

# Calculating Radiative Recombination Continuum From a Hot Plasma

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When an electron collides with an atom or ion, it may

- excite the atom/ion ( $I + e \rightarrow I^* + e$ )
- ionize the atom/ion ( $I + e \rightarrow I^+ + 2e$ )
- scatter inelastically ( $I + e \rightarrow I + e + \gamma$ )
- recombine radiatively ( $I + e \rightarrow I^- + \gamma$ )
- recombine dielectronically ( $I + e \rightarrow I^{-*}$ )

This memo will focus on the penultimate process, where an electron collides and recombines with an ion, emitting a photon in the process. The energy of this photon will equal the kinetic energy of the electron plus the binding energy of the newly-recombined electron. Since the kinetic energy of the electron is not quantized, this forms a continuous spectrum with sharp edges at the binding energy of the levels.

The power emitted per keV by this process is (Tucker & Gould 1966):

$$\frac{dE}{dt dV d\omega} = \frac{dP}{dE} = n_e n_{Z,j+1} E_\gamma \sigma_n^{rec}(E_e) v_e \frac{f(v) dv}{dE_\gamma} \quad (1)$$

where  $n_e$  is the electron density,  $n_{Z,j+1}$  is the density of the ion ( $Z, j+1$ ) (where  $Z$  is the atomic number of the ion, and  $j+1$  is the ionization state),  $E_\gamma$  is the energy of the emitted photon,  $\sigma_n^{rec}(E_e)$  is the recombination cross section to level  $n$  at the electron energy  $E_e$ ,  $v_e$  is the electron velocity and  $f(v)dv$  is the number of electrons with velocities in the range  $(v, v + dv)$ . In most cases,  $f(v)$  is the Maxwell-Boltzmann distribution,

$$f(v)dv = 4\pi \left( \frac{m}{2\pi kT} \right)^{3/2} v^2 \exp\left(-\frac{mv^2}{2kT}\right) dv \quad (2)$$

Equation (1) can be simplified considerably. If we define  $I_{Z,j,n}$  to be the binding energy for an electron in level  $n$  of the ion ( $Z, j$ ), and use the fact that  $E_e = 0.5m_e v_e^2$ , we get that

$$\frac{dv_e}{dE_\gamma} = \frac{1}{m_e v_e} \quad (3)$$

Using this result, and substituting the Maxwell-Boltzman equation for  $f(v)$ , we can rewrite (1) as

$$\frac{dP}{dE} = n_e n_{Z,j+1} 4 \left( \frac{E_\gamma - I_{Z,j,n}}{kT} \right) \sqrt{\frac{1}{2\pi m_e kT}} \sigma_n^{rec}(E_\gamma - I_{Z,j,n}) \exp\left(-\frac{E_\gamma - I_{Z,j,n}}{kT}\right) E_\gamma \quad (4)$$

Equation (4) completely describes the spectrum of the radiative recombination continuum (RRC). However, cross sections for recombination are not generally calculated by the atomic physics community; photoionization cross sections are. As photoionization and recombination are inverse processes,

$$I_{Z,j,n} + \gamma \xleftrightarrow{\quad} I_{Z,j+1} + e^- \quad (5)$$

they can be related using detailed balancing. Raymond & Smith (1977) state that:

$$\frac{\sigma_{Z,j,n}^{ph}(\nu)}{\sigma_{Z,j,n}^{rec}(v_e)} = \frac{m_e^2 c^2 v_e^2}{E_\gamma^2} \frac{g_{Z,j+1}}{g_{Z,j,n}}. \quad (6)$$

Here,  $\sigma_{Z,j,n}^{ph}(\nu)$  is the photoionization cross section for the ion ( $Z, j$ ) in state  $n$  for a photon with frequency  $\nu$ , and  $\sigma_{Z,j+1}^{rec}(v_e)$  is the recombination cross section for an electron with velocity  $v_e$  to combine with an ion ( $Z, j+1$ ) (assumed to be in the ground state) to create an ion ( $Z, j$ ) in state  $n$ . Additionally,  $m_e$  is the mass of the electron,  $c$  the speed of light,  $E_\gamma$  is the energy of the photon, and  $g_{Z,j+1}$  and  $g_{Z,j,n}$  are the statistical weights for the ( $Z, j+1$ ) ion in its ground state and the ( $Z, j$ ) ion in state  $n$ , respectively.

