MAX-PLANCK-INSTITUT FÜR PLASMAPHYSIK

GARCHING BEI MÜNCHEN

X-ray Pulse Height Analysis

F. Pohl

IPP 6/193 February 1980

Die nachstehende Arbeit wurde im Rahmen des Vertrages zwischen dem Max-Planck-Institut für Plasmaphysik und der Europäischen Atomgemeinschaft über die Zusammenarbeit auf dem Gebiete der Plasmaphysik durchgeführt.

X-ray Pulse Height Analysis

Abstract

This report gives a detailed description of a computer program for pulse height analysis (PHA) in tokamak experiments. The program yields the electron temperature and the ζ-factor in two energy intervals which have to be free of impurity lines and recombination steps. In such intervals the logarithm of the emissivity F is a linear function of the quantum energy E = hv:

$$\ln F = \alpha + \beta E$$

Information from numerous experimental data is used for rather exact determination of the two coefficients α and β. For this purpose the experimental values are first smoothed. The user of the program then has the option of performing the Abel inversion first. He may, however, also call an iteration procedure in which α and β are obtained direct from the experimental data. The accuracy of this iteration method is in some cases much better than that of conventional Abel inversion.

Furthermore, the densities of the metal ions Ti, Cr, Fe, Ni are estimated from the electron temperature, electron density and the K_α lines. It should be noted, however, that this estimate is very rough because the necessary data, e.g. $\langle \sigma v \rangle$, are not very exactly known.

Table of Contents

1. INTRODUCTION

The report describes a computer program for pulse height analysis (PHA) in tokamak experiments. Data such as raw spectra, aperture parameters etc. are used to determine the electron temperature and the ζ-factor with a good degree of accuracy and also the order of magnitude of the densities of the impurities Ti, Cr, Fe, Ni. It is not possible to estimate the oxygen ion density, as shown at the end of Sec.23.

The report is in three parts:

Part A (Secs. 2 and 3) describes how the spectral function U is produced from the detector signals (eq. (2.4)).

In Part B (Secs. 4 to 11) information on the plasma parameters (e.g. electron temperature) is derived from the spectral function U.

Part C (Secs. 12 to 23) describes the individual subroutines and also details either not treated in Parts A and B or else not fully enough.

The experimental layout is shown schematically in Sec.2. The X-ray quanta emerge from the plasma along the line of sight, pass through the two apertures 1 and 2 (Fig. 1) and the filter and enter the detector. Not only are the photons detected in the detector, their energy is also measured. The resulting pulses are sorted in the analog-digital convertor (ADC) according to height or photon energy $E = h\nu$; the result is the raw spectrum R of the detector. If the raw spectrum R is multiplied by an appropriate normalization factor (see eqs. (2.5) and (2.6)), one obtains the normalized spectrum U_B, which only differs from the ideal spectral function U by statistical errors. In order to obtain the spectral function U in a wide energy interval, we superpose in eq. (2.4) the spectra of several detectors. This superpositioning is performed in the OVLAP subroutine (Sec. 14). This yields the spectral function U(L,J) at given "reference" energy mesh points (eq. (14.1)) and probe positions P_L. This result is transferred to the SESNIC subroutine for further processing.

First the function is smoothed (GLATT subroutine, Sec. 15) because the number of parameters sought (within a clean energy window there are two, namely α and β) is much smaller than the number of mesh points (a few dozen).

The problem of finding the emissivity F or α and β from the spectral function U by ABEL-Inversion (eq. 4.1) is mathematically not well posed, if U is given only at a few mesh points. In order to regularize the problem, we have to introduce an ansatz for U or for T_e and S etc. This can be done by various methods. The choice of this method is a matter of taste. We describe in Secs. 4, 5, 17, 18 and 19 several methods which the user can call by choosing a parameter (NABEL; see Sec. 18).

In Secs. 7 and 8 collection of formulae describe how the X-ray emissivity F depends on the plasma parameters. Equation (7.2) is mostly used in the form

