The Free-Bound Continuum

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This document presents how the free-bound continuum is calculated in CHIANTI, paying particular attention to the value of the numerical constants and the units employed in CHIANTI. The method used by the Mewe code is also presented and differences highlighted.

1 The free-bound emission formula

Consider an ion Z^{+z+1} which we term the *recombining ion*, and an ion Z^{+z} which we term the *recombined ion*. A continuum of radiation is produced when an electron collides with the recombining ion to produce the recombined ion. In terms of energy we have

$$E = E_{\rm e} + I_i + E_{j'} \tag{1}$$

where E is the energy of the emitted photon, $E_{\rm e}$ the energy of the incoming electron, I_i the energy required to ionize the recombined ion from level i, and $E_{j'}$ is the energy of the j' level of the recombining ion. We use j' to denote an arbitrary level of the recombining ion, and i to denote an arbitrary level of the recombined ion.

We define the free-bound continuum emissivity, $P_{\rm fb}$, from the energy carried off by photons in a unit plasma volume into unit solid angle per unit time:

$$\mathcal{E} = P_{\rm fb} {\rm d}E_{\rm e}\, {\rm d}t\, {\rm d}V\, {\rm d}\Omega. \tag{2}$$

For incoming electrons with a energy distribution, $f(E_{\rm e})$, and a plasma with an electron number density $n_{\rm e}$ and a recombining ion number density n_{+z+1} we have

$$P_{\rm fb} = \sum_{i,j'} \frac{E}{4\pi} n_{+z+1} n_{\rm e} v_{\rm e} f(E_{\rm e}) \sigma^{\rm fb}_{j'i}. \tag{3}$$

where $v_{\rm e}$ is the velocity of the incoming electron ($m_{\rm e}v_{\rm e}^2/2 = E_{\rm e}$). For CHIANTI we are interested in the continuum emissivity per wavelength interval, $P_{{\rm fb},\lambda}$:

$$P_{{\rm fb},\lambda} = \sum_{i,j'} \frac{E}{4\pi} \frac{hc}{\lambda^2} n_{+z+1} n_{\rm e} v_{\rm e} f(E_{\rm e}) \sigma^{\rm fb}_{j'i}. \tag{4}$$

Inserting for a Maxwellian velocity distribution gives

$$P_{{\rm fb},\lambda} = \sum_{i,j'} \frac{E}{4\pi} \frac{E^2}{hc} n_e n_{+z+1} \frac{E_{\rm e}}{kT} \frac{4}{(2\pi m_e kT)^{1/2}} \sigma^{\rm fb}_{j'i} \exp\left(-\frac{E_{\rm e}}{kT}\right) \tag{5}$$

For practical purposes recombination is assumed to only take place from the ground state of the recombining ion. We will thus refer to cross-sections as $\sigma^{\rm fb}_i$, dropping the j'.

Now the principle of detailed balance (Rybicki & Lightman, Eq. 10.62) gives

$$\frac{\sigma^{\rm fb}_i}{\sigma^{\rm bf}_i} = \frac{E^2}{m_e^2 c^2 v_e^2} \frac{\omega_i}{\omega_0} = \frac{E^2}{2 m_e c^2 E_{\rm e}} \frac{\omega_i}{\omega_0} \tag{6}$$

where the w_i (i =1,2,...) are the statistical weights of the levels of the recombined ion, and w_0 is the statistical weight of the ground level of the recombining ion. The total free-bound continuum emissivity from the recombinations is then

$$P_{\mathrm{fb},\lambda} = \frac{1}{4\pi} n_e n_{+z+1} \frac{2}{hkc^3 m_\mathrm{e}\sqrt{2\pi k m_\mathrm{e}}} \frac{E^5}{T^{3/2}} \sum_i \frac{\omega_i}{\omega_0} \sigma_i^{\mathrm{bf}} \exp\left(-\frac{E-I_i}{kT}\right) \tag{7}$$

This expression can be compared to Eq. 1a of Mewe et al. (1986) which has a λ^{-2} dependency in contrast to the λ^{-5} dependence above ($E \propto \lambda^{-1}$). This is because Mewe's equation implicitly assumes the λ^3 dependence of the cross-section (see also Sect. 2.2).

