a list of lines which contribute to opacity in a given wavelength region, together with their approximate equivalent widths. Synthetic spectrum is not calculated.
   $= -2$ – the "iron curtain" option, ie. a monochromatic opacity for a homogeneous slab of a given T and n_e

   IDSTD – index of the "standard depth" (ie the depth at which the continuum optical depth is of the order of unity) (for detailed explanation see the guide for TLUSTY)

   IPRIN – determines the amount of output:
   $= 0$ – standard output: condensed output on unit 6 (basics + error messages), no output on unit 36 (depths of formation); normal output on 16 (equivalent widths); normal output on 12 (identification table)
   > 0 – more output:
   $= 1$ – emergent flux on unit 6, no unit 36
   $= 2$ – identification table + flux on unit 6, no unit 36
   $= 3$ – as before, plus unit 36 (depths of formation);
   < 0 – less output:
   $= -1$ – no output on unit 16
   $= -2$ – no output on units 16 and 12

2. The second line of input contains the following parameters

INMOD – indicator of the type of input model atmosphere:
= 0 – input model atmosphere as a Kurucz model (read by procedure INKUR) = 1 – input model atmosphere is a model calculated by the program TLUSTY (read by procedure INPMOD)
= 2 – input model is a model of the vertical structure of one ring of an accretion disk

INTRPL – switch indicating whether the input model has to be interpolated to the present depth scale (for details see the guide for TLUSTY)

ICHANG – switch indicating whether the populations from the input model have to be updated (for details see the guide for TLUSTY)

ICHEMC – switch indicating that new chemical composition will be read from unit 56

3. The third line of input contains the following parameter

IOPHLI – switch for treatment the Lyman line far wings
= 0 – only Stark broadening of far wings of Lyman lines
= 1 – normal treatment of Lyman lines – Stark + natural broadening; complete redistribution.
If the special line broadening parameter HYDPRF (see below) is set to a non-zero value (i.e. one uses Schoening's hydrogen Stark broadening tables), coding of IOPHLI=1 will add only natural broadening of Lyman lines (that is, Stark broadening is not taken twice).

4. The fourth line of input contains the following parameters

IFREQ – switch for choosing the scheme of numerical solution of the radiative transfer equation
$\leq$ 10 – the DFE (discontinuous finite element) scheme (subroutines RTEDFE and RTECD).
$>$ 10 - Feautrier scheme (subroutine RTE)

INLTE – indicator of the treatment of LTE or NLTE
= 0 – pure LTE (no lines in NLTE)
$\neq$ 0 – NLTE option, ie one or more lines treated in the exact or approximate NLTE approach

ICONTL – a relatively un important switch indicating whether the Lyman and Balmer lines are considered as the continuum opacity source
= 1 – Lyman and Balmer lines are considered as a continuum opacity source
$\neq$ 0 – Lyman and Balmer lines are not considered as an continuum opacity source

INLIST – dummy variable, set to 0 (kept for historical reasons)

IFHE2 – the He II opacity switch.
= 0 – no pseudocontinuum (i.e. the merging of high series members near the series limits); only lines contained in the line list are taken into account; and moreover with classical Stark broadening (which is inaccurate!)
$>$ 0 – the pseudocontinuum is taken into account (by means of occupation probabilities); and all lines are taken with more exact Stark + Doppler broadening. The lines from the line list are replaced by hard-wired data from SYNSPEC. In other words, He II is treated completely analogously to hydrogen. This is usually a recommendable option, but may cause numerical problems (underflows etc.) for low effective temperatures.

5. The fifth line of input contains the special line broadening parameters:

   IHYDPR – a switch for special hydrogen line broadening table.
   $= 0$ – SYNSPEC uses an approximate Stark broadening treatment (after Hubeny, Hummer, & Lanz 1995).
   > 0 – specifies the unit number for the special hydrogen line broadening table (Schoening, priv.comm) for the first four Lyman lines, and the first eight Balmer lines.

   IHE1PR – a switch for special He I line broadening table.
   $= 0$ – SYNSPEC uses an approximate Stark broadening treatment. > 0 – specifies the unit number for the special He I line broadening table (after Barnard, Cooper, and Shamey) for four lines: λ 4471, 4388, 4026, and 4922 Å.