$$\ln F_C = \alpha + \beta E \qquad (1.1)$$

with

$$S = e^{\alpha} \qquad (1.2)$$

$$T_e = - 1./\beta \qquad (1.3)$$

$$E = h\nu \, .$$

It is hoped here that there are large E-intervals without lines or recombination edges in which α and β are independent of E; these intervals are called "clean energy windows" (see Sec. 5, Fig. 4). It should be noted that the linearity (1.1) is often satisfied very well, but that the interpretation (1.2 and 1.3) is wrong: e.g. with pure hydrogen plasma owing to the E dependence of the Gaunt factor (7.10), but possibly also when, for instance, there are metal impurities whose ζ factor for $E < 2$ keV strongly depends on E; see Sec. 9, Fig. 11 for Fe. In Sec. 9 the contribution of the iron to the ζ factor is calculated on the basis of the curves given in Ref. /2/ for the partial densities in corona equilibrium. At the end of the section we discuss how questionable these curves are and what errors are to be expected owing to the absence of corona equilibrium in the tokamak. It is not known whether similar curves are available for other metals. Under the circumstances we have given approximation formulae for the recombination part R_{fb} of the iron (eq. (9.7)) and used them for the other metals Ti, Cr and Ni as well (Sec. 22, METAL subroutine). When better data become available, the numerical coefficients involved will then just have to be replaced in the METAL routine by others. The cross-section $\langle \sigma v \rangle$ for the K_α line radiation is only known within a factor of 2 to 4; see, for example, the two curves of LOTZ and GRIEM in Sec. 11, Fig. 13. Accordingly, the values given for the ion densities by our IMPUR subroutine are also only known within a factor of 2 to 3. Here, too, better values have to be awaited. Under these circumstances Sec. 10 on oxygen recombination radiation is superfluous; it has only been retained for the sake of completeness, and in Sec. 23 we give a method (eqs. (23.4 and 23.5)) by which the oxygen density may yet perhaps be estimated if the metal ion densities are known. Only the following ion species are considered in our program:

hydrogen	(Z = 1)	
oxygen	(Z = 8)	
titanium	(Z = 22)	(1.4)
chromium	(Z = 24)	
iron	(Z = 26)	
nickel	(Z = 28)	

It should be noted that, for example, a strong cobalt line at 7.0 keV can spoil the method of determining the continuum part that is described in Sec. 21, Fig. 24. - As already mentioned, the METAL subroutine is used to determine or, to be more correct, estimate the contribution of the metals Ti, Cr, Fe and Ni, listed in (1.4), to the ζ factor. The difference between the ζ factor and the contribution of the metals is ascribed to the oxygen and hydrogen. This conclusion is, of course, wrong when, for example, carbon is present, but also when tungsten or molybdenum is present, because their density cannot be determined by IMPUR according to the method described in Sec. 11. But even if only the ion species listed in (1.4) are present oxygen determination is mostly impossible at the present time: if, for example, the contribution of the metals is about 5 to 10 and the total ζ factor is 11, any value between 1 and 6 is possible for the difference and hence for the oxygen density. Finally, the parameters calculated with our program and the inaccuracy roughly expected are presented below:

ß, T_e	5 - 10 %	electron temperature
S, ζ	10 - 20 %	ζ -factor
$n_{22}..n_{28}$	factor 2 - 3	metal ion densities
Z_{ME}	factor 3 ?	contribution of metal ions to ζ factor
n_8	factor 10 ?	oxygen ion density

The ζ factors are calculated for two separate clean energy windows which should be free of impurities so that eq. (1.1) is valid there. It is hoped to obtain the recombination edge from the difference of the ζ factors.

2. SPECTRA

Here we define the terms "raw spectrum", "normalized spectrum", "spectral function" etc. as used in the description of the computer program. We start with the scheme of the experimental setup.

Figure 1 shows the plasma cross-section and a detector comprising two apertures, a filter and a counter. The two apertures 1 and 2 define a narrow cone whose axis we call the "line of sight" of the detector. The distance p of the line of sight from the plasma centre is called the "position" of the detector. Behind the aperture 2 is a filter which is more or less opaque to soft X-radiation, but admits hard X-radiation (see Sec. 13). The radiation which has passed through the two apertures and the filter enters the PHA system.