## Detailed Balance

Equation (6) can be derived from first principles, as was first shown by Milne (1924). We begin with the assumption that the system is in thermal equilibrium. In this case the emission due to spontaneous and stimulated recombination is balanced by the ionization of the recombined ions (see also Cowen 1980; Shu 1991):

$$n_{Z,j,n} \frac{4\pi B_\nu(T)}{h\nu} \sigma_{Z,j,n}^{ph}(\nu) d\nu = v_e f_e(v_e) n_e n_{Z,j+1} \left\{ \sigma_{Z,j+1}^{rec}(v) + \alpha^{stim} B_\nu(T) \right\} \quad (7)$$

Here,  $B_\nu(T)$  is the Planck blackbody emission function, and  $f(v)$  is the Boltzman equation (2). The  $\alpha^{stim}$  term allows for stimulated recombination. Written in expanded form, Equation (7) becomes

$$n_{Z,j,n} \sigma^{ph}(\nu) \frac{8\pi h\nu^3/c^2}{e^{\frac{h\nu}{kT}} - 1} d\nu = 4\pi v^3 \left[ \frac{m_e}{2\pi kT} \right]^{3/2} \exp\left(-\frac{m_e v^2}{2kT}\right) dv n_e n_{Z,j+1} \left\{ \sigma^{rec}(v) + \alpha^{stim}(v) \frac{2h\nu^3/c^2}{e^{\frac{h\nu}{kT}} - 1} \right\}. \quad (8)$$

Cancelling common terms and solving for  $\sigma^{ph}(\nu)$ , we get

$$\sigma^{ph}(\nu) = \frac{n_e n_{Z,j+1}}{n_{Z,j,n}} \left( e^{\frac{h\nu}{kT}} - 1 \right) \frac{c^2 v^3}{2\nu^2} \left( \frac{m_e}{2\pi kT} \right)^{3/2} \exp\left(-\frac{m_e v^2}{2kT}\right) \frac{dv}{d\nu} \left\{ \sigma^{rec}(v) + \alpha^{stim}(v) \frac{2h\nu^3/c^2}{e^{\frac{h\nu}{kT}} - 1} \right\} \quad (9)$$

Equation (9) can be simplified further using the Saha equation

$$\frac{n_{Z,j+1}}{n_{Z,j,n}} = \frac{2g_{Z,j+1}}{g_{Z,j,n}} \frac{(2\pi m_e kT)^{3/2}}{h^3 n_e} \exp\left(-\frac{I_{Z,j,n}}{kT}\right), \quad (10)$$

which is applicable because of the assumption of thermal equilibrium. Substituting this in gives

$$\sigma^{ph}(\nu) = \frac{2g_{Z,j+1}}{g_{Z,j,n}} \frac{(2\pi m_e kT)^{3/2}}{h^3} \frac{c^2 \nu^3}{2\nu^2} \left(\frac{m_e}{2\pi kT}\right)^{3/2} \exp\left(-\frac{\frac{1}{2}m_e \nu^2 + I_{Z,j,n}}{kT}\right) \frac{d\nu}{d\nu} \left\{ \sigma^{rec}(\nu) + \alpha^{stim}(\nu) \frac{2h\nu^3/c^2}{e^{\frac{h\nu}{kT}} - 1} \right\}. \quad (11)$$