   IHE2PR – a switch for special hydrogen line broadening table.
   $= 0$ – SYNSPEC uses an approximate Stark broadening treatment (after Hubeny, Hummer, & Lanz 1995).
   > 0 – specifies the unit number for the special He II line broadening table (Schoening, priv.comm) for transitions 2-3; 3-4 to 3-10; and 4-5 to 4-15.

6. The sixth line of input contains the following parameters:

   ALAM0 – the short-wavelength limit (in Å) of the synthetic spectrum (in Å).

   ALAM1 – the long-wavelength limit of the synthetic spectrum (in Å).

   CUTOF0 – the cutoff for a line opacity (i.e. a line is allowed to contribute to the total opacity within the distance of $\Delta\lambda =$ CUTOFF (in Å) from the line center. Recommended value is 10 - 20 Å.

   CUTOFS – dummy variable (kept for historical reasons)

   RELOP – the minimum value of the ratio (opacity in the line center)/(opacity in continuum), for which is the line taken into account (usually 10^{-4} to 10^{-3})

   SPACE – the maximum distance of two neighboring frequency points for evaluating the spectrum (in Å).

7. The following record is required only if the user wants to change the value of turbulent velocity from that considered in the input file for TLUSTY (either Unit 5 – in the old format, or the non-standard flag file – in the new format):

   VTB – turbulent velocity (in km/s) (notice that the standard model atmosphere input also contains the turbulent velocity. That value is overwritten by VTURB.

8. The following record is present only in case the specific intensities are required. It contains three numbers:

   NMU0 – number of angles for evaluating specific intensity; angles are expressed as directional cosines μ)
   > 0 – and if also ANG0> 0, angles (μ's) equidistant between 1 and ANG0
   > 0 – and if also ANG0< 0, angles (μ's) equidistant between 0.7 and ANG0, and sinuses equidistant for others
   < 0 – angles are read in the next record

   ANG0 – minimum μ (see above)

IFLUX – mode for evaluating angle-dependent intensities and the corresponding flux:
= 0 – no specific intensities are evaluated; only usual flux is stored (unit 7 and 17)
= 1 – specific intensities are evaluated; and stored on unit 18
= 2 – (interesting only for the case of macroscopic velocity field); specific intensities evaluated by a simple formal solution (RESOLV)

Unit 56: Abundance change

The structure of the file has been changed with respect to the previous versions. It is now much simpler. The first record specifies the number of chemical elements for which the abundances are going to be changed; then for each such element there is one record which specifies the atomic number, and the corresponding abundance. The abundance value is coded is in TLUSTY:

- if the value is positive, it means the abundance by number, relative to hydrogen;
- if the value is zero, it is set to the solar abundance;
- if the value is negative, the absolute value then means the relation with respect to the solar abundance (e.g., -5.5 means 5.5 times the solar abundance, etc.).

Unit 19: Line list

The line list has a very similar format to the original Kurucz and Peytremann (1975) tables; however we use recent Kurucz (1990) data, moreover updated and supplemented by more accurate data wherever available.

The structure of the file is very simple: for each spectral line, there are one (or two) records, which contain the following parameters (the description is again taken verbatim as appears in subroutine `INILIN`.

```
C
C    ALAM    - wavelength (in nm)
C    ANUM    - code of the element and ion (as in Kurucz-Peytremann)
C              (eg. 2.00 = HeI; 26.00 = FeI; 26.01 = FeII; 6.03 = C IV)
C    GF      - log gf
C    EXCL    - excitation potential of the lower level (in cm*-1)
C    QL      - the J quantum number of the lower level
C    EXCU    - excitation potential of the upper level (in cm*-1)
C    QU      - the J quantum number of the upper level
C    AGAM    = 0. - radiation damping taken classical
C            > 0. - the value of Gamma(rad)
C    GS      = 0. - Stark broadening taken classical
C            > 0. - value of log gamma(Stark)
C    GW      = 0. - Van der Waals broadening taken classical
C            > 0. - value of log gamma(VdW)
C    INEXT   = 0  - no other record necessary for a given line
C            > 0  - next record is read, which contains:
c
C    WGR1,WGR2,WGR3,WGR4 - Stark broadening values from Griem (in Angst)
C                   for T=5000,10000,20000,40000 K, respectively;
C                   and n(el)=1e16 for neutrals, =1e17 for ions.
C    ILWN    = 0  - line taken in LTE (default)
C            > 0  - line taken in NLTE, ILWN is then index of the
C                   lower level
C            =-1  - line taken in approx. NLTE, with Doppler K2 function
C            =-2  - line taken in approx. NLTE, with Lorentz K2 function
```

```
C    IUN     = 0  - population of the upper level in LTE (default)
C             > 0  - index of the lower level
C    IPRF    = 0  - Stark broadening determined by GS
C             < 0  - Stark broadening determined by WGR1 - WGR4
C             > 0  - index for a special evaluation of the Stark
C                    broadening (in the present version only for He I -
C                    see procedure GAMHE)
```