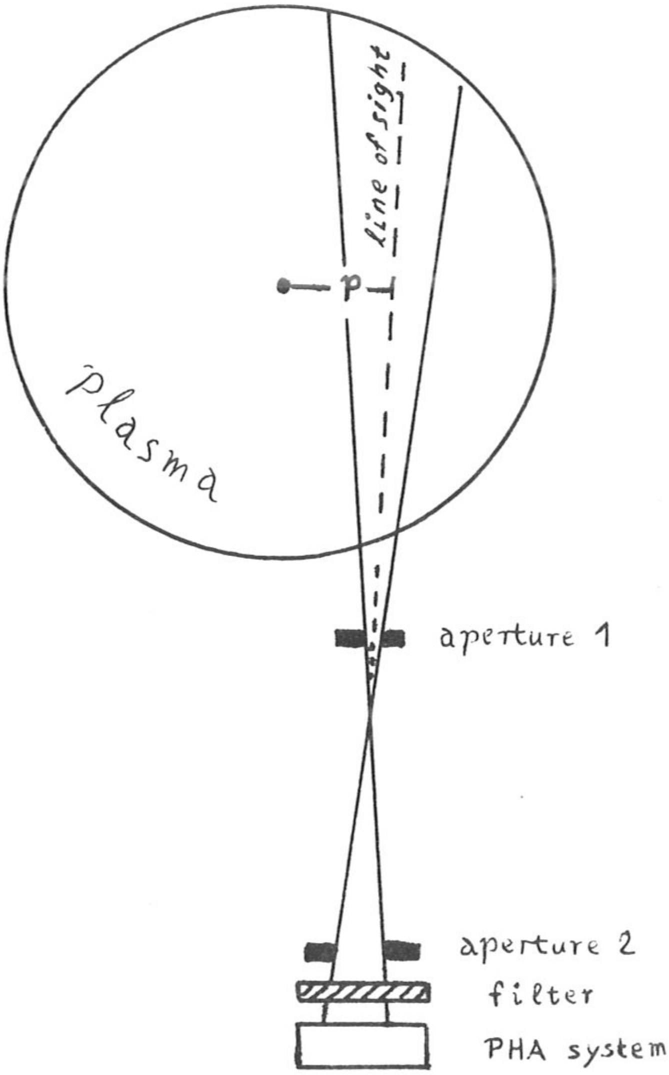


Fig. 1

The PHA system contains an energy scale divided into equal intervals which we call "energy channels" (see eq.(14.2)). The counter records the number of X-ray quanta $E = h\nu$ per energy channel. One can imagine a counter behind each energy channel. (When, for example, a quantum arrives and its energy is incident on channel J = 57, counter No. 57 is advanced by 1.). This yields the following result:

Channel No. 1 recorded 0 quanta
Channel No. 2 recorded 1 quanta (2.1a)
Channel No. 3 recorded 3 quanta

etc.

Figure 1a shows a PHA system with six energy channels; in actual fact such systems have 256 energy channels. The energy channels are counted or designated by the channel number J, the channel width being denoted by DE. When a quantum with an energy $h\nu$ arrives from the interval $E_0+DE(J-\frac{1}{2}) \leq h\nu \leq E_0+DE(J+\frac{1}{2})$ counter No. J is advanced by 1. We now define "raw spectrum" as the number of quanta in the energy channel.

Figure 1b shows the raw spectrum for the case treated in Fig. 1a. The dashed line is the idealized raw spectrum.

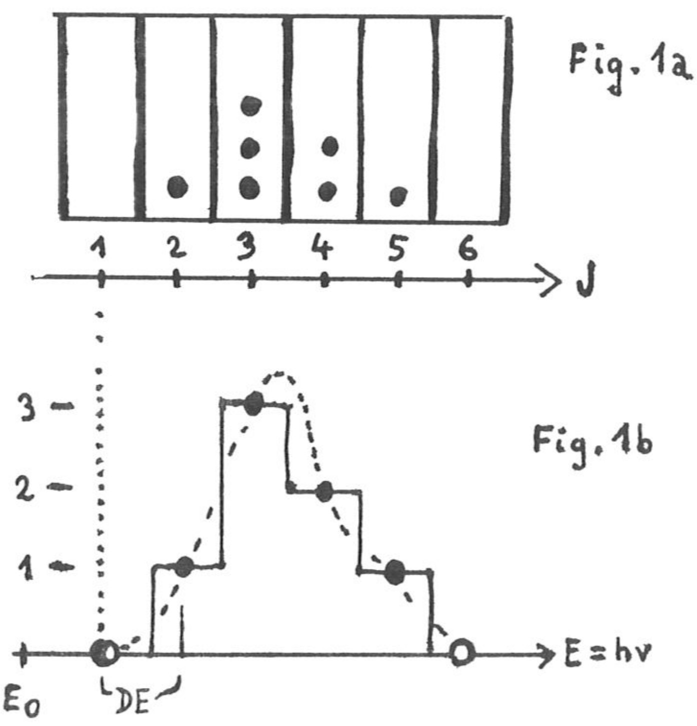


Figure 1b already shows the essential properties of the raw spectra: they vanish for low energies $E = h\nu$ as a result of filtering exp(FILTER) (see Sec. 13, eq. (13.2)). Furthermore, they vanish for high energies $h\nu$ because of the Saha factor $\exp(-h\nu:kT_e)$ (see Sec. 7, eqs. (7.2) and (7.3)). The intervening energy interval - in Fig. 1b channels 3 and 4- are called the "sensitive regime" of the detector. This is usually a few keV. This is not much compared with the total regime of about $2 \lesssim h\nu \lesssim 20$ keV to be recorded or measured. Several detectors with different sensitivity regimes are therefore used: detector 1, for example, is sensitive to low energies, this being achieved with small aperture radii and weak filtering, while detector 2 is sensitive to high energies, this being achieved with strong filtering and large aperture radii.

Such control of the photon flux by the choice of aperture radius is necessary because the PHA system can only handle a limited maximum photon flux. Each detector thus yields a raw spectrum, denoted by $R^{(I)}$, where I is the detector number. In the foregoing example I = 1 thus stands for the detector sensitive to low energies, and I = 2 for the one sensitive to high energies. Each of these detectors has its own energy channels, channel width DE_I and zero displacement EO_I, and so these quantities have the index I; see Sec. 14.

The spectral function U emitted by the plasma - to be defined later in eq. (2.4) - depends on the position p in addition to the plasma parameters such as temperature, density etc. If the plasma spectrum is to be measured over a wide energy range with several detectors, we thus have to locate the detectors at the same position p. It is shown in Figs. c and d how this is done.

