
|SRON| – SPEX

Continuum Radiation Processes

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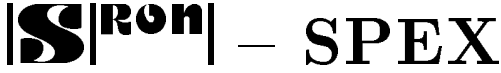
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CONTINUUM RADIATION PROCESSES

1 Introduction

The continuum emission from an optically thin plasma includes three components:

- free-free emission (“bremsstrahlung”) (subroutine BREMS)
- free-bound emission (subroutine FREEBOUND)
- two-photon emission (subroutine TWOFOT)

The subroutine CONEM adds bin-wise the three components to calculate the total continuum spectrum. In the following sections we will shortly deal with the three processes.

The *structure* of the subroutine CONEM is as follows. After initialisation of some constants, which is done the first time the routine is called, the subroutine calculates some temperature-dependent coefficients for each of the ions and emission processes involved. Then a large loop over the input energy array follows; for each energy, a loop over all ions in which the free-free, two-photon and free-bound Gaunt factor is calculated is done.

There are some cut-offs in the program to avoid unnecessary calculation of negligible quantities and arithmetic overflow. These are as follows. The relevant scale parameters are C_{\max} and U_{\max} . C_{\max} (currently put to .001) is a cut-off for too small amplitudes of the Gaunt factor. U_{\max} (currently put to 69.0, or $e^{U_{\max}} = 9.25 \times 10^{29}$) is a factor which governs all exponential factors. Continuum emission is only calculated for photon energies

$$E/kT < U_{\max}.$$

2 Bremsstrahlung (subroutine BREMS)

Compared to the old version of the code (Mewe, Gronenschild, van den Oord 1985) which have sometimes relative errors of some 15 % we have improved the accuracy of the continuum emissivity to an overall accuracy of 1 %. This improvement is discussed below. Moreover, because the subroutine calculating the continuum emission was far most the most CPU time consuming part of the code in the older version, its speed has been enhanced by a factor of $\gtrsim 4$.

In the last section we show which elemental abundances are used as a standard in the calculations.

2.1 Algorithm

The algorithm in the subroutine BREMS is

$$P_{ff} = 3.031014 \times 10^{-1} Y \frac{G_{ff} e^{-E/T}}{E \sqrt{T}}, \quad (1)$$

where P is the emission in 10^{44} photons/s/keV, Y is the total emission measure in 10^{64} m^{-3} , E is the photon energy in keV, and T is the electron temperature in keV. G_{ff} is the total, energy-averaged Gaunt factor summed over all ions and calculated by the subroutine GAUNTF. The constant can be derived from the quantities as given by Rybicki and Lightman (1979) (eq. 5.14b) if converted to SI units and by taking the correct transformations from K to keV and Hz to keV.

3 Free-free Gaunt factor calculations (subroutine GAUNTF)

3.1 Improvements

Gronenschild and Mewe (1978) have given a formula for the *free-free Gaunt factor*, based upon the Born approximation and a correction factor. This formula contained a modified Bessel function, square roots and logarithms and was the largest contributor to the CPU time consumed, since the formula was evaluated for each ion contributing to the emission and for all energy bins. The formula was an approximation to the calculations of Karzas and Latter (1961) and had an accuracy of better than 15 %. Karzas and Latter presented their results only graphically; since then, Carson (1988) presented extensive tables of the free-free Gaunt factor, reproducing the results of Karzas and Latter.

Table 1 shows the differences of Gronenschild and Mewe's Gaunt factor with the exact results of Carson. It is evident that especially in the temperature range of 10^4 – 10^7 K (for Hydrogen) and for $E > kT$ the errors can be quite substantially. Therefore we have chosen to calculate the free-free Gaunt factor by interpolation of Carson's table. With bilinear interpolation of the logs of the Gaunt factor on Carson's logarithmic energy and temperature grid the required accuracy of 1 % was reached. Carson lists the Gaunt factor in the energy range $10^{-4}kT < E < 100kT$. For larger energies no Gaunt factor is required since the exponential prefactor cuts off the spectrum at high energies. For lower energies, we used the asymptotic dependence $G = a(\gamma^2) + (\sqrt{3}/\pi) \ln(E/kT)$, where $\gamma^2 = Z^2 \text{Ryd}/kT$. As stated before, the present calculations are nonrelativistic; Carson's tables are valid for $T < 136$ keV ($10^{-4} < \gamma^2 < 100$). For larger temperatures (better: smaller γ^2), we simply took the minimum value for $\gamma^2 = 10^{-4}$. Similarly, for very low temperatures ($T < 0.136$ eV, or about 1000 K) we took the maximum value for γ^2 . But in this regime the calculations are irrelevant anyhow since then the atoms are essentially neutral, so free-free radiation is impossible.