This can be simplified further by cancelling common factors, and we also use the relationship  $h d\nu = m_e \nu d\nu$  to get:

$$\begin{aligned} \sigma^{ph}(\nu) &= \frac{g_{Z,j+1}}{g_{Z,j,n}} \frac{m_e^2 c^2 \nu^2}{h^2 \nu^2} \exp\left(\frac{h\nu}{kT}\right) \left\{ \sigma^{rec}(\nu) \left(\exp\left(\frac{h\nu}{kT}\right) - 1\right) + \alpha^{stim}(\nu) \left(\frac{2h\nu^3}{c^2} - 1\right) \right\} \\ &= \frac{g_{Z,j+1}}{g_{Z,j,n}} \frac{m_e^2 c^2 \nu^2}{h^2 \nu^2} \left\{ \sigma^{rec}(\nu) + \exp\left(-\frac{h\nu}{kT}\right) \left( \alpha^{stim}(\nu) \left(\frac{2h\nu^3}{c^2}\right) - \sigma^{rec}(\nu) \right) \right\} \end{aligned}$$

But since  $\sigma^{rec}(\nu)$  and  $\alpha^{stim}(\nu)$  are atomic constants, they cannot depend on the temperature of the medium, or on its equilibrium state. Therefore the following relationship must hold:

$$\alpha^{stim}(\nu) = \frac{c^2}{2h\nu^3} \sigma^{rec}(\nu), \quad (14)$$

which leads to our desired result, Equation (6).

## Spectral Calculation

Radiative recombination gives rise to a continuum of emission, with a minimum energy equal to the binding energy of the ion in its final state. The power emitted per unit energy at an energy  $E_\gamma$  is given by

$$\frac{dP}{dE}(E_\gamma) = n_e n_{Z,j+1} E_\gamma \sigma_{Z,j+1 \rightarrow Z,j,n}^{rec}(E_e) v_e f(\nu) \frac{d\nu}{dE_\gamma}, \quad (15)$$

where  $E_e$  is the initial electron energy, and  $v_e$  the initial electron velocity. Using Equation (6), we can restate this in terms of the photoionization cross section  $\sigma_{Z,j,n}^{ph}$ :

$$\frac{dP}{dE}(E_\gamma) = \frac{4\pi}{c^2} (2\pi m_e kT)^{-3/2} n_e n_{Z,j+1} E_\gamma^3 \frac{g_{Z,j,n}}{g_{Z,j+1}} \exp\left(-\frac{E_\gamma - I_{Z,j,n}}{kT}\right) \sigma_{Z,j,n}^{ph}(E_\gamma). \quad (16)$$

After substituting in values for the constants, we get:

$$\frac{dP}{dE}(E_\gamma) = 1.31 \times 10^8 \text{ erg cm/s/keV } n_e n_{Z,j+1} \left(\frac{E_\gamma}{\text{keV}}\right)^3 \frac{g_{Z,j,n}}{g_{Z,j+1}} \exp\left(-\frac{E_\gamma - I_{Z,j,n}}{kT}\right) \left(\frac{T}{1\text{K}}\right)^{-3/2} \sigma_{Z,j,n}^{ph}(E_\gamma). \quad (17)$$

## Practical Consideration

Given the photoionization cross section, the ionization energy, and the statistical weights of the levels involved it is trivial to use Equation (17) to calculate the emission due to radiative recombination. However, a number of complications remain:

1. The photoionization cross sections have not been calculated for all levels of all ions.
2. Each ion has an infinite number of bound states which an electron could recombine into; some method of cutting off the level calculation must be done.
3. Calculating the power emitted per energy bin should properly be done as an integral of  $dP/dE$  over the bin. However, this requires a substantial amount of computation that will slow down the entire code.

We will consider each of these problems and discuss how they have been addressed.

## Cross Sections

The most substantial problem in creating any plasma emission code is the lack of accurate atomic data. Verner & Yakovlev (1995) used a Hartree-Dirac-Slater (HDS) code to calculate the partial photoionization cross section for all subshells  $nl$  of all ions with  $Z \leq 30$ . We use these results to calculate recombination to the ground state of each ion. A subsequent paper (Verner *et al.* 1996) enhanced these results near threshold by including data from the Opacity Project. However, much of the improvement is due to including autoionization resonances. In the context of recombination, these will be considered in this code as dielectronic recombination, not radiative recombination. Therefore, for our purposes the HDS code data which does not include resonances is more appropriate.