Figs. c and d
Plasma torus and lines of sight of three detectors with the same position p

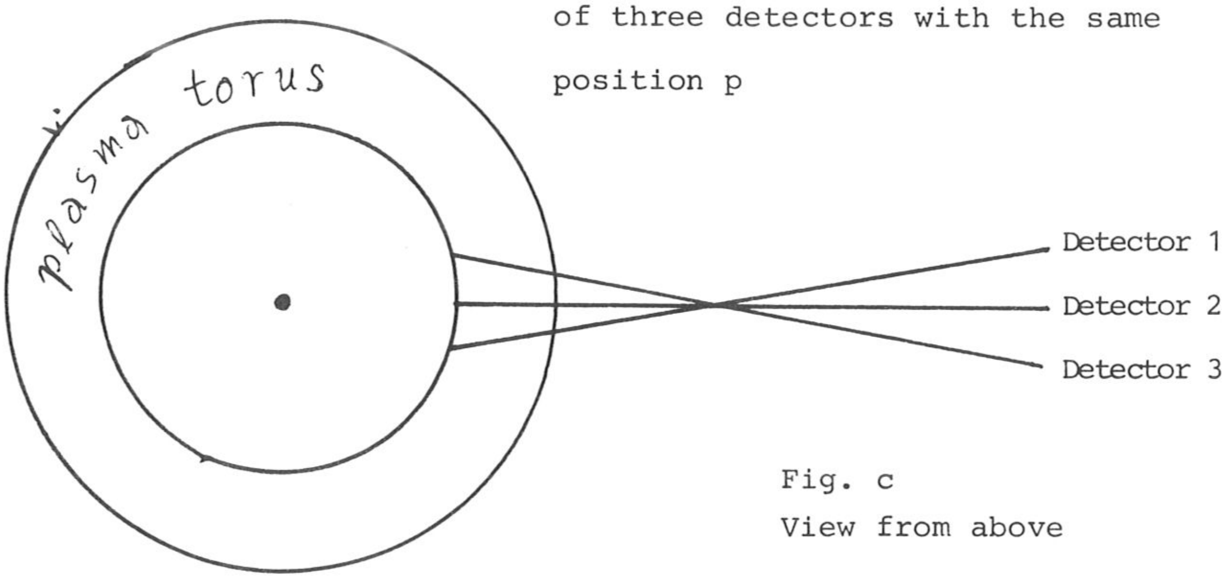


Fig. c
View from above

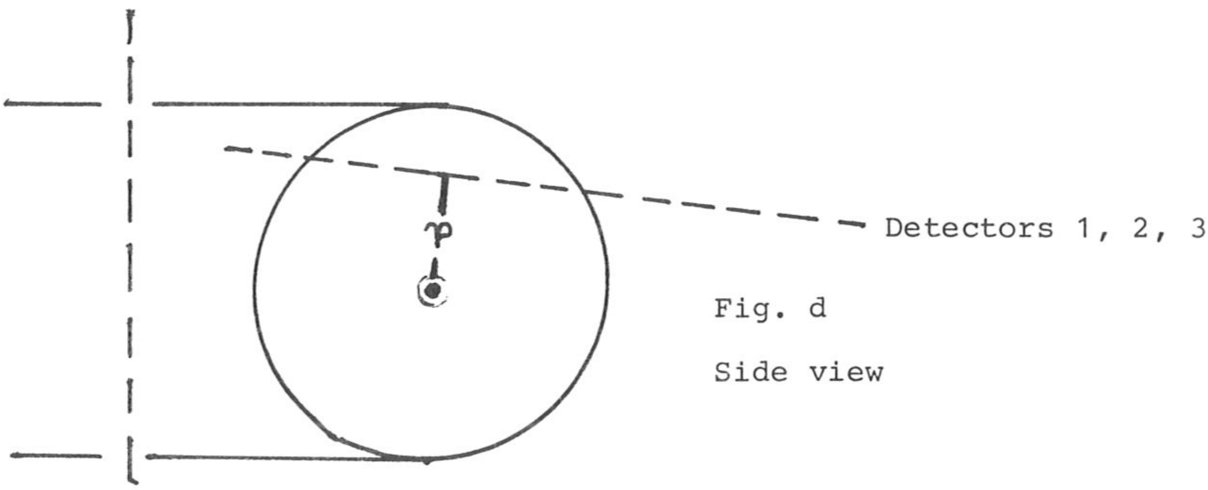


Fig. d
Side view

The idealized raw spectra and the spectral function U differ by an instrument function, which will be treated later in eqs. (2.5) and (2.6). When the raw spectra actually measured are multiplied by this instrument function, one obtains the normalized spectra $U_B^{(I)}$. We now consider how to obtain the spectral function U from the $U_B^{(I)}$. For this purpose we draw in a schematic example Fig. e.