The calculations of Carson are non-relativistic. Relativistic corrections were calculated by Kylafis and Lamb (1982), eqn. (B4). These authors calculate the relativistic correction with respect to the Born approximation. The relative accuracy of the Born approximation (in the non-relativistic limit) with respect to the results of Carson is shown in Table 2. As is obvious, the Born approximation is good for high energies, and for that reason Kylafis and Lamb made the same approximations as for

Table 1: Comparison of free-free Gaunt factor of Gronenschild and Mewe (1978) ($G_{ff,GM}$) with Carson (1987) ($G_{ff,C}$). The tabulated quantity is $G_{ff,GM}/G_{ff,C} - 1$.

$E/kT \setminus Z^2\text{Ryd}/kT$	-4.00	-3.00	-2.00	-1.00	.00	1.00	2.00
-4.00	-.002	.003	.027	.052	.048	.026	-.002
-3.50	-.003	.003	.028	.054	.053	.031	-.004
-3.00	-.003	.003	.029	.056	.057	.035	-.010
-2.50	-.003	.003	.028	.056	.060	.037	-.023
-2.00	-.004	.001	.026	.052	.058	.036	-.038
-1.50	-.005	-.001	.020	.039	.047	.034	-.040
-1.00	-.006	-.003	.009	.012	.023	.035	-.020
-.50	-.007	-.003	-.000	-.029	-.016	.040	.007
.00	-.002	.010	.006	-.063	-.069	.029	.023
.50	.020	.053	.044	-.066	-.121	-.005	.018
1.00	.080	.137	.092	-.035	-.135	-.053	-.005
1.50	.219	.243	.049	-.037	-.079	-.081	-.035
2.00	.489	.269	-.278	-.252	.047	-.029	-.063

Table 2: Comparison of free-free Gaunt factor $G_{ff,Born}$ in the non-relativistic Born approximation with Carson (1987) ($G_{ff,C}$). The tabulated quantity is $G_{ff,Born}/G_{ff,C} - 1$.

$E/kT \setminus Z^2\text{Ryd}/kT$	-4.00	-3.00	-2.00	-1.00	.00	1.00	2.00
-4.00	-.001	-.001	.003	.026	.102	.245	.441
-3.50	-.001	-.001	.003	.028	.114	.277	.506
-3.00	-.001	-.001	.003	.030	.125	.312	.576
-2.50	-.002	-.002	.001	.029	.133	.343	.638
-2.00	-.002	-.005	-.005	.019	.130	.356	.660
-1.50	-.004	-.009	-.019	-.007	.097	.319	.594
-1.00	-.006	-.017	-.044	-.062	.012	.196	.401
-.50	-.010	-.030	-.083	-.158	-.143	-.024	.097
.00	-.015	-.047	-.133	-.282	-.351	-.299	-.238
.50	-.021	-.065	-.184	-.400	-.549	-.551	-.523
1.00	-.026	-.080	-.226	-.487	-.689	-.732	-.721
1.50	-.030	-.090	-.253	-.542	-.769	-.841	-.843
2.00	-.032	-.097	-.270	-.573	-.812	-.898	-.912

Table 3: Comparison of relativistic free-free Gaunt factor ($G_{ff,Rel.}$) with the nonrelativistic Born approximation ($G_{ff,Born}$) The tabulated quantity is $G_{ff,Rel.}/G_{ff,Born} - 1$. Numbers in italics are for photon energies larger than 400 keV, where the approximation to the relativistic Gaunt factor breaks down.

