CHIANTI

An Astrophysical Database for Emission Line Spectroscopy

CHIANTI TECHNICAL REPORT No. 3

Computing a synthetic spectrum with CHIANTI

Version 1.5, 27 Jun 2023, Peter Young

This software note describes how a synthetic spectrum is computed by the CHIANTI IDL software.

1 Software routines

The two key IDL routines used to create a spectrum are `ch_synthetic` and `make_chianti_spec`. The end result from `make_chianti_spec` is a structure that contains a spectrum expressed as wavelength vs. intensity. Some key points to note are:

1. `ch_synthetic` computes emission line intensities for all of the lines within the user-specified wavelength range, but without including the element abundance.
2. `make_chianti_spec` takes the line intensities from `ch_synthetic`, folds in the element abundances, adds a line spread function, and computes a 1D spectrum. Optionally, it adds a continuum comprised of free-free, free-bound and two-photon emission.

The reason for splitting the computation process between two routines is because `ch_synthetic` is usually quite slow, while `make_chianti_spec` is quite fast. Therefore the user can vary the abundances or line spread function (pixel size, line broadening) within `make_chianti_spec` without having to re-compute the emission line intensities again.

Note that the widget-based routine `ch_ss` calls `ch_synthetic` and `make_chianti_spec` to compute spectra. Generally new users are recommended to use `ch_ss`.

2 Which lines are included in the final spectrum?

An important point to note is that the default options for making a spectrum with `make_chianti_spec` do *not* yield a spectrum containing all of the transitions in CHIANTI.

In the database we distinguish between "observed" and "theoretical" wavelengths. The former are atomic transitions for which the two levels have known energies (for example, the levels have energies listed in the NIST database). The latter are atomic transitions for which one or both of the levels do not have known energies. Only lines with *observed* wavelengths are included in the spectrum produced by `make_chianti_spec`. To include the lines with theoretical wavelengths, you should give the keyword `/all`.

The reason for this behavior is that theoretical wavelengths can be inaccurate by several Angstroms, and so the user may inadvertently mis-identify an emission line in a real spectrum by comparison with the CHIANTI spectrum.

However, increasingly the CHIANTI team uses so-called "best-guess" energies for levels without known energies. In this case the theoretical wavelengths may actually be quite accurate (within a fraction of an Angstrom).

The recommendation is that if you interested in the broad properties of a spectrum, such as the total radiative loss in the spectrum, then you should use the `/all` keyword. If you are more interested in a specific portion of the spectrum where accurate line identifications are crucial then you should not use the `/all` keyword.

The behavior described above only applies to `make_chianti_spec`. The routine `ch_synthetic` *always* returns the complete set of transitions in the CHIANTI models.

3 The contribution function

For this document the contribution function, $G(T, N_{\rm e})$, for an emission line of wavelength, λ, that corresponds to the atomic transition from an upper level with index j to a lower level with index i is defined as

$$G(T, N_{\rm e}) = \frac{1}{4\pi}\frac{hc}{\lambda}\frac{n_j(T, N_{\rm e})}{N_{\rm e}}F(T)A_{ji} \tag{1}$$

where T is the plasma temperature, $N_{\rm e}$ is the electron number density, h is the Planck constant, c the speed of light, n_j is the population of the upper emitting level of the transition relative to the total population of the ion, F is the ionization fraction of the emitting ion, and A_{ji} is the radiative decay rate for the transition. Note that the expression does not include the element abundance. The contribution function can be computed by the CHIANTI IDL routine `gofnt`, setting the `/noabund` keyword. Note that `ch_synthetic` does not actually call `gofnt`, but computes the contribution function from scratch.

With the above definition of G, the intensity of the emission line for an isothermal plasma is given by

$$I = \epsilon G N_{\rm e} N_{\rm H} h \tag{2}$$

where ϵ is the abundance of the emitting element relative to hydrogen, $N_{\rm H}$ is the number density of hydrogen (i.e., neutral hydrogen and protons), and h is the column depth of the plasma.