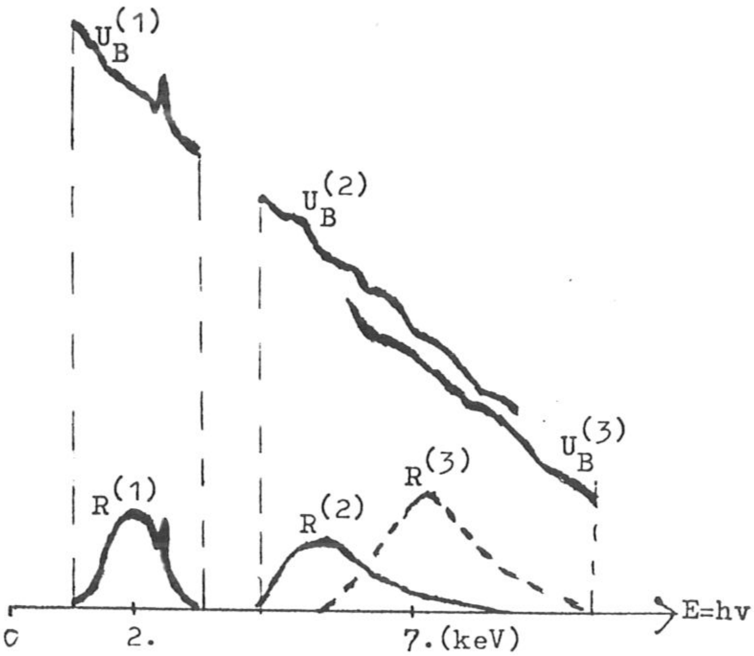


Abb. e
Raw spectra $R^{(I)}$ and normalized spectra $U_B^{(I)}$ of three detectors located at the same position p.

In this example we have no other information on the vicinity of hv = 2 keV than the spectrum of detector 1. We therefore set

$$U = U_B^{(1)} \quad \text{for } h\nu \approx 2.\text{keV}\,. \tag{2.1}$$

The situation is different in the vicinity of 7 keV, where two spectra are available. We form

$$U = G^{(2)}\, U_B^{(2)} + G^{(3)}\, U_B^{(3)} \tag{2.2}$$

and now ask how best to select the weighting factors $G^{(2)}$ and $G^{(3)}$.

We now put forward the following rather sloppy and arbitrary argument: the raw spectra as photon numbers per energy interval are the more exact and informative the larger they are. The raw spectra themselves are therefore the appropriate weighting function, e.g.

$$G^{(2)} = \frac{R^{(2)}}{R^{(2)} + R^{(3)}} \qquad (2.3)$$

The objection will now be raised that the relative inaccuracy of a raw spectrum is $1/\sqrt{R}$, and so weighting should be done with $\sqrt{R}$. We nevertheless stick to eq. (2.3), not because the objection is unjustified, but because taking the root requires a lot of computing time (see Sec. 14 on OVLAP routine).

If the foregoing is generalized, one obtains

$$U = \frac{\sum_I R^{(I)} \; U_B^{(I)}}{\sum_I R^{(I)}} \qquad (2.4)$$

The summation covers all detectors I located at the same position p. In Secs. 4 and 13 we call these detectors "probe", and the U formed from their spectra "probe signal" or "spectral function". We regard eq. (2.4) as the definition of the spectral function U from the spectra of the detector of a probe.

We now describe the instrument function by means of which the normalized spectrum U_B is obtained from the raw spectrum R of a detector. One has

$$U_B = U_o \frac{NW/NG}{t(N) - t(N-1)} R \qquad (2.5)$$

where

$$U_o = 4\pi \frac{E}{DE} \frac{\exp(FILTER)}{S} \qquad (2.6)$$

We now explain the individual factors.

We start with U_o, which contains all time-independent factors. For this purpose we define the emissivity F as the radiation power per plasma volume element and energy interval (see Sec. 3, eq. (3.6)). F thus has the dimension $cm^{-3}\ s^{-1}$. In addition, according to eq. (3.11) one has $U = \int F\,dx$, where dx stands for a line element of the line of sight of the detector. U has the dimension $s^{-1}\ cm^{-2}$. Comparing the two defintions:

U = radiation energy per energy interval per cm^2 per s

R = quantum number per energy channel,

it is seen that U_o must be proportional to $\frac{E}{DE} = \frac{\text{quantum energy}}{\text{channel width}}$.

The proportionality to $4\pi / \Delta S \Delta \Omega$ is thoroughly justified in Sec. 3. Furthermore, it should be noted that

R prop. exp(-FILTER)

from which it follows that

U_o prop. exp(+FILTER). (see Sec. 13)

In addition, R must be proportional to the observation time t(N) - t(N-1): the longer the observation time the larger are the raw spectra. To study the time development of an ASDEX discharge, the user reads in times t(N), N = 1,..NMAX, the meaning of which can be schematically described as follows: at the time t = t(N-1) all counters from Fig. 1a are set to zero. During the time t(N-1) to t(N) the detector is exposed to X-radiation, thus producing a raw spectrum. This is read off at time t(N) and put into the computer (see OVLAP routine, statement ISN 0013). The counters are then returned to 0 and the game starts all over again.