$E/kT \setminus Z^2 \text{Ryd}/kT$	-4.00	-3.00	-2.00	-1.00	.00	1.00	2.00
-4.00	.108	.006	.000	.000	.000	.000	.000
-3.50	.111	.006	.000	.000	.000	.000	.000
-3.00	.116	.006	.001	.000	.000	.000	.000
-2.50	.123	.006	.001	.000	.000	.000	.000
-2.00	.132	.007	.001	.000	.000	.000	.000
-1.50	.146	.008	.001	.000	.000	.000	.000
-1.00	.171	.009	.001	.000	.000	.000	.000
-.50	.222	.012	.001	.000	.000	.000	.000
.00	.366	.018	.002	.000	.000	.000	.000
.50	<i>.987</i>	.039	.003	.000	.000	.000	.000
1.00	<i>5.536</i>	.125	.008	.001	.000	.000	.000
1.50	<i>63.045</i>	.655	.026	.002	.000	.000	.000
2.00	<i>1211.239</i>	<i>5.694</i>	.107	.007	.001	.000	.000

the Born approximation (apart of course from relativistic effects). Table 3 lists Kylafis and Lamb's correction factor (minus 1) and it is evident from this table that in some parts of our parameter space (especially for high temperatures) the correction factor can not be neglected. Discarding the difference between the non-relativistic Born approximation and Carson's results at the temperatures and energies where the relativistic correction is important, we simply approximated the true Gaunt factor by Carson's value times Kylafis and Lamb's correction factor. *Note:* The correction of Kylafis and Lamb is calculated for Hydrogen. Since at high temperatures all ions are nearly completely stripped of electrons, $Z^2 \geq 4$ for all ions other than Hydrogen, and thus the corresponding γ^2 is also 4 times larger, resulting in a much smaller relativistic correction.

3.2 Algorithm

The subroutine GAUNTFF calculates the total free-free Gaunt factor as a function of electron energy E , as well as the energy-averaged Gaunt factor (over a Maxwellian distribution with electron temperature T), and summed over all ions.

The algorithm uses bi-linear interpolation of the logs of the Gaunt factor $G_{ff}(\gamma^2, u)$ for the contribution from a particular ion Z^{+z} on a log-log grid in γ^2 and u . Here we define:

$$u = E/kT, \quad \gamma^2 = z_n^2 E_H, \tag{2}$$

where the effective charge z_n (of the recombining ion Z^{+z} is defined from

$$E(Z, z - 1, n) = E_{\text{H}} z_n^2 / n^2, \quad (3)$$

E_{H} being the ionization energy of hydrogen, and $E(Z, z - 1, n)$ (or in short notation E_n , the "edge" energy) the ionization energy from the level with principal quantum number n in the recombined ion $Z^{+(z-1)}$. In the expression for γ^2 we take $n = n_0$, the quantum number of the ground state, hence $z_n = z n_0$.

We note that all these quantities are defined by Carson (1988) and in papers III (Gronenschild, Mewe 1978) and VI (Mewe, Lemen, van den Oord 1986). The Gaunt factors g_{ff} for the individual ions are calculated using Carson's tables plus a relativistic correction as described by Kylafis and Lamb (1982) (see §3.1.) and then added (cf. paper VI, eq. 3), with the exception that we normalise here everything to the Hydrogen density instead of the electron density.

First we determine the sum $S = \sum_i C_i z_i^2$ where i denotes the ions, C_i the concentration of the ion ($i \equiv Z^{+z}$) with respect to Hydrogen, and z_i^2 the square of the effective charge for this ion. In the final calculation, only ions with $C_i z_i^2$ values larger than $.001S$ are taken into account.

The ion concentrations are calculated by solving the ionization balance (see SRON/SPEX/TRPB02) using the ionization and recombination rate coefficients as calculated with the code of Arnaud and Rothenflug (1985) (which is applicable only for the 14 most abundant elements). As an additional option we can use for the special case of iron the ion concentrations calculated by Arnaud and Raymond (1992) which seem an improvement at least for the iso-electronic sequences from H to Ne (H.E. Mason, private communication, 1994). In the future we will calculate new rate coefficients for all elements with atomic number $Z \leq 30$.

The cut-offs in the program to avoid unnecessary calculation of negligible quantities and arithmetic overflow are described by the following scale parameters: C_{max} and U_{max} . C_{max} (currently put to .001) is a cut-off for too small amplitudes of the Gaunt factor. U_{max} (currently put to 69.0, or $e^{U_{\text{max}}} = 9.25 \times 10^{29}$) is a factor which governs all exponential factors.