Calculating recombination to non-ground states requires data on the cross section of excited ions. In the case of hydrogenic ions, the exact cross section can be calculated (Karzas & Latter 1961; Boardman 1964). However, for more complex ions, only very limited data is available. The most complete set of data is by Clark, Cowan, & Bobrowicz (1986), who calculated the configuration-averaged photoionization cross sections for all subshells between 1s and 5g for He-like through Al-like ions. One restriction on the data, however, is that it is only valid for ions more than three times ionized. As a result of the configuration averaging, however, some important data is not available. For example, a triplet of lines from the  $n = 2$  level of He-like ions exists that is very strong in many astrophysical environments. It consists of a resonance line ( $1s2p \ ^1P_1 \rightarrow 1s^2 \ ^1S_1$ ), a forbidden line ( $1s2s \ ^3S_1 \rightarrow 1s^2 \ ^1S_1$ ), and an intercombination line ( $1s2s \ ^3P_1 \rightarrow 1s^2 \ ^1S_1$ ). In addition, the  $n = 2$  level also has the strictly forbidden transition  $1s2s \ ^1S_1 \rightarrow 1s^2 \ ^1S_1$  which gives rise to two-photon emission. The Clark *et al.* data, however, does not distinguish between the triplet and the

singlet states, and so will not allow us to calculate the ratio of the forbidden and resonance lines.

Table 1 lists the sources of the cross sections used in the code to date. The most important issue for the code is not the calculation of the continuum emission, which (except in the case of a photoionized plasma) is usually smaller than the bremsstrahlung emission. Rather, recombination can affect level populations and thereby change line ratios.

### Level Cutoffs

Each ion has an infinite number of bound states but also has a finite total recombination rate. Therefore, the cross section for recombination must drop rapidly as a function of  $n$ . Of course, as stated above very little data exists beyond the ground state recombination rate. Despite this shortage of data on cross sections on excited ions, we can approximate the recombination to excited levels when necessary by using a hydrogenic model (see Péquignot, Petitjean, & Boisson 1991). This is also the method used by *SPEX* (Mewe & Kaastra 1994). However, we use a different method than theirs to determine the maximum level to consider for recombination.

The maximum radiative RRC occurs near the ionization energy of the level, since that is where the cross section tends to be large and because of the exponential damping term (see Eq. 4). Therefore, when asking if recombination to a given level will be important we can examine only the case of zero-energy electrons, where the emitted photon's energy comes entirely from the binding energy of the level. In this case, we care only about the hydrogenic cross section at threshold. Using Kramer's semiclassical approximation, this is

$$\sigma_n(E_{th}) = 7.91 \times 10^{-18} \text{ cm}^2 \frac{n}{Z_{\text{eff}}^2} \quad (18)$$

where  $Z_{\text{eff}}$  is the is the atomic number  $Z$  of the element under consideration minus the number of electrons  $j$  screening its charge. When we use this approximation to the cross section, Equation (17) becomes:

$$\begin{aligned} \frac{dP}{dE}(I_{Z,j,n}) &= 1.31 \times 10^8 \text{ erg cm/s/keV } n_e n_{Z,j+1} \left(\frac{I_{Z,j,n}}{\text{keV}}\right)^3 \frac{g_{Z,j,n}}{g_{Z,j+1}} \left(\frac{T}{1\text{K}}\right)^{-3/2} \sigma_{Z,j,n}^{ph}(I_{Z,j,n}) \\ &\approx 5.21 \times 10^{-15} \text{ erg cm}^3/\text{s/keV } n_e n_{Z,j+1} \left(\frac{Z_{\text{eff}}^4}{n^3}\right) \frac{1}{g_{Z,j+1}} \left(\frac{T}{1\text{K}}\right)^{-3/2} \end{aligned} \quad (20)$$

where we also used the fact that  $g_{Z,j,n} = 2n^2$ . As this shows, the importance of higher  $n$  states to the radiative recombination continuum drops off as  $1/n^3$ .