Evaluating the numerical constant in Eq. 7 (Appendix B) and specifying units for the physical parameters gives

$$P_{\mathrm{fb},\lambda} = \frac{3.0992 \times 10^{-46}}{4\pi} n_\mathrm{e} n_{+z+1} \left(\frac{E}{\mathrm{cm}^{-1}}\right)^5 \left(\frac{\mathrm{K}}{T}\right)^{3/2} \sum_i \frac{\omega_i}{\omega_0} \left(\frac{\sigma_i^{\mathrm{bf}}}{\mathrm{Mb}}\right) \exp\left(-\frac{E-I_i}{kT}\right) \tag{8}$$

$$[\mathrm{ergs\ cm^{-3}\ s^{-1}\ \AA^{-1}\ sr^{-1}}].$$

Note that a mega-barn (Mb) is 10^{-18} cm^2. Specific details of how this formula is used in CHIANTI are given in the following section.

2 CHIANTI implementation

2.1 Freebound and Freebound_ion

Eq. 8 gives the free-bound emission from a single ion in a plasma with specified number densities for the ion and electrons . To compute the total emission from all ions it is necessary to sum over all ions, and the CHIANTI method is to calculate the contribution from each individual ion with the IDL routine FREEBOUND_ION and then combine these together to calculate the final continuum with FREEBOUND. There are two cases to consider: (i) the continuum for a plasma at a single temperature, and (ii) the continuum from a plasma with a differential emission measure defined.

Considering case (i) first, we define

$$C_{\mathrm{fb},\lambda}(T) = \frac{3.0992 \times 10^{-46} \times 10^{40}}{4\pi} \left(\frac{E}{\mathrm{cm}^{-1}}\right)^5 \left(\frac{\mathrm{K}}{T}\right)^{3/2} \sum_i \frac{\omega_i}{\omega_0} \left(\frac{\sigma_i^{\mathrm{bf}}}{\mathrm{Mb}}\right) \exp\left(-\frac{E-I_i}{kT}\right) \tag{9}$$

which has units of 10^{-40} ergs cm^3 s^{-1} Å^{-1} sr^{-1}. This is the quantity calculated by FREEBOUND_ION and represents the continuum emission from a unit volume of plasma containing only a single ion with a unit density.

For a plasma containing a range of ions and elements at unit density the continuum emission is then

$$\mathcal{P}_{\mathrm{fb},\lambda}(T) = \sum_{j=1}^{j=30} A_j \sum_{k=1}^{k=j} F_{j,k}(T) C^{jk}_{\mathrm{fb},\lambda}(T) \tag{10}$$

where A_j is the element abundance of element j, and $F_{j,k}$ is the ionization fraction of ion k of element j (elements up to zinc are included in CHIANTI). This is the quantity calculated by FREEBOUND for case (i). The units are 10^{-40} ergs cm^3 s^{-1} Å^{-1} sr^{-1}. Note that, if the user wants to calculate the continuum emission from an isothermal plasma with an electron density

n_e, then it is necessary to multiply Eq. 10 by $n_e n_H$ where n_H is the number density of hydrogen. This step is automatically performed by the CHIANTI routines CH_SS, CH_SYNTHETIC, and CH_ISOTHERMAL.

For case (ii) the user specifies a differential emission measure curve, $\phi(T)$, which is defined at a number of discrete temperatures, T_m. The continuum emission is then:

$$\mathcal{P}_{\mathrm{fb},\lambda} = \sum_{j=1}^{j=30} A_j \sum_{k=1}^{k=j} \sum_m F_{j,k}(T_m) C_{\mathrm{fb},\lambda}^{jk}(T_m) \phi(T_m)\, \Delta(\log_{10} T) \ln 10\, T_m \tag{11}$$

where the T_m are *required* to have a fixed spacing in $\log_{10} T$, indicated by the quantity $\Delta(\log_{10} T)$ in the above equation. E.g., $\log T_0 = 6.0$, $\log T_1 = 6.1$, $\log T_2 = 6.2$, etc. If the temperatures are not evenly spaced, then the calculation will not proceed. The units of $\mathcal{P}_{\mathrm{fb},\lambda}$ are 10^{-40} ergs cm^{-2} s^{-1} Å^{-1} sr^{-1}.

In the call to freebound, the differential emission measure values are specified with the keyword DEM_INT, e.g.,

```
IDL> freebound, temp, wvl, int, dem_int=dem_int
```

the intensity array, INT, (corresponding to $\mathcal{P}_{\mathrm{fb},\lambda}(T)$) will be returned as an array of size NWVL × NT. Only if the keyword /SUMT is given will the continuum intensities by summed over temperature:

```
IDL> freebound, temp, wvl, int, dem_int=dem_int, /sumt
```

2.2 Evaluation of the cross-sections

In computing the quantity $C_{\mathrm{fb},\lambda}$, the photoionization cross-sections, σ_i^{bf} are needed. These are the photoionization cross-sections for transitions from the ground state of the recombining ion to the states i of the recombined ion. For the transitions to the ground state of the recombined ion ($i = 1$) we use the photoionization cross-sections of Verner & Yakovlev (1995). For excited states we use the Gaunt factors of Karzas & Latter (1961). States here are actually configurations with progressive excitations of the outer electron. E.g., for C III we have $2s^2$, $2s2p$, $2s3s$, …, $2s5g$. The energies of each level define the edges in the recombination spectrum. The level IDs and energies are given in the CHIANTI .FBLVL files.