The *free-free* emission is only calculated if

$$Z_{eff}^2 X_{(Z,z)} > C_{\text{max}}$$

where Z_{eff} is the effective charge of the ion and $X_{(Z,z)}$ its relative abundance to the total Hydrogen density. Should in any case the photon energy be larger than 511.003 keV, then the relativistic correction of Kylafis and Lamb to the free-free Gaunt factor is calculated assuming $E = 511.003$ keV (this is actually done in the program which generates the free-free Gaunt-factor table).

4 Free-bound Gaunt factor calculations (subroutine FREEBOUND)

4.1 Improvements

Mewe, Lemen and van den Oord (1986) approximated the *free-bound Gaunt factor* by assuming that the individual Gaunt factor $g_{fb}(n)$ for each (excited) state with principal quantum number n did

not depend upon energy, and that the edge energies $E_n = E_{n_0+1}$ for $n > n_0 + 1$, where n_0 is the principal quantum number of the ground state. Here we take into account the full energy dependence of $g_{fb}(n)$, and also the correct edge energies for all $n \leq 15$. As in Mewe, Lemen and van den Oord, we approximate for the excited states $\zeta_n = 2n^2$, and $z_n = z$, the charge of the recombining ion Z^{+z} .

The individual gaunt factors $g_{fb}(n, E)$ were tabulated by Karzas and Latter (1961). We found the following approximation to their results:

$$g_{fb}(n, E) = (((a_{n,4}x + a_{n,3})x + a_{n,2})x + 1)xa_{n,1}$$

where

$$x \equiv 1/(1 + \sqrt{E/E_1})$$

and

$$E_1 \equiv n^2 E_n = E_H z_n^2.$$

The above formula has an absolute accuracy of < 0.0059 for all n (for $n = 1$ even better than 0.0004). Since in most of the energy region of interest the Gaunt factor is of order unity, this absolute error is sufficiently small for our purposes. (The relative error is everywhere better than 0.023, with the largest value occurring for very large energies).

The difference between the "old" free-bound Gaunt factor and the new one can be up to 5–10 %.

4.2 Algorithm

The subroutine FREEBOUND calculates the free-bound recombination continuum spectrum.

The background of the calculation can be found in Rybicki and Lightman (1979), p. 282–285. From this we deduce (with slightly different notation)

$$\sigma_{bf} = \frac{32\pi\alpha^3 a_0^2 m_e c^2 I^2}{3\sqrt{3}nE^3} g_{bf}. \quad (4)$$

This defines the relation between the bound-free (photo-ionisation) cross section σ_{bf} and the corresponding Gaunt factor g_{bf} . In this equation α is the fine-structure constant and a_0 is the Bohr radius. Further I is the ionisation potential of the particular (excited) level towards which the recombination takes place, and E is the energy of the corresponding photon. Further n is the principal quantum number of the level towards which the recombination occurs. Equation (4) can directly be derived from equations (10.55) and (10.56) of Rybicki and Lightman (RL hereafter).

Similar to (10.55) of RL, the ionisation energy I is related to the effective charge z by

$$I = \frac{z^2 E_H}{n^2}, \quad (5)$$

where E_H is the Rydberg energy (N.B. $E_H \equiv \alpha^2 m_e c^2 / 2$).

Expressing energies in keV, and σ_{bf} in barns (10^{-28} m²), equation (4) can be rewritten as

$$\sigma_{\text{bf}} = 107581.2 \frac{I^2 g_{\text{bf}}}{n E^3}. \quad (6)$$

Using RL (10.57), inserting the Maxwell distribution (10.60) and using the Milne relation (10.62), we get for the free-bound emissivity (photons/volume/time/energy)

$$S(E) = \frac{\sqrt{2} E^2 C_i g_n \sigma_{\text{bf}}}{\sqrt{\pi} (m_e k T)^{3/2} c^2} e^{(I-E)/kT}. \quad (7)$$

Here C_i is the concentration of the recombining ion with respect to Hydrogen, g_n is the statistical weight of the recombining level (defined here as the number of vacancies before recombination in that particular level).

Expressing energies in keV and $S(E)$ in 10^{-20} photons/s/m³/keV, this equation can be rewritten as

$$S(E) = 2.070764 \times 10^{-4} C_i g_n \sigma_{\text{bf}} E^2 T^{-3/2} e^{(I-E)/T}. \quad (8)$$

For recombination to the ground level (principal quantum number n_0), we use the photo-ionisation cross sections as determined in subroutine FOTION, and apply equations (6) and (8).