Finally, it should be mentioned that not all quanta reaching the counter in Fig. 1 are recorded. Consequently, the "true" number NW of quanta is larger than the number NG of quanta recorded. But we do not pay any attention to this and in the OVLAP routine we set in ISN 0014

$$NW/NG = 1. \qquad (2.7)$$

In practical applications this statement will be replaced by another in which NW/NG is either read in or calculated in a subroutine.

3. SOLID ANGLE FORMULA FOR $\Delta S \Delta \Omega$

Here the quantity $\Delta S \Delta \Omega$ from Secs. 2 and 13 (BLENDE subroutine) is calculated.

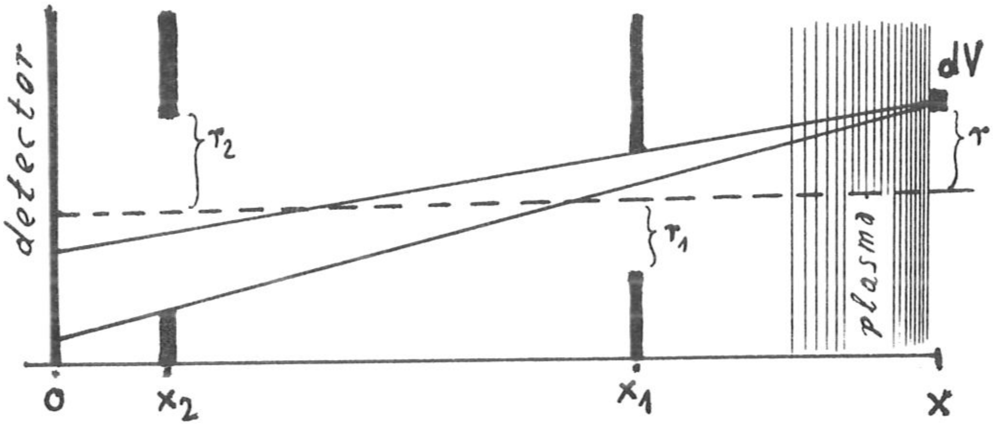


Figure 2 shows

at x = 0 the detector,

at $x = x_1, x_2$ apertures with radius r_1, r_2 ,

the axis through the aperture centres (dahsed),

a plasma volume element dV at a distance r from the axis.

Assumptions

1) The detector is equally sensitive everywhere.

2) The plasma emissivity F only depends on x, thus not on r. In visual terms, this means that the straight lines drawn in Fig. 2 are so close together (a few mm) that in a figure like Fig. 1 they merge into one straight line, namely the line of sight of the detector.

Required

To determine the radiation power which passes through the apertures and enters the detector.

First we deal with the radiation power arriving at the detector from the volume element dV.

Viewed from dV, the two apertures appear as circles with apparent radius[1] (in units of angle):

$$v_1 = r_1 / (x-x_1) \qquad (3.1)$$

and $$v_2 = r_2 / (x-x_2)$$

whose centres are at the apparent distance

$$d = \frac{r\ (x_1-x_2)}{(x-x_1)\ (x-x_2)} \qquad (3.2)$$

from one another (see Fig. 3).

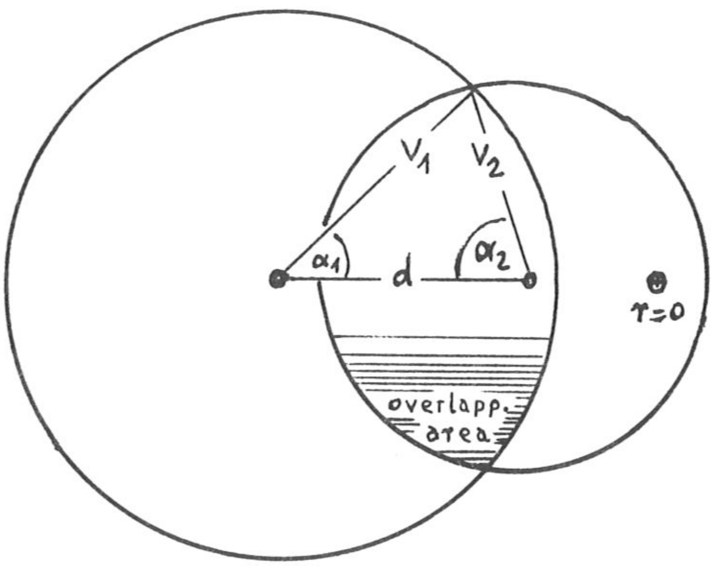


Fig. 3

The two aperture cross-sections, viewed from dV

[1] As an example from astronomy it is mentioned that the sun and moon, viewed from the earth, both have the same apparent radius of about 15'. In partial eclipses overlapping areas similar to those in Fig. 3 can often be seen.