The hydrogen density can be expressed in terms of the electron density by making use of the CHIANTI IDL routine `proton_dens`. For example the call

```
IDL> nh_ne=proton_dens(ltemp,abund=!abund_file, ioneq=!ioneq_file, /hydrogen)
```

computes the ratio of the hydrogen density to the electron density at the log T value specified by `ltemp` and using the default CHIANTI abundance and ionization equilibrium files. The ratio is approximately constant for log $T \geq 5.0$ with a value around 0.85, which will vary depending on the abundance file used. (Note: if you do not give the /hydrogen keyword then the routine returns the proton-to-electron ratio.)

4 The emission line contribution to the spectrum

In computing an emission line intensity within the CHIANTI software there are two distinct cases. The first is the emission measure (EM) case (also referred to as the isothermal case), and the second is the differential emission measure, DEM, case. These are discussed below.

The equations for the line intensity given below include the element abundance (ϵ), but the reader should note that the intensity computed by `ch_synthetic` does not include the abundance. It is only included when `make_chianti_spec` is called.

4.1 The EM case

This is when the sight-line contains one or more plasma components that are each isothermal. For each plasma, the user specifies a temperature, T, and emission measure, Φ, value using the keyword inputs `logt_isothermal` and `logem_isothermal` to `ch_synthetic`. Note that the emission measure is defined as $\Phi = N_{\rm e} N_{\rm H} h$. If `logem_isothermal` is not specified by the user, then a value of $\Phi = 1$ is assumed.

For a set of temperatures, T_k, the intensity computed by `ch_synthetic` is given by

$$I = \epsilon \sum_k G_k \Phi_k \tag{3}$$

The user has options to set $N_{{\rm e},k}$ to be constant for each temperature (through the `density=` keyword), for the pressure, $P_k = T_k N_{{\rm e},k}$ to be constant (through the `pressure=` keyword), or for each $N_{{\rm e},k}$ to be specified individually through the `model_file=` keyword.

4.2 DEM case

A DEM curve, $\phi(T)$, is specified through an input file that gives the DEM value as a function of temperature. Examples are found in the `chianti/dbase/dem` directory within the database. The name of the DEM file is sent to `ch_synthetic` through the `dem_name=` optional input. If `dem_name` is not specified, then a widget will appear allowing you to manually choose a DEM file.

The CHIANTI definition of $\phi(T)$ is

$$\phi(T) = N_{\rm e} N_{\rm H} \frac{{\rm d}h}{{\rm d}T} \tag{4}$$

and so it is assumed that the input DEM when creating the synthetic spectrum is specified in this form. It is quite common for DEM codes to yield the alternative $N_{\rm e}^2$ form of the DEM, so in this case the DEM should be multiplied by $N_{\rm H}/N_{\rm e}$ before being input to `ch_synthetic`.

The DEM curve does not need to be specified on a uniform temperature grid; `ch_synthetic` will automatically interpolate the input DEM curve onto the temperature grid at which the ion balance curves are defined.

The expression for computing the line intensity from the DEM curve, is:

$$I = \epsilon \int_T G(T) \phi(T) {\rm d}T \tag{5}$$

$$= \epsilon \sum_{k=1}^{k=n} G_k \phi_k \delta T_k \tag{6}$$

$$= \ln 10 \, \epsilon \sum_{k=1}^{k=n} G_k \phi_k T_k \delta(\log_{10} T). \tag{7}$$

Up to CHIANTI 6, $\delta(\log_{10} T)$ was always 0.1, i.e., temperatures were always specified on a log scale set at 0.1 dex intervals. The temperature scale was fixed by the temperatures in the ion balance file. With CHIANTI 6, a new ion balance was added with temperatures set at 0.05 dex intervals.

See Appendix B for a discussion of the integration method used for the DEM case.

5 The line spread function

The routine `make_chianti_spec` computes the synthetic spectrum by taking the intensity values calculated by `ch_synthetic`, multiplying them by the element abundance values and then dispersing over the wavelength bins by assuming a Gaussian line spread function. Note that the dispersion is done on a per-Angstrom basis rather than a per-pixel basis, i.e., the intensity is given by erg cm^{-2} s^{-1} sr^{-1} Å^{-1}.