For recombination to non-groundlevel states with $n = n_0$ (e.g. to $2p$ if the ground level is $2s$) and also for recombination to higher excited states ($n > n_0$), we use the Hydrogenic approximation for the ionisation potential I as well as for the bound-free Gaunt factor g_{bf} . After calculating the Gaunt factor, equations (6) and (8) are applied.

For the ionisation potential I of the ground state we use the ionisation energies E_{n_0} of Lotz (1968) as used throughout this work. Formally we write

$$n = n_0 : \quad I = E_{n_0} \equiv \frac{E_{\text{H}} z_0^2}{n_0^2}. \quad (9)$$

For the ionisation potential for states with $n = n_0$ but not the ground state we use the same ionisation energy E_{n_0} .

For the ionisation potential for $n > n_0$ we use the Hydrogenic approximation (cf. paper VI):

$$n > n_0 : \quad I = \frac{E_{\text{H}} z^2}{n^2}, \quad (10)$$

with z the net charge of the recombining ion (e.g. $z = 12$ for recombination of Fe XIII).

The statistical weight g_n is defined as the number of vacancies in the level towards which recombination occurs, before recombination. We approximate this for ions in the ground state. The statistical weight of the ground state is denoted here by g_0 , the total statistical weight of all levels with $n = n_0$ is gn_0 (this last quantity was denoted ζ_0 in paper VI). If the ground states towards which recombination occurs contains m electrons in the outermost subshell after recombination, we get values for g_n of $3 - m$, $7 - m$ and $11 - m$ in cases where the ground state is an s , p or d -shell, respectively.

Similarly, if the ground state contains M electrons after recombination in all subshells with the same principal quantum number n_0 , we get values for gn_0 of $3 - M$, $11 - M$, $19 - M$ and $33 - M$ for recombination towards n_0 equal to 1, 2, 3, and 4, respectively.

For levels with $n > n_0$, we take

$$g_n = 2n^2. \quad (11)$$

There are many excited levels towards which recombination can take place; we do not take into account all of these levels since this would require an enormous amount of cpu time. The Gaunt factors g_{bf} in equation (4) are all of order unity. Also, the exponential factor in equation (7) is at most 1 (for $E = I$). Inserting (4) and (10) into (7), omitting multiplicative constants which are equal for all levels of all ions and taking g_{bf} and the exponential factor of order unity, we find that for given photon energy E the recombination rate towards level n of each ion is proportional to

$$w_{ni} \equiv C_i g_n z^4 / n^5. \quad (12)$$

In particular, for $n > n_0$ we get after inserting (11) into (12):

$$n > n_0 : \quad w_{ni} = \frac{2z^4}{n^3} C_i \quad (13)$$

and for $n = n_0$ we have

$$n = n_0 : \quad w_{n_0i} = \frac{g_{n_0} z_0^4}{n_0^5} C_i. \quad (14)$$

At the beginning of the process, we calculate

$$W \equiv \sum_i \sum_{n=n_0}^{\infty} w_{ni}. \quad (15)$$

We use only recombination towards those levels, for which $w_{ni} > \epsilon W$, where ϵ is a small number (in practice, we take $\epsilon = 10^{-4}$).

The sum over n in (15) is (apart from the factor C_i) pre-calculated and stored. The sum over n is written as the sum of the n_0 contribution plus all higher levels, which are evaluated with

$$2z^4 C_i \Sigma(n_0) \equiv \sum_{n=n_0+1}^{\infty} w_{ni} = 2z^4 C_i \left[\sum_{n=1}^{\infty} \frac{1}{n^3} - \sum_{n=1}^{n_0} \frac{1}{n^3} \right]. \quad (16)$$

The first sum can be calculated using Riemann's ζ -function as

$$\sum_{n=1}^{\infty} \frac{1}{n^3} = \zeta(3) = 1.2020569031 \dots \quad (17)$$

Finally, for the calculation of the Hydrogenic Gaunt factors g_{bf} we refer to the approximation made in §4.1.