Unit 8: Model atmosphere

The program accepts either a TLUSTY model atmosphere (Unit 7 output there), or Kurucz model atmosphere in the new format (tapes distributed by R. Kurucz starting from the late 1980's and early 1990's; Kurucz's CD ROMs). We stress that the first depth point in a Kurucz model is removed because it has been calculated by ATLAS incorrectly (showing a sharp decrease of temperature between the second and the first point). While this feature is likely inconsequential in the context of Kurucz's programs, which use an integral method to solve the radiative transfer equation, it may sometimes cause large numerical problems in our scheme which uses the Feautrier (i.e. differential) scheme (see Mihalas 1978).

4 Output

There are several output files. By default, all the output files are generated as ASCII files for portability.

- Unit 6 – Standard output
- Unit 7 – Synthetic spectrum - flux
- Unit 10 – Synthetic spectrum - specific intensities (optional)
- Unit 12 – Identification table
- Unit 14 – Identification table (hydrogen lines only; if any)
- Unit 15 – Identification table for molecular lines (optional)
- Unit 16 – Equivalent widths for all 'sets'
- Unit 17 – Theoretical continuum flux
- Unit 18 – Theoretical continuum specific intensities (optional)

Unit 6: Standard output.

This a general log of the model construction procedure, It contains tables displaying the input data, some performance (and possibly error) messages, and optionally prints several tables of the emergent spectrum. In most cases, these tables are self-explanatory. The amount of output is controlled by the parameter IPRIN (input from unit 55).

Unit 7 and 17: Emergent flux

These are the basic output files. Unit 7 contains a detailed synthetic spectrum, and consists of a simple table of wavelength versus flux, for all wavelength points considered. The wavelength is expressed in Å, and the flux is expressed as H_λ, in erg cm^{-2}s^{-1}Å^{-1}. Unit 17 has an analogous format, and contains the flux for the *theoretical continuum.*

Both files may serve as an input to another program ROTINS, which performs rotational and instrumental convolutions, and sets up files for a plot.

Unit 10 and 18: Emergent specific intensity

These files are produced only if the user so requires (IFLUX=1 in Unit 55 input). The angles (specified as $\mu = \cos\theta$, where θ is the angle of propagation with respect to the normal to the surface), are specified by the user (also in unit 55). The output specific intensities are expressed in erg cm^{-2}s^{-1}Hz^{-1}sterad^{-1} (notice the difference from the flux - units 7 and 17 - which is given in the wavelength units). The structure of the files is as follows: for each wavelength, there are two or more lines of output, depending on the number of angles. The first line contains the wavelength (in Å) and the flux, the second line the first five specific intensities, and each following line specific intensities for five subsequent angle points. The last line contains *mod*(NANGLE,5) entries.

Units 12 and 14: Identification table

The structure of the file is as follows: for each selected spectral line, there is one output record, which contains 12 entries: the first two numbers are internal indices of the line (the first one in the indexing of lines in the given "set"; the second one in the global indexing - these numbers are normally not interesting for a user, unless there are some problems); the following entries are; wavelength (in Å); spectroscopic identification of an atom and ion; log gf; excitation potential of the lower level (in cm^{-1}); ratio of the line center opacity to the continuum opacity at the standard depth (given by IDSTD - input from unit 55); approximate equivalent width (in mÅ) – calculated by the classical theory, using the values at the standard depth; a visual identification of expected line strength (with increasing value of the approximate equivalent width the labels are respectively a blank, a dot, a star, two or more stars). The next two numbers are indices of NLTE levels in the case that the line was treated in NLTE. Finally, the last number is the depth of formation, i.e. the depth index for which the monochromatic optical depth in the line center is closest to 2/3).
The file is not produced if the input parameter IPRIN≤ -1.