For example, the specific intensity in wavelength bin i is given by

$$I_{\lambda,i} = If(\lambda_i) = \frac{I}{\delta\lambda}\exp\left(-\frac{(\lambda_i-\lambda)^2}{2\sigma^2}\right) \tag{8}$$

where I is the integrated line intensity, $f(\lambda)$ is the line spread function, $\delta\lambda$ is the size of a wavelength pixel in Angstroms, and σ is the gaussian width of the emission line. The gaussian width is related to the full-width at half-maximum (FWHM), W, by $W = 2\sqrt{2\ln 2}\sigma$. For CHIANTI we set W to be

$$W^2 = W_{\rm t}^2 + W_{\rm i}^2 \tag{9}$$

where $W_{\rm i}$ is the instrumental width that is set with the `instr_fwhm` keyword, and $W_{\rm t}$ is the thermal width given by:

$$\left(\frac{W_\lambda}{\text{Å}}\right) \approx \frac{7.14\times10^{-7}}{\sqrt{N}}\left(\frac{T}{\rm K}\right)^{1/2}\left(\frac{\lambda}{\text{Å}}\right) \tag{10}$$

where N is the atomic weight of the element in atomic mass units. The latter is returned by the CHIANTI IDL routine `get_atomic_weight`. By default the instrument width is zero unless set with the `instr_fwhm` keyword.

6 Adding the continuum

There are three components to the continuum calculated by CHIANTI: free-free, free-bound and two-photon. The continua are calculated through the IDL routines `freefree`, `freebound` and `two_photon`, each of which is called by `make_chianti_spec`.

The individual continuum emissivities (as returned by the three continuum IDL routines) are given by $P_{\rm ff}$, $P_{\rm fb}$ and $P_{\rm pp}$, and the specific intensity for the EM case is given by

$$I_\lambda = 10^{-40}\sum(P_{\rm ff}+P_{\rm fb}+P_{\rm pp})\Phi_k. \tag{11}$$

The factor 10^{-40} is required due to a quirk of the CHIANTI continuum routines that multiples the output by 10^{40}.

For the DEM case, the specific intensity is given by:

$$I_\lambda = 10^{-40}\ln 10\,\delta(\log_{10}T)\sum(P_{{\rm ff},k}+P_{{\rm fb},k}+P_{{\rm pp},k})T_k\phi_k. \tag{12}$$

The continuum routines each have optional inputs `em_int` and `dem_int` that enable the EM and DEM values to be directly input, allowing the specific intensities to be returned (although with the 10^{40} factor not corrected).

7 The output structures

The routines `ch_synthetic` and `make_chianti_spec` both send their output to IDL structures, and we give some information about their contents here.

Consider the following simple example of computing a synthetic spectrum for O VI in the wavelength range 1030–1040 Å.

```
IDL> ch_synthetic,1030,1040,press=1e15,sngl='o_6',logt_iso=5.6,logem_iso=27.0, $
         output=output
IDL> make_chianti_spec,output,lambda,spectrum,instr_fwhm=0.2,abund_name=!abund_file
```

The structure `output` contains a number of tags with the input parameters for `ch_synthetic`. The list of emission lines that has been calculated is stored in the tag `lines`, which is itself a structure. In CHIANTI 10.0.2 there are 207 lines that have been calculated for O VI. For each line the wavelength and intensity (tags `wvl` and `int`) are given. The units for each are given by the tags `output.wvl_units` and `output.int_units`. However, the intensity does not include the element abundance (see Section 4), so you should instead retrieve the intensity from the `spectrum` structure.

The `spectrum` structure is very similar to `output`, but it adds additional tags (`lambda` and `spectrum`) for the 1D spectrum that has been calculated and the additional inputs.