The cut-offs in the program to avoid unnecessary calculation of negligible quantities and arithmetic overflow are described by the following scale parameters: C_{max} and U_{max} . C_{max} (currently put to .001) is a cut-off for too small amplitudes of the Gaunt factor. U_{max} (currently put to 69.0, or $e^{U_{\text{max}}} = 9.25 \times 10^{29}$) is a factor which governs all exponential factors.

Free-bound emission is only calculated if the edge energy E_n satisfies

$$\begin{aligned} E_n/kT &< E/kT < U_{\text{max}}, \\ (E - E_n)/kT &< U_{\text{max}}, \\ a_{n,1} \zeta_0 z_0^4 X_{(Z,z)} \frac{E_H}{kT} e^{E_{n_0}/kT} / n_0^5 &< C_{\text{max}} \end{aligned}$$

for the ground state and

$$2a_{n,1} z^4 X_{(Z,z)} \frac{E_H}{kT} e^{E_n/kT} / n^3 < C_{\text{max}}$$

for excited states, and if at the energy E the relative contribution of higher states compared to the sum of all non-zero lower states exceeds C_{max} .

5 Two-photon emission (subroutine TWOFOT)

5.1 Improvements

We have also improved the *two-photon Gaunt factor* calculations. Gronenschild and Mewe (1978) approximated the spectral distribution function ψ with the square root of a cosine, i.e.

Table 4: **Two photon spectral distribution function $\psi(x)$**

x	Gronenschild-Mewe	H-like	He-like
0.00	0.00	0.00	0.00
0.05	1.04	0.92	0.47
0.10	1.46	1.48	1.18
0.20	2.01	2.10	2.07
0.30	2.36	2.41	2.54
0.40	2.56	2.56	2.78
0.50	2.62	2.60	2.86

$$\psi(x) = 2.623 \sqrt{\cos[\pi(x - 0.5)]}, \quad (18)$$

where $x = E/E_i$, E is the photon energy in keV and E_i is the excitation energy in keV of the $1s-2s$ transition involved. The accuracy of that approximation is some 14 %. In the current code we interpolate directly in the table of Spitzer and Greenstein (1961) for Hydrogenic ions, and in a graph in Dalgarno and Drake (1969) for the Helium-like ions. An accuracy of better than 0.007 times the maximum of the probability distribution function $\psi(x)$ is reached if we interpolate linearly on a grid of 51 points spaced evenly from $x = 0$ to $x = 1$. An impression of the differences with the old version is given in Table 4.

In the old version of the program an error was made with the two-photon emission of Calcium. Instead of taking the ionic concentrations for the H- and He-like ions, the concentrations for the Li- and Be-like ions were taken. This error has now been removed.

Finally we modified the normalisation of the two-photon emissivity. The contribution to the total two-photon Gaunt factor of ion (Z, z) can be written as

$$G_{2p,Z,z}(E) = 164995 \frac{E}{E_{Z,z}^2} \psi\left(\frac{E}{E_{Z,z}}\right) f_{ij} \bar{g}\left(\frac{E}{E_{Z,z}}\right) e^{(E-E_{Z,z})/kT}, \quad (19)$$

where the constant is $3\pi^2 a_0 m_e^2 c^3 / (2000eh)$ and all input quantities are in SI, and the photon energy E is expressed in keV, f_{ij} is the oscillator strength and $\bar{g}(y)$ the average excitation gaunt factor.

We take f_{ij} from Mewe (1977), which differs in the last digit from Gronenschild and Mewe (1978), i.e. $f=0.415$ for H-like ions and $f = 0.830(1 - 1.34/Z)$ for He-like ions. For the average Gaunt factor we follow Mewe (1972) which seems to be different from Mewe and Schrijver (1978): for the Helium sequence, $\bar{g} = 0.05$ (and not 0.045 as taken by Gronenschild and Mewe (1978) and in the old code); for the Hydrogen sequence, $\bar{g} = 0.055$ for Carbon and higher elements, and g is the expression for the Gaunt factor of Mewe (1972) with $A = 0.08$, $B = -0.16$, $C = 0.11$, $D = 0$ for He II.