Unit 16: Equivalent widths

As discussed in Sect. 3.1, this file contains a list of total equivalent widths (in mÅ) for all individual 'sets', i.e. frequency intervals containing 120 wavelength points and set up automatically by the program.
The file is not produced if the input (unit 55) parameter IPRIN≤ -2.

5 Details of NLTE treatment of lines

By default, the *line* source function is treated in LTE, i.e. is assumed to be given by the Planck function. Notice that the *total* monochromatic source function is given as a weighted sum of all contributions from the corresponding line source functions, the continuum source function, and that

for electron scattering. The latter two are by default treated in NLTE for NLTE model atmospheres. As far as the lines are concerned, the program allows for two kinds of NLTE treatment:

1. **exact NLTE**, which is possible only if the given line is a transition between levels which were treated in NLTE in the input model atmosphere. If only one level was the NLTE level, the other one is taken with an LTE population (i.e. in LTE with respect to the ground state of the next ion, which, may or may not be an explicit level in TLUSTY).

   The corresponding level indices are communicated to SYNSPEC either

   - "manually" – by modifying the line list. i.e. by explicitly putting the indices of NLTE levels for each line (the additional line of the line list input – see Sect. 3);
   - automatically – in this case SYNSPEC itself finds the corresponding level indices based on the level energies. For species for which the NLTE level considered by TLUSTY are actually "superlevels" (many genuine levels merged together and treated as one - see Hubeny and Lanz 1995), SYNSPEC needs an additional input file (Units 13) to identify the relevant ions and to communicate the limiting level energies used by TLUSTY (see Sect. 5.1).

2. **approximate NLTE**, where the source function is assumed to be given by an analytical expression following from the second-order escape probability theory (see Sect. 5.2). Again, the choice of line to be treated in this way is either

   - manual – i.e. by modifying the line list adding an additional line with the lower level index set to ILWN $= -1$ – see Sect. 3);
   - automatic – the so-called "implied NLTE" option. In this case a whole group of lines is treated in the second-order escape probability theory, without the necessity of changing the line list. The available options are specified in detail below.

5.1 Exact NLTE treatment of lines

Exact NLTE treatment of lines is switched on by setting the parameter INLTE > 0. Switching INLTE to positive values for an LTE model atmosphere does not have any effect. If INLTE $= 0$ is coded for an input NLTE model atmosphere, the synthetic spectrum is calculated assuming the input (NLTE) populations used for evaluating the continuum opacities, but LTE Saha-Boltzmann populations are used for computing line opacities. The exceptions are hydrogen lines which cannot be put to LTE (SYNSPEC treats hydrogen lines more as a continuum than as lines. Similarly, the He II lines are treated in NLTE even if INTE=0, if the parameter IFHE2 is set to 1 (for an input NLTE model, obviously). In other words, if IFHE2 $= 1$, the He II lines are treated in the exactly the same manner as the hydrogen lines, i.e. regardless of the line list (Unit 19) - all the necessary information about He II lines is hardwired in the program.

5.1.1 Assignment of NLTE level indices

A TLUSTY model contains a number of atomic level populations, which are ordered in the way specified by the standard input. A given atomic energy level is referred to in TLUSTY by its global index. In contrast, the atomic energy levels in the line list communicated to SYNSPEC (Unit 19) are quite independent of the list of levels TLUSTY has worked with. This does not create any problems for computing continuum opacities, because they are evaluated according the same

procedures as in TLUSTY. The only problem is to correctly assign level indices to the bulk of lines listed for a given NLTE atom/ion in the line list. As mentioned above, there are two possibilities:

i) the manual assignment. In this case, the input line list has to be modified as described above (setting ILWN and possibly IUPN to actual level indices). This option is useful if there are only very few NLTE lines, and/or if the set of NLTE levels adopted in TLUSTY is very small. However, this way is rather cumbersome, because the user has to keep in mind that different TLUSTY models may have different NLTE levels, so the line list for SYNSPEC has to be carefully checked. Obviously, incompatible NLTE level indices may easily lead to spurious emission lines and all kinds of unexpected and funny results.