In addition, the intensities in `lines.int` now include the element abundance. An extra tag (`peak`) gives the peak amplitude of the line in the spectrum, and the units are given by `spectrum.units[1]`. Note that `lines` contains less lines than `output.lines` (15 lines for CHIANTI 10.0.2). This is because the default behavior of `make_chianti_spec` is to not include lines with theoretical wavelengths (Section 2). To include all of the O VI lines you will need to set the `/all` keyword.

Some care has to taken with `lambda` in the call to `make_chianti_spec`. If it does not exist, then it is returned as the wavelength vector (the same as `spectrum.lambda`). If you call the routine again, however, then `lambda` will exist and it will be treated as an input that specifies the wavelength array. This can cause confusion if you run the synthetic spectrum software multiple times in the same IDL session. It is good practice to delete `lambda` before running `make_chianti_spec` unless you want to always use the same the wavelength array.

8 Speeding up the calculation

Calculating a synthetic spectrum with `ch_synthetic` can take several minutes. There are two options for speeding up the calculation: (1) using population lookup tables, and (2) switching off autoionization rates.

Population lookup tables are described in CHIANTI Technical Report No. 16, and they are implemented in `ch_synthetic` through the /lookup keyword. For *Solarsoft* users, the lookup tables are provided in the CHIANTI distribution. For standalone users, the lookup tables can be downloaded from the CHIANTI webpage (`https://chiantidatabase.org/download`).

Autoionization rates are provided for the H, He and Li isoelectronic sequences and lead to significantly larger models as they require levels above the ionization threshold that are normally not

Table 1: Time taken to compute a spectrum with ch_synthetic.

	Regular	/lookup	/no_auto
Time taken (s)	319	42	123

included in the CHIANTI models. The rates are important for modeling X-ray satellite lines, but for longer wavelength spectra the rates are generally not important. By switching them off with the /no_auto keyword the synthetic spectrum calculation is faster.

Table 1 compares the times taken to compute a synthetic spectrum using the regular calling sequence, the /lookup keyword and the /no_auto keyword. The call used was

```
IDL> ch_synthetic,1,100,output=output,press=1e16,dem=dem_name
```

where the DEM file used was `flare.dem`. The author performed these calculations in June 2023 with CHIANTI 10.1 and he used a 2023 MacBook Pro with an M2 Max processor.

9 Additional information

9.1 Emission line formation temperature (Tmax)

The output structure returned by `ch_synthetic` contains the tag `line.tmax`, which contains the formation temperature (logarithmic value) of the emission line in the spectrum. This temperature is obtained by multiplying the contribution function by the DEM function and finding the temperature at which the function has its maximum value. It thus accurately represents the true formation temperature of the emission line, and may be significantly different from the temperature obtained from the peak of the ionization fraction, $F(T)$, which is commonly denoted by $T_{\max}$.

9.2 Satellite lines

The standard model for a CHIANTI ion has a number of *bound* atomic states, i.e., states that are energetically lower than the ionization energy of the ion. Ions also have unbound or *autoionizing* states above the ionization energy. As the name suggests, these states can spontaneously decay through the ejection of an electron to yield a new ion with a higher charge state. The states can also decay by *radiative stabilization* to a bound state. This latter process results in *satellite lines*. These are named because they lie close to strong resonance lines of the ionized ion. For example, the Fe XXV resonance line at 1.8504 Å has several strong satellite lines of Fe XXIV nearby between 1.853 and 1.873 Å.

Autoionizing states are excited through dielectronic capture from the next highest ionization stage and/or inner-shell excitation of the ion. Depending on the properties of the state, one or both of these mechanisms can be significant. In both cases, the formation temperature of the satellite line that comes from the state is higher than that of standard resonance line of the ion.

In the output structure returned by `ch_synthetic`, the tag `lines.snote` gives the emitting ion of the emission line. For satellite lines, an "s" is appended to the ion name and is printed to the line list generated by the routine `ch_line_list`, and it also appears in the output of the `ch_ss` GUI. Satellite lines can also be identified by their higher $T_{\max}$ values compared to the resonance lines of the same ion.