The Karzas & Latter (1961) cross-sections for each excited configuration of an ion are evaluated in CHIANTI with the expression:

$$\sigma_i^{\mathrm{bf}} = 1.077294 \times 10^{-1} . 8065.54 \times 10^3 \left(\frac{I_i}{\mathrm{cm}^{-1}}\right)^2 \left(\frac{\mathrm{cm}^{-1}}{E}\right)^3 \frac{g_{\mathrm{bf}}}{n_i} \qquad [\mathrm{Mb}] \tag{12}$$

where I_i is the energy required to remove the excited electron in the orbital $n_i l_i$, E the energy of the emitted photon and g_{bf} the bound-free Gaunt factor of Karzas & Latter (1961). Note that a mega-barn (Mb) is 10^{-18} cm^2. The constants are evaluated in Appendix A.

Within CHIANTI, the routines VERNER_XS() and KARZAS_XS() yield the cross-sections in Mb.

One can see how the Verner data affects the continuum from an ion by using the /noverner keyword in freebound_ion. E.g.,

```
IDL> wvl=findgen(100)+1.
IDL> freebound_ion, 1e6, wvl, int1, 6, 5
```

```
IDL> freebound_ion, 1e6, wvl, int2, 6, 5, /noverner
IDL> plot,wvl,int1
IDL> plot,wvl,int2,line=2
```

2.3 The Verner & Yakovlev data

Verner & Yakovlev (1995) provide photoionization cross sections for each orbital of the ground configuration of all ions of all elements up to and including zinc. For example, for Fe XIV with ground configuration $1s^2 2s^2 2p^6 3s^2 3p$ five cross sections are given, for removing $1s$, $2s$, $2p$, $3s$ and $3p$ orbitals, respectively. For the free-bound calculations only the transition that produces the ground configuration of Fe XV, $1s^2 2s^2 2p^6 3s^2$, is needed and so we only use the Verner & Yakovlev (1995) cross-sections for the removal of the $3p$ orbital.

For this reason, the Verner & Yakovlev (1995) data file contained in !xuvtop/continuum/verner_short.txt is a subset of the original Verner & Yakovlev (1995) data file.

2.4 Statistical weights

For the CHIANTI implementation the statistical weights, w_i, are taken as the weights of the 'levels' involved in the transitions. These levels are actually configurations and so the weights of the configurations are computed.

For example, for Fe XV recombining to Fe XIV, recombination takes place from the ground 'level' of Fe XV (i.e., the ground configuration, $3s^2$) to 'levels' of the form $3s^2 nl$ in Fe XIV where $n \leq 5$. The statistical weight of the Fe XV ground level, w_0, is 1 and those of the Fe XIV levels are $w_1 = 6$ ($3s^2 3p$), $w_2 = 10$ ($3s^2 3d$), $w_3 = 2$ ($3s^2 4s$), etc.

3 Mewe method

Mewe uses the Karzas & Latter method for the bound-free cross section, and he quotes the formula

$$\sigma_i^{\rm bf} = 1.075812 \times 10^{-23} \left(\frac{I_i}{\rm keV} \right)^2 \left(\frac{\rm keV}{E} \right)^3 \frac{g_{\rm bf}}{n_i} \qquad [{\rm m}^2] \tag{13}$$

where n_i is the principal quantum number of level i, $g_{\rm bf}$ is the bound-free gaunt factor, and the other quantities are the same as in the previous section. The constant is evaluated in Appendix A. Mewe assumes the $g_{\rm bf}$ values are 1.

In the hydrogenic approximation, we write

$$I_i = \frac{E_{\rm H}(z+1)^2}{n_i^2} \tag{14}$$

where $z+1$ is the net charge of the recombining ion.

Eq. 7 is thus written as

$$P_{{\rm fb},\lambda} = \frac{1.075812 \times 10^{-23}}{4\pi} n_e n_{+z+1} \frac{2}{hkc^3 m_{\rm e} \sqrt{2\pi k m_{\rm e}}} \frac{E^2\, E_{\rm H}}{T^{3/2}} \sum_i \frac{\omega_i}{\omega_0} \frac{(z+1)^4}{n_i^5} \exp\left(-\frac{E - I_i}{kT} \right) \tag{15}$$

Now, at this point Mewe sets ω_0 to 1 and $\omega_i = \zeta(Z, z+1, n)$, the number of vacancies in the nth shell of the recombined ion before recombination. To understand this latter quantity, consider O^{+3} recombining into O^{+2}. The ground configuration of O^{+3} is $2s^2 2p$, and it captures an electron into the $n = 2$ shell. It has 5 free p orbitals that it can enter, and so $\zeta(8, 3, 2) = 5$.