ii) Therefore, the automatic assignment of level indices is much more advantageous. It is simply switched on by setting the parameter INLTE to a non-zero value (1 or 2 – see below), as before, but *not modifying the line list at all.* There are four different types of lines:

- **Hydrogen**: As discussed above, the hydrogen lines are always evaluated using the TLUSTY populations (NLTE or LTE, depending on the input model atmosphere); the user has no means to change that

- **Helium**: For a NLTE model, and for INLTE$\geq$1, the level indices are *always* assigned automatically. (Note: this feature was present already in the previous versions). Helium lines may be put to LTE, even in a NLTE model (if the user really wants to do that), by coding INLTE=0, except for the He II lines when IFHE2 is set to 1.

- **Light elements**, i.e. other elements, not treated in TLUSTY by means of superlevels (typically C, N, O, Si, Mg, etc.): the level assignment is done automatically; no additional input is necessary. If, however, the user chooses to change the corresponding entry in the line list, the level indices given there take precedence over the indices set up automatically. The latter procedure is useful in cases when one deals with very complicated atomic energy level systems for which the automatic procedure may give incorrect results.

  The automatic level assignment is based solely on level energies. It assumes that all actual energy levels with energies between $(E_i + E_{i-1})/2$ and $(E_i + E_{i+1})/2$ [or between 0 and $(E_2 - E_1)/2$ if $i = 1$, i.e. the ground state] have the *same b-factor* (NLTE departure coefficient) as level i; index i refers to the level considered by TLUSTY. In other words, all levels found in the line list with energies in the above range are assigned index ILWN=i.

  There are two different treatments of the highest levels, which are selected by means of the value of the flag INLTE:

  i) for INLTE=1, the limiting energies for the last TLUSTY NLTE level i of an ion are $(E_i - E_{i-1})/2$ and $E_i + (E_i - E_{i-1})/2$. In other words, all levels with energies between $E_i + (E_i - E_{i-1})/2$ and the ionization limit are assigned the index ILWN=0, i.e. are treated in LTE.

  ii) for INLTE=2, the lower limiting energy for the last explicit NLTE level is the same, while the upper limiting energy is the ionization energy. In other words, all actual levels with energy between $(E_i - E_{i-1})/2$ and the ionization limit are assigned index ILWN=i (i being the last NLTE level of the ion); i.e. all high levels share the same b-factor with the last explicit TLUSTY level.

- **Iron-peak elements**, i.e. elements with superlevels: In this case, the assignment of level (i.e. superlevel) indices is similar. However, since the superlevels for TLUSTY were constructed taking into account level parity, and energy limits, these energy limits have to be

communicated to SYNSPEC on a separate input file. We refer to its unit numbers as 13, but this can be easily changed, since the actual input file has the unit numbers INLLEV, which is assigned value 13 in subroutine `NLTSET`. The structure of Unit 13 is as follows: the first line specifies the number of ions with superlevels – NNION (for instance, NNION=3 if Fe IV, Fe V, and Fe VI were treated with superlevels). Then there are NNION blocks, each containing the header with the atomic number (e.g. 26 for iron), and the ion number (zero for neutrals, 1 for once ionized, etc.). The next line contains a single number, NEVEN, specifying the number of *even* superlevels. This is followed by NEVEN records lines which each contains the index of the superlevel, the upper limit of energy, and the mean energy of the superlevel. The same input is then provided for *odd* levels. All energies are expressed in cm^{-1}.

5.1.2 Laser lines

The laser effect, namely the situation where the line opacity (treated as absorption minus stimulated emission) is negative, is an effect which may arise solely in NLTE situations. Indeed, in LTE, the line center opacity is proportional to $n_i^*[1-\exp(-h\nu/kT)]$ times a positive constant, and is therefore always positive. In NLTE, it is given by $(n_i - g_i n_j/g_j)$ times the same constant. The expression in the brackets does not have to be positive. Such a situation often happens for transitions between very high states of an atom.