The energies of the 1s-2s transition are modified slightly with respect to the old version; they are calculated as $0.75I$ for the H-sequence, where I is the ionisation potential. For the He-sequence, we took the energy E_i of the He6-line (in the notation of Paper V), i.e. the transition $1s - 2s(^3S)$. For He-F, this energy was derived from the tables of Moore, For Ne-Si, S, Ar, Ca and Fe we took the data from paper V, for the other elements we interpolated in a where $E_i = \frac{3}{4}(Z - a)^2 E_H$ where Z is the atomic number (a ranges from -0.606 for He to -0.43 for Cu). $F(Z)$ is very smooth in Z , e.g. for Be, C, O, Ne, Mg, Si, S, Ar, Ca and Fe (steps of 2 in Z from Be-Ca, step of 6 from Ca to Fe) it equals 13.18, 11.96, 11.45, 11.17, 11.01, 10.88, 10.80, 10.75, 10.69, and 10.61 eV (Fe). The value for Ni as given in paper V is probably slightly too high, since it yields $f(28) = 10.63$ eV. We have used $f = 10.61$ eV for all elements from Fe-Zn.

Warning: the two-photon emission of H I and He I still has to be implemented!

5.2 Algorithm

The algorithm to calculate the two-photon continuum spectrum is described above in more detail. However, here we differ from that notation: the two-photon emission spectrum $S(E)$ (units 10^{44} photons/s/keV) can be written as

$$S(E) = kC_i Y \frac{f_{ij} e^{-y} \bar{g}(y)}{\sqrt{T} E_i^2} \psi_i(x), \quad (20)$$

where Y is the emission measure in units of 10^{64} m^{-3} , $x = E/E_i$, E is the photon energy in keV, E_i is the excitation energy in keV of the 1s-2s transition involved, $y = E_i/T$ where T is the electron temperature, $\bar{g}(y)$ is the temperature-averaged excitation Gaunt factor for the 1s-2s transition (see e.g. Mewe *et al.* paper VI), and f_{ij} is the corresponding oscillator strength. Further k is a normalisation constant, equal to

$$k = \frac{2^{9/2} \pi^{3/2} a_0^2 E_H^2}{(3m_e)^{1/2}} 10^{20} (1\text{keV})^{1/2} = 5.000965 \times 10^4, \quad (21)$$

where all quantities in eq. 21 are to be taken in SI units.

$\psi(x)$ is the probability distribution for the two photons emitted, normalised to

$$\int_0^1 \psi(x) dx = 2. \quad (22)$$

Finally we note that eq. 20 is only valid for $0 \leq x \leq 1$.

As noted before, the function ψ is tabulated at 51 equally spaced points from 0 to 1 and is interpolated linearly in x . This yields an absolute accuracy of better than 0.007 times the maximum of ψ at $x = 0.5$. (Note that $\psi(0) = \psi(1) = 0$ and further that $\psi(x) = \psi(1 - x)$).

The two-photon emission is calculated for the H-sequence and the He-sequence. For the H-sequence we determine ψ directly by interpolation from the table of Spitzer and Greenstein (1961) for Hydrogenic ions, and for the He-like ions from a graph in Dalgarno and Drake (1969).

The cut-offs in the program to avoid unnecessary calculation of negligible quantities and arithmetic overflow are described by the following scale parameters: C_{\max} and U_{\max} . C_{\max} (currently put to .001) is a cut-off for too small amplitudes of the Gaunt factor. U_{\max} (currently put to 69.0, or $e^{U_{\max}} = 9.25 \times 10^{29}$) is a factor which governs all exponential factors.

The *two-photon* emission is only calculated if

$$164995 E_{Z,z}^{-1} f_{ij} \bar{g}\left(\frac{E}{E_{Z,z}}\right) X_{(Z,z)} = G_{2p,Z,z}(E) \frac{E_{Z,z}}{E} e^{(E_{Z,z}-E)/kT} \phi\left(\frac{E}{E_{Z,z}}\right) X_{Z,z} > C_{\max}$$

and if

$$E/kT < E_{2p}/kT < U_{\max}.$$

6 Abundances

The subroutine SETABU determines the elemental abundances with respect to Hydrogen from the abundances relative to the Solar values. The element abundance is defined as the quantity:

$$A(Z) = {}^{10} \log[n_s(Z)/n_s(H)] + 12 \quad (23)$$

where Z is an arbitrary element, H denotes hydrogen, and n_s is the density (atoms per unit volume) of the current element in the sun. By definition,