The two circles have in common the overlapping area

$$A = v_1^2 \left[\alpha_1 - \sin\alpha_1 \cos\alpha_1 \right] + v_2^2 \left[\alpha_2 - \sin\alpha_2 \cos\alpha_2 \right] \quad (\text{if } v_1 - v_2 \leq d \leq v_1 + v_2)$$

where

$$\cos\alpha_1 = (d^2 + v_1^2 - v_2^2) \;/\; 2v_1 d$$

$$\cos\alpha_2 = (d^2 + v_2^2 - v_1^2) \;/\; 2v_2 d$$

If $d = v_1 - v_2$,

it holds that

$$A = \pi v_2^2 .$$

The radiation power of dV is

$$dP = F\,dV \;(\text{erg sec}^{-1}\;\text{erg}^{-1})$$

This radiation power is emitted uniformly in all directions. All directions together form the solid angle 4π . Only the fraction

$$d^2P = \frac{A}{4\pi} F\,dV \qquad (3.6)$$

passes through both apertures and reaches the detector.

The next question is what radiation power do <u>all</u> volume elements <u>at distance x</u> transmit to the detector. These volume elements together form a disc. The contribution of the disc is

$$P_x = \int_0^{2\pi} d\varphi \int_0^{r_{max}} dr \quad r \frac{A}{4\pi} F \, dx$$

where

$$dV = dx \, d\varphi \quad dr \, r.$$

According to the assumption 2) F dx may be put in front of the integral. r_{max} is obtained by putting the largest possible value $v_1 + v_2$ for d in eq. (3.2):

$$r_{max} = \frac{r_1(x-x_2) + r_2(x-x_1)}{(x_1-x_2)}$$

Integration yields

$$P_x = \frac{dx \; F}{4\pi} \frac{\pi r_1^2 \;\; \pi r_2^2}{(x_1-x_2)^2} = \frac{dx \; F}{4\pi} \; \Delta S \Delta \Omega \tag{3.9}$$

where

$$\Delta S \Delta \Omega = \frac{\pi r_1^2 \;\; \pi r_2^2}{(x_1-x_2)^2} \tag{3.10}$$

(solid angle formula)

The total contribution of all volume elements located on the line of sight, i.e. visible from the detector through the two apertures, is

$$L = \int P_x dx = \frac{\Delta S \Delta \Omega}{4\pi} \int F \, dx. \tag{3.11}$$

According to Ref. /3/, Sec. 1 one has

$$\int F \, dx = 2 \int_p^a \frac{dr \;\; r \;\; F}{\sqrt{r^2-p^2}} = U \quad ; \qquad \text{see (4.5)}$$

One thus gets

$$L = \frac{\Delta S \Delta \Omega}{4\pi} \quad U \, . \qquad (3.12)$$

Relation to the raw spectra

According to eqs. (2.1) - (2.5) one has

$$\frac{R}{t(N) \; -t(N-1)} = \int dE \; L/E$$

$$\approx \frac{\Delta E}{E} L$$

$$= \frac{\Delta S \Delta \Omega}{4\pi} \; \frac{\Delta E}{E} \quad U \qquad (3.13)$$

$$U_o = \frac{4\pi}{\Delta S \Delta \Omega} \; \frac{\Delta E}{E} \qquad (3.14)$$

without taking filtering and NW/NG into account,
L being the power per energy interval, and L/E the photon number per energy interval per s.

4. ABEL INVERSION FACTOR A_Z

In the first part of this report (Secs. 2 and 3) the spectral function U was obtained from the raw spectra and other parameters. The second part (Secs. 4 to 11) deals with the evaluation of the spectral function U.

If the plasma is transparent to X-radiation and U is a symmetric function of the probe position p, it can be assumed that the plasma is circularly symmetric. The emissivity F then only depends on the space via r, the latter being the distance from the plasma centre. In this case Abel's integral equation in the form

$$U(p) = 2 \int_p^a \frac{dr\ r\ F(r)}{\sqrt{r^2-p^2}} \quad , \qquad (4.1)$$

is valid, where a is the plasma radius. U and F depend not only on p or r but also on the photon energy E = hv (see Sec. 7). Now under certain conditions there are intervals, already referred to as clean energy windows, in which

$$\ln F(r,E) = \alpha(r) + \beta(r)\ E \qquad (4.2)$$

is valid, i.e. in which ln F is at least approximately a linear function of the photon energy E = hv. α and β may depend in which of the energy windows they are calculated; see Sec. 12, Fig. 14. One of the most important tasks of the programs in this report is to determine α and β from the spectral function U. For this purpose we offer several methods which the user can select by the choice of the parameter NABEL; see Sec. 18 on ALPBET subroutine. The simplest concept is to solve Abel's integral equation (4.1) for F and then determine α and β by a least square fit (see Secs. 16 and 19). For this purpose one has to introduce for U an interpolation ansatz between two mesh points (probe positions) P_L. What is then obtained from the Abel inversion for F often drastically depends on the choice of the interpolation ansatz, particularly in the plasma boundary regions. We have therefore developed a completely different method in which F is not calculated at all, α and β being determined direct from the spectral function U. For this purpose we define a function $A_Z(p)$ by means of the equation

$$U(p) = 2a\ F(p) \sqrt{\frac{1-\hat{p}^2}{A_Z(p)}} \qquad (4.3)$$

where $\hat{p} = p/a$. (4.4)