In some cases, the effect is real, but in many cases the laser effect may be spurious due to an insufficient number of processes populating and depopulating the upper states taken into account by TLUSTY. It may therefore be necessary to neglect, in some cases, the spurious negative opacity, which may produce large spurious emissions in otherwise quite unsuspicious lines. The basic numerical problem occurs when the zero point in the opacity from the transitions between the negative and positive values happens to be very close to an atmospheric depth grid point, which results in a spuriously large (sometime infinite) source function.

SYNSPEC thus allows the possibility to switch off all laser lines. More precisely, the line opacity is given as proportional to $\max[0, (n_i - g_i n_j/g_j)]$. This is switched on by coding a value of the parameter INLTE (input from unit 55) greater than 10. The program then resets the value of INLTE to *mod*(INLTE, 10). Since the DFE (discontinuous finite element) and the Feautrier scheme treat the transfer equation differently, the programs allows the four following options:

- $0 \leq$ INLTE < 10 – laser lines turned off; DFE scheme;
- $10 \leq$ INLTE < 20 – laser lines allowed, DFE scheme;
- $20 \leq$ INLTE < 30 – laser lines turned off; Feautrier scheme;
- $30 \leq$ INLTE < 40 – laser lines allowed; Feautrier scheme.

In the two latter cases, the parameter IFREQ is reset to IFREQ=11, regardless of the original input value.

5.2 Approximate NLTE treatment of lines

SYNSPEC allows the user to consider an approximate NLTE treatment even for LTE models, or for NLTE models but for lines of atoms/ions which were not treated in NLTE in the model construction. This is done by means of the second-order escape probability theory (see, e.g., Rybicky 1988), where

the line source function is given by the analytical expression

$$S_L = B_{\nu_0}(T(\tau)) \left(\frac{\epsilon}{\epsilon + (1 - \epsilon K_2(\tau)} \right)^{1/2}$$

where $B(T)$ is the Planck function at the local temperature and at the line center frequency ν_0; τ is the frequency-averaged optical depth in the line; ϵ is the photon destruction probability; and $K_2(\tau)$ is the kernel function. For the destruction probability, we adopt an approximation due to Kastner (1981), which expresses ϵ as an analytical function of the temperature, electron density, and the line wavelength. The kernel function is evaluated as described by Hummer (1981). We adopt the K_2 function for Doppler broadening. Although the above equation is, strictly speaking, valid for a constant-property atmosphere, we apply it with local values of T and $n_{\rm e}$ for a depth-dependent atmosphere.

The approximate NLTE treatment is switched on, analogously to the case of an exact treatment, either manually or automatically. The manual case again consists in modifying the corresponding entry in the line list, coding ILWN$=-1$.

The automatic treatment is switched on by coding a negative value for the global NLTE switch INLTE. This is called the *implied NLTE option*. There are several possibilities

- INLTE$=-2$ – all lines of all elements with IAT ≤ 20 (IAT being the atomic number), and excitation energy $E_i \leq 1000{\rm cm}^{-1}$ are treated in approximate NLTE. This option means that all resonance lines of all ligth elements are treated in the second-order escape probability formalism.

- INLTE$=-3$ – similar, but for all atoms (not limited to IAT below 20).

- INLTE$=-4$ – all lines in approximate NLTE. This option does not usually have any practical meaning; it is included for possible pedagogical purposes.

6 Detailed photoionization cross-sections

Most of the continuum opacity is treated in exactly the same way as in TLUSTY. These standard continuum opacity sources are assumed to be slowly varying functions of wavelength. Consequently, all the individual bound-free opacity contributions are evaluated at the endpoints of the current 'set', and the opacity within the set is evaluated by a linear interpolation between those two values. Since the set typically spans 0.5 - 2 Å(and much less in the EUV region), the linear interpolation of the continuum opacity is usually quite satisfactory.

However, with the advent of a mass production of detailed photoionization cross-section, provided e.g. by the Opacity Project, it is desirable to be able to consider full details of these cross-sections in the spectrum synthesis. Of course, all the options to include photoionization cross-sections, including those from the Opacity Project, which are considered in TLUSTY, are compatible with SYNSPEC as well. The only additional feature SYNSPEC offers is to read very detailed cross-sections and to consider them without losing their fine structure features. This is accomplished by three possible ways:

i) Input of detailed data for levels or superlevels considered by TLUSTY. This is done analogously as in TLUSTY (see the corresponding manual) by considering IFANCY for the given transition to be greater than 49, in which case IFANCY (transported as array IBF) has the meaning of the unit number of the input of detailed cross-sections. Although the structure of input is the same as for TLUSTY, the tables themselves may now be much more detailed.