For O^{+6} recombining into the $n = 2$ shell of O^{+5}, all 8 orbitals ($2 \times 2s$ and $6 \times 2p$) are free, and so $\zeta(8, 6, 2) = 8$. The values of ζ for recombinations into the lowest n shells for all ions are given by Mewe et al. (1986).

This is all well and good, but the values of ζ bare no relation to the real statistical weights, ω_0 and ω_i! E.g., again for the example of O^{+3} recombining into O^{+2}, the total weight for the entire ground configuration of O^{+3} $2s^2 2p$ is 6. The total weight for the O^{+4} $2s^2 2p^2$ configuration is 15. The ratio ω_i/ω_0 is thus 2.5, compared to $\zeta = 5$.

4 Topbase

Topbase contains photoionization cross-sections resolved into LS states for many ions. It's not at all clear in the Topbase literature, but it seems that the cross-sections are summed into all final states of the recombining ion. I've guessed this from the Si I data where I've compared what Topbase has to what was published in Nahar & Pradhan (1993, JPhysB 26, 1109). In particular, Fig. 2a of this work shows resolved cross-sections for final states of the recombining ion. There's a distinctive spike at around 0.48 Ryd that is due to the first excited state, and this is seen in the Topbase data, implying that the cross-sections are summed. The Topbase data are not useful for calculating the free-bound continuum since we only want cross-sections for transitions into the ground state of the recombining ion.

References

Karzas, W. J., & Latter, R. 1961, ApJS, 6, 167

Mewe, R., Lemen, J. R., & van den Oord, G. H. J. 1986, A&AS, 65, 511

Verner, & Yakovlev 1995, A&AS, 109, 125

A Evaluating the Karzas & Latter constant

Eq. 12 gives the expression used in CHIANTI for evaluating the Karzas & Latter (1961) bound-free cross sections. Where does the constant come from?

From the original Karzas & Latter (1961) paper, Eq. 39 gives:

$$\sigma_n^{\rm bf} = \frac{2^4}{3\sqrt{3}} \frac{e^2}{mc\nu} \frac{1}{n} \left(\frac{\rho^2}{1+\rho^2} \right)^2 g_{\rm bf} \tag{16}$$

which is the cross-section for removing an electron from the nl orbital with an incoming electron of energy $E_{\rm e}$. Now $\rho^2 = \eta^2/n^2 = Z^2 E_{\rm H}/E_{\rm e} n^2$. The ionization energy from a hydrogenic energy level is $I_n = Z^2 E_{\rm H}/n^2$. Since $E = E_{\rm e} + I_n$ and $E = h\nu$, then

$$\sigma_n^{\rm bf} = \frac{2^4}{3\sqrt{3}} \frac{he^2}{mc} \frac{1}{n} \frac{I_n^2}{E^3} g_{\rm bf} \tag{17}$$

where we have written I_n for the ionization energy for an electron in the n shell.

For the evaulation of the constants, we first note that in the Gaussian system of units, the charge e has the units of g$^{1/2}$ cm$^{3/2}$ s^{-1}. We know that $e = 1.602177 \times 10^{-19}$ C in SI units, and to convert this to gaussian units we multiply by 3×10^9 (see the Appendix in Priest's book for more information about this), giving $e = 4.806532 \times 10^{-10}$ g$^{1/2}$ cm$^{3/2}$ s^{-1}.

Now $m = 9.109390 \times 10^{-28}$ g, $h = 6.6260755 \times 10^{-27}$ erg s, and $c = 2.99792458 \times 10^{10}$ cm s^{-1}. The numerical constant evaluates to 3.0792015, and so we have

$$\sigma = 1.7260293 \times 10^{-28} \left(\frac{I_n}{\rm erg} \right)^2 \left(\frac{\rm erg}{E} \right)^3 \frac{g_{\rm bf}}{n} \qquad [{\rm cm}^2] \tag{18}$$

Note that energies are specified in ergs in Gaussian units.