To decide where to stop calculating the recombination continuum, we compare the RRC emission at threshold to the bremsstrahlung emission at the same energy. If the RRC emission is less than some chosen fraction of the bremsstrahlung for this level, then we assume that recombination to this and all higher levels of this ion are negligible. **We still must do a study to discover the appropriate value of this constant, and how much emission is missed for a given value.**

## Integrating $dP/dE$

After the choice of data is made and the maximum  $n$  level to calculate recombination to has been chosen, one further issue exists: how to estimate the total emission in a given energy bin. The exact method would be to integrate the emission over the bin:

$$\Lambda_{RRC}(E_{\text{bin}}) = \int_{E_0}^{E_1} \frac{dP}{dE}(E)dE \quad (21)$$

where  $E_0, E_1$  are the minimum and maximum energies for the bin, respectively. However, doing a numerical integration is slow and if  $dP/dE$  is nearly constant over the bin energies, unnecessary.

We calculate the emission as follows:

1. Calculate the emission at the bin edges
2. If the two results differ by less than some constant  $\epsilon$ , average them and multiply by the bin width to get the total emissivity.
3. If the results differ by more than  $\epsilon$ , then use a numerical integration routine to calculate the emissivity.
4. If a numerical integration is used, the code returns a low-level warning to the user (which may be safely ignored) suggesting that a finer binning should be used to measure the RRC emission accurately.

**We still need to make an estimate of what  $\epsilon$  should be.**

## References

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Table 1: Sources of photoionization cross section data for all levels

Ion	H	He	C	N	O	Ne	Mg	Al	Si	S	Ar	Ca	Fe	Ni
I	H													
II	N	H												
III	-	N												
IV	-	-												
V	-	-	C	C	C	C	C	C	C	C				
VI	-	-	H	C	C	C	C	C	C	C	C			
VII	-	-	N	H	C	C	C	C	C	C	C			
VIII	-	-	-	-	H	C	C	C	C	C	C	C		
IX	-	-	-	-	N	C	C	C	C	C	C	C		
X	-	-	-	-	-	H	C	C	C	C	C	C		
XI	-	-	-	-	-	N	C	C	C	C	C	C		
XII	-	-	-	-	-	-	H	C	C	C	C	C		
XIII	-	-	-	-	-	-	N	H	C	C	C	C		
XIV	-	-	-	-	-	-	-	N	H	C	C	C	C	
XV	-	-	-	-	-	-	-	-	N	C	C	C	C	
XVI	-	-	-	-	-	-	-	-	-	H	C	C	C	C
XVII	-	-	-	-	-	-	-	-	-	N	C	C	C	C
XVIII	-	-	-	-	-	-	-	-	-	-	H	C	C	C
XIX	-	-	-	-	-	-	-	-	-	-	N	C	C	C
XX	-	-	-	-	-	-	-	-	-	-	-	H	C	C
XXI	-	-	-	-	-	-	-	-	-	-	-	N	C	C
XXII	-	-	-	-	-	-	-	-	-	-	-	-	C	C
XXIII	-	-	-	-	-	-	-	-	-	-	-	-	C	C
XXIV	-	-	-	-	-	-	-	-	-	-	-	-	C	C
XXV	-	-	-	-	-	-	-	-	-	-	-	-	C	C
XXVI	-	-	-	-	-	-	-	-	-	-	-	-	H	C
XXVII	-	-	-	-	-	-	-	-	-	-	-	-	N	C
XXVIII	-	-	-	-	-	-	-	-	-	-	-	-	-	H
XXIX	-	-	-	-	-	-	-	-	-	-	-	-	-	N

Sources:

**H** Exact hydrogenic solution available

**C** From Clark, Cowen & Bobrowicz, 1986, ADNDT, 34, 3, 419

**N** None needed; no electrons to photoionize.