ii) An analogous input as in the previous case, the only difference is that the corresponding ions were not treated explicitly by TLUSTY. For instance, even if iron was not treated explicitly in the TLUSTY (or any other) model explicitly, we may still use detailed iron photoionization cross-sections when calculating the synthetic spectrum. In this case, the unit number for the input is 54, and its structure is:
the first line specifies the number of such ions – NUNIT. There are now NUNIT lines, each containing three parameters, ATIR, INSA, NQHTR, where ATIR is the ion indication (as in the line list, for instance 26.02 means Fe III); INSA is the unit number for input of cross-sections, and NQHTR is the number of cross-sections for the given ion. The reason why we adopted such a seemingly overcomplicated system (a need for several input files) is that the unit 54 serves only as a pointer to other files, which were already prepared for their potential use for explicit (super)levels. It is therefore desirable not to change them.

The input from units INSA is quite analogous to those for explicit (super)levels. They are discussed in the TLUSTY manual, we repeat it for convenience here as well:
1st line – IIAT, IIZ, NSUP, where IIAT is the atomic number; IIZ ionic charge, and NSUP the number of cross-sections. The value of NQHTR should be equal to or smaller than NSUP; if not, the program prints a warning message and resets the value of NQHTR to NSUP. The advantage of distinguishing these two values is that SYNSPEC can, in principle, use only a subset of cross-sections prepared for TLUSTY. Then there are NQHTR blocks, each starting with a header line which specifies the level index, energy (in cm^{-1}), statistical weight, and number of frequency points in which the cross-section is given, NFCRR. This is followed by NFCRR records, each containing frequency (in Hz) and the cross-section (in $10^{-18}\mathrm{cm}^{-2}$). For more details refer to subroutine `SIGAVS`.

iii) A similar input of detailed cross-sections. It was historically the first actual implementation of detailed cross-sections to SYNSPEC, and is kept essentially due to historical reasons. This system again requires one driver Unit input (Unit 57), which then points to other unit numbers. The structure of Unit 57 is given by the instructions which are copied here from subroutine `READPH`:

```
PARAMETER (IPHT0=57)
READ(IPHT0,*,END=50,err=50) NPHT
IF(NPHT.LE.0) RETURN
READ(IPHT0,*,END=50) (IPHT(I),I=1,NPHT)
READ(IPHT0,*,END=50) (APHT(I),I=1,NPHT)
READ(IPHT0,*,END=50) (EPHT(I),I=1,NPHT)
READ(IPHT0,*,END=50) (GPHT(I),I=1,NPHT)
READ(IPHT0,*,END=50) (JPHT(I),I=1,NPHT)
```

where NPHT is the number of cross-sections; IPHT unit numbers for the detailed cross-section tables; APHT the atom/ion indication (as in the line list; for instance 14.01 means Si II); EPHT the level energy (in cm^{-1}); GPHT the statistical weight; and JPHT, if non-zero, is the index of the given level in the TLUSTY indexing of levels. If JPHT=0, the level is not among the explicit levels considered by TLUSTY, and is therefore taken in LTE.

The structure of the individual files IPHT is very simple; it is just a table of wavelength (in Å) versus cross-section (in $10^{-18}\mathrm{cm}^{-2}$). The table may have an arbitrary length; the total number of entries is not required by SYNSPEC and therefore does not have to be specified.

7 Summary of changes with respect to version 36

There are three basic changes:

- Fully universal scheme for computing theoretical spectra for stellar atmospheres (generated by TLUSTY or for Kurucz models), or for accretion disks (generated by TLUSDISK).
- A possibility of using the Opacity Project ionization fractions and therefore deduced partition functions. This allows the user to consider all degrees of ionization, up to fully stripped ions, of the species considered by the opacity project (H, He, C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, Cr, Mn, Fe, Ni) – see Sect. 6.
- Full compatibility with TLUSTY, version 195, i.e. allowing for two different input format – the "old" one (used in TLUSTY and SYNSPEC so far), and "new" one – see "TLUSTY: A User's Guide, Version 195" (Hubeny and Lanz 1997).

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