To derive the expression used by Mewe, the energy units must be converted to keV and the cross-section expressed in m^2. This gives

$$\sigma = \frac{1.7260293 \times 10^{-32}}{1.60219 \times 10^{-9}} \left(\frac{I_n}{\rm keV} \right)^2 \left(\frac{\rm keV}{E} \right)^3 \frac{g_{\rm bf}}{n} \qquad [{\rm m}^2] \tag{19}$$

$$\sigma = 1.077294 \times 10^{-23} \left(\frac{I_n}{\rm keV} \right)^2 \left(\frac{\rm keV}{E} \right)^3 \frac{g_{\rm bf}}{n} \qquad [{\rm m}^2] \tag{20}$$

For CHIANTI we express the energies in cm^{-1} and the cross-section in Mb, giving

$$\sigma = 1.077294 \times 10^{-1} . 8065.54 \times 10^3 \left(\frac{I_n}{{\rm cm}^{-1}} \right)^2 \left(\frac{{\rm cm}^{-1}}{E} \right)^3 \frac{g_{\rm bf}}{n} \qquad [{\rm Mb}] \tag{21}$$

B Evaluation of emissivity constant

The constant terms from Eq. 7 are

$$\alpha = \left(\frac{2}{\pi} \right)^{1/2} \frac{1}{hk^{3/2} (m_{\rm e}c^2)^{3/2}} \tag{22}$$

We use $k = 8.61735 \times 10^{-8}$ keV K^{-1}, $h = 4.1356692 \times 10^{-18}$ keV s, and $m_{\rm e}c^2 = 510.999$ keV, giving

$$\alpha = 6.602427 \times 10^{23} \qquad [\mathrm{keV}^{-4}\ \mathrm{K}^{3/2}\ \mathrm{s}^{-1}] \tag{23}$$

In CHIANTI we will specify the photon energies in cm^{-1}, so we need a conversion factor which is 1.23984×10^{-7} (converts cm^{-1} into keV). This gives

$$\alpha = 1.560162 \times 10^{-4} \qquad [\mathrm{cm}^4\ \mathrm{K}^{3/2}\ \mathrm{s}^{-1}] \tag{24}$$

The cross-sections, σ, are given in Mb and the cm^2-to-Mb conversion factor is 10^{-18}. To convert a cm^{-1} to Å gives a factor 10^{-8} and, for the emissivity in energy units, a further factor of 1.986×10^{-16} is required. Thus the constant becomes 3.0992×10^{-46} erg cm^8 Mb^{-1} s^{-1} $\mathrm{Å}^{-1}$ $\mathrm{K}^{3/2}$. This is what is defined at the beginning of the FREEBOUND_ION routine.

The CHIANTI v.4 paper Eq. 12 actually gives a constant of 3.0992×10^{-52}, but this is wrong.

B.1 keV units

In the CHIANTI software we also want to produce the continuum in units erg cm^{-3} s^{-1} keV^{-1}. Eq. 8 becomes

$$P_{\mathrm{fb}} = \alpha \left(\frac{n_\mathrm{e}}{\mathrm{cm}^{-3}}\right) \left(\frac{n_{+z+1}}{\mathrm{cm}^{-3}}\right) \left(\frac{E}{\mathrm{cm}^{-1}}\right)^3 \left(\frac{\mathrm{K}}{T}\right)^{3/2} \sum_i \frac{\omega_i}{\omega_0} \left(\frac{\sigma_i^{\mathrm{bf}}}{\mathrm{Mb}}\right) \exp\left(-\frac{E - I_i}{kT}\right) \tag{25}$$

where I note the E^3 rather than E^5, and the numerical constant α is given by

$$\alpha = \left(\frac{2}{\pi}\right)^{1/2} \frac{c}{k^{3/2}(m_\mathrm{e}c^2)^{3/2}} \tag{26}$$

after removing the hc factor. This is evaluated to:

$$\alpha = 8.185629 \times 10^{16} \qquad [\mathrm{keV}^{-3}\ \mathrm{K}^{3/2}\ \mathrm{cm}\ \mathrm{s}^{-1}] \tag{27}$$

we need to leave one of the keV^{-1}, but the other two are converted into cm, as before, giving

$$\alpha = 1.258298 \times 10^{-3} \qquad [\mathrm{keV}^{-1}\ \mathrm{K}^{3/2}\ \mathrm{cm}^3\ \mathrm{s}^{-1}] \tag{28}$$

Now, taking into account the cm^2 to Mb conversion, and the cm^{-1} to erg conversion, the constant becomes

$$\alpha = 2.499479 \times 10^{-31} \qquad [\mathrm{keV}^{-1}\ \mathrm{K}^{3/2}\ \mathrm{erg}\ \mathrm{Mb}^{-1}\ \mathrm{cm}^6\ \mathrm{s}^{-1}] \tag{29}$$