$$A(H) = 12. \quad (24)$$

For a non-solar plasma the relative abundance $R(Z)$ with respect to the solar photosphere value is given by

$$R(Z) \equiv \frac{n(Z)/n(H)}{n_s(Z)/n_s(H)}, \quad (25)$$

where $n(Z)$ is the density of the element in the non-solar plasma, and the absolute abundance $C(Z)$ with respect to H is thus given by

$$C(Z) = R(Z) 10^{A(Z)-12}. \quad (26)$$

In the old versions of our code, the solar abundances were from Allen (1973), who referred to work from the early sixties. In an intermediate code, we adopted the values for the abundances from Ross and Aller (1976), where also a discussion on the accuracy of this standard set is found.

There are indications that in the hotter upper solar atmosphere (the X-ray emitting corona) the abundances of the elements with a low first ionization potential (FIP) could be larger by a factor of up to three due some enrichment process (fractionation in the chromosphere between the corona and the photosphere, see e.g. discussions by Feldman (1992) and Hénoux and Somov (1992)). However, in the current code, we use as a standard the solar photospheric abundances of Anders and Grevesse (1989). Table 5 lists the 30 elements (H–Zn) used in this program and the abundances (number of nuclei per Hydrogen nucleus) according to Anders and Grevesse (1989).

In the current code, we have an option to use different standard abundances. Determining parameter is ABUNSET; by default, this parameter is 0 (Anders and Grevesse); values of 1 and 2 correspond to Allen and Ross and Aller, respectively. The relative multiplication factors to be applied when using the other abundances are listed in table 6. Finally we give in Table 7 some more recently determined values taken from Grevesse *et al.* (1992).

7 References

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Table 5: **Elemental abundances** $A(Z)$

Element	Anders and Grevesse (1989)
H	$\equiv 1$
He	.0977
Li	1.45×10^{-11}
Be	1.15×10^{-11}
B	3.98×10^{-8}
C	3.63×10^{-4}
N	1.12×10^{-4}
O	8.51×10^{-4}
F	3.63×10^{-8}
Ne	1.23×10^{-4}
Na	2.14×10^{-6}
Mg	3.80×10^{-5}
Al	2.95×10^{-6}
Si	3.55×10^{-5}
P	2.82×10^{-7}
S	1.62×10^{-5}
Cl	3.16×10^{-7}
Ar	3.63×10^{-6}
K	1.32×10^{-7}
Ca	2.29×10^{-6}
Sc	1.26×10^{-9}
Ti	9.77×10^{-8}
V	1.00×10^{-8}
Cr	4.68×10^{-7}
Mn	2.45×10^{-7}
Fe	4.68×10^{-5}
Co	8.32×10^{-8}
Ni	1.78×10^{-6}
Cu	1.62×10^{-8}
Zn	3.98×10^{-8}

Table 6: Other elemental abundances $R(Z)$ relative to Anders and Grevesse (1989)

Element	Allen (1973)	Ross and Aller (1976)
H	1.00	1.00
He	0.87	0.65
Li	0.35	0.69
Be	0.89	1.00
B	2.51	0.32
C	0.91	1.15
N	0.81	0.78
O	0.78	0.81
F	1.10	1.00
Ne	0.68	0.30
Na	0.83	0.89
Mg	0.69	1.02
Al	0.83	1.12
Si	0.93	1.26
P	1.17	1.12
S	0.98	0.98
Cl	1.26	1.00
Ar	1.74	0.28
K	0.68	1.10
Ca	0.87	0.98
Sc	1.32	0.87
Ti	1.38	1.15
V	2.51	1.05
Cr	1.51	1.10
Mn	1.02	1.07
Fe	0.85	0.68
Co	1.51	0.95
Ni	1.12	1.07
Cu	1.95	0.71
Zn	0.40	0.71

Table 7: **Elemental abundances** $A(Z)$

Element	Grevesse <i>et al.</i> (1992)
H	$\equiv 1$
He	.095
C	3.55×10^{-4}
N	9.33×10^{-5}
O	7.41×10^{-4}
F	3.63×10^{-8}
Ne	1.20×10^{-4}
Cl	3.16×10^{-7}
Ar	3.31×10^{-6}
Sc	1.58×10^{-9}
Ti	1.10×10^{-7}
Fe	3.24×10^{-5}

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