References

Hannah, I. G., & Kontar, E. P. 2012, A&A, 539, A146, doi: 10.1051/0004-6361/201117576

A Document history

Ver. 1.5, 27-Jun-2023. Added Sect. 9.

Ver. 1.4, 11-May-2023. Added Sect. 8; moved the Latex file to Overleaf; changed the figure to png format.

Ver. 1.3, 03-Jan-2023. Added Sect. 7; expanded introduction to Sect. 4.

Ver. 1.2, 01-Nov-2021. Added Sect. 2.

Ver. 1.1, 07-Dec-2020. The /hydrogen keyword has been added to the call to `proton_dens`; added $\phi(T)$ definition to Sect. 4.2.

Ver. 1.0, 25-Apr-2019. Initial release version.

B Integration method

From Equation 5 we see that the integration over the contribution function and the DEM function is approximated by a sum over a set of temperature bins. If the bins are set to be log $T = 5.0$,...,6.0 at 0.1 dex intervals, then it can be seen that the first bin covers the temperature range log $T = 4.95$ to 5.05, and the last bin covers log $T = 5.95$ to 6.05. The intensity from Equation 5 thus effectively represents an integration from log $T = 4.95$ to 6.05.

If the trapezoidal rule had been used for the integration, then the integration range of log $T = 5.0$ to 6.0 would have been strictly applied, and the result would differ from the CHIANTI method by the amount

$$\Delta I = -0.23\epsilon \frac{f(\log T = 5.0) + f(\log T = 6.0)}{2} \tag{13}$$

where $f = G\phi T$. If the contribution function peaks between the end-points of the DEM, then ΔI will generally be small. However, if the contribution function peaks outside of the end-points then it is likely that ΔI will be significant. Tests show that it can be up to half of the intensity derived using the CHIANTI method.

This issue is illustrated in Figure 1 where the CHIANTI quiet Sun DEM curve is plotted together with the contribution function for Ca XVII λ192.83. The last data point for the DEM is at log $T =$ 6.6 and it can be seen that the contribution function is sharply rising at this temperature. When the two functions are convolved the dominant contribution to the Ca XVII intensity comes from the log $T = 6.6$ temperature bin.

Why not use the trapezoidal rule for performing the integration? Most DEM methods used by solar physicists (see Hannah & Kontar, 2012, for an example) discretize the temperature range into bins, thus the output DEM values do not represent spline points of a continuous function but are essentially average values over the bin used by the method. This is consistent with the approach of Equation 5.

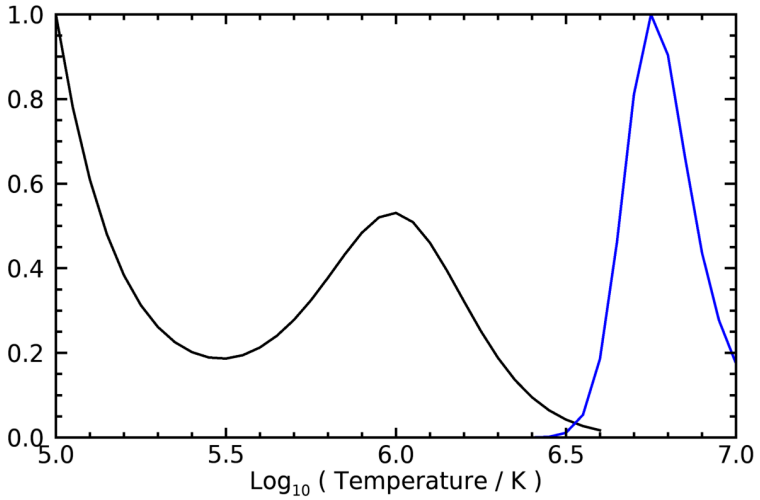

Figure 1: The black curve shows the CHIANTI quiet Sun differential emission measure curve, and the blue curve shows the contribution function for Ca XVII λ192.83. Both curves are normalized to make their maximum values 1, and the Y-axis has a linear scaling.