Substituting eq. (4.3) in eq. (4.2) yields

$$\alpha(r) + \beta(r)\ E = \ln U - \ln \left\{ 2a \sqrt{\frac{1-\hat{p}^2}{A_Z(p)}} \right\} . \qquad (4.5)$$

This is the initial equation for the iteration method described in Sec. 17. The disadvantage of this method is that, basically, one does not know anything about A_Z and has to introduce arbitrary assumptions. Numerical tests have shown, however, that the method is quite insensitive to wrong determination of A_Z. If, for example, one sets $A_Z = 1$, this makes ß(r) about approx. 10 to 20 % inaccurate. If A_Z is carefully determined, the inaccuracy in determining α and ß can be reduced to just a few per cent. We therefore now determine A_Z for a few special cases in which the Abel integration (4.1) can be performed exactly or as an analytic approximation.

The simplest case is $$F(r) = (1-\hat{r}^2)^n \tag{4.6}$$
with integer n and $$\hat{r} = r/a \quad . \tag{4.7}$$

It follows that $$U(p) = U_o(1-\hat{p}^2)^{n+1/2} \tag{4.8}$$

where $$U_o = a \sum_{m=0}^{n} (-1)^m \binom{n}{m} \frac{2}{2m+1} \tag{4.9}$$

$$U_o \approx \frac{2a}{\sqrt{1.+(1.+0.273 \frac{n+1}{n+1.17})n}} \tag{4.10}$$

and hence

$$A_Z = 1. + (1.+ 0.273 \frac{n+1}{n+1.17})n \tag{4.11}$$

In this case A_Z thus does not depend on p at all. The approximation (4.10) is valid for all real $n \gtrsim - 0.6$; test calculations showed that the inaccuracy of eq. (4.10) is

for $n \geq - 0.5$ at most 3×10^{-4}

for $n \geq 3$ at most 1×10^{-4} .

Now it is known from laser scattering measurements that the temperature is a profile function of type (4.6) in good approximation. We therefore calculated A_Z for the following case (see Sec. 7):

$$F = S\, e^{-x} \tag{4.12}$$

where
$$x = E/kT_e = x(r) \tag{4.13}$$
$$S = S_o (1-\hat{r}^2)^C \tag{4.14}$$
$$kT_e = T_o (1-\hat{r}^2)^H \tag{4.15}$$

In this case A_Z only depends on C, H, and $x = x(p)$. S_o and T_o do not appear. The numerical results can be described by the approximation formula

$$A_Z = 1.+ \left(1.+ 0.273 \frac{n+1.}{n+1.17}\right) n + Z \tag{4.16a}$$

where
$$n = C + H\, x \qquad \text{b)}$$
$$Z = \frac{H}{1.+ \frac{C+H}{y}} \qquad \text{c)}$$
$$y = \frac{1.8\, x^E\, H^2}{1.+ 0.83\, H} \qquad \text{d)}$$
$$E = 0.5 + 0.03\, C + \frac{0.46}{1.+H} \qquad \text{e)}$$

The inaccuracy is mostly less than 1 %. Errors of $>$ 1 % occur almost only at very small H values ($H \lesssim 0.01$). We program this formula in the AZRUT subroutine. One therefore just has to modify the AZRUT routine if a better method of determining A_Z is wanted later; all other programs remain unchanged.

Testing was done by determining the profile number n by a least square fit from given data U, where U(p) was <u>not</u> of the profile type. We then determined A_Z according to eq. (4.11) and finally α and β from eq. (4.5) by a least square fit. The inaccuracy in determining α and β was about 10 %.

5. CALCULATION OF α AND β

The X-ray emissivity F of a contaminated plasma consists of a continuum component F_C and a line component F_L:

$$F = F_C + F_L \tag{5.1}$$

If oxygen, carbon, Ti, Cr, Fe, and Ni are the only impurities and, in particular, heavy metals such as tungsten, molybdenum etc. are absent, there are two ranges, namely $2 \lesssim E \lesssim 4$ keV and $10 \lesssim E$ (keV) (see Fig. 4) in which (5.2)
the impurity lines and edges are absent, and hence it holds that

$$F_L = 0 \quad F = F_C \quad . \tag{5.3}$$

Furthermore, in these regions (5.2) ln F is approximately a linear function of the quantum energy E = hv:

$$\ln F\ (r,E) = \alpha(r) + \beta(r)\ E \tag{5.4}$$

(see eq. (7.2) and Fig. 4).

In Fig. 4 ln F is plotted versus E schematically for a plasma containing Ti, Cr, Fe and Ni.

Intervals in which ln F depends linerarly on the photon energy E = hv are called "clean energy windows". α and β can assume different values in different energy windows and must therefore have a window index. This is dealt with in Sec. 12, Fig. 14. Here we confine ourselves to mesh points located in the same window and omit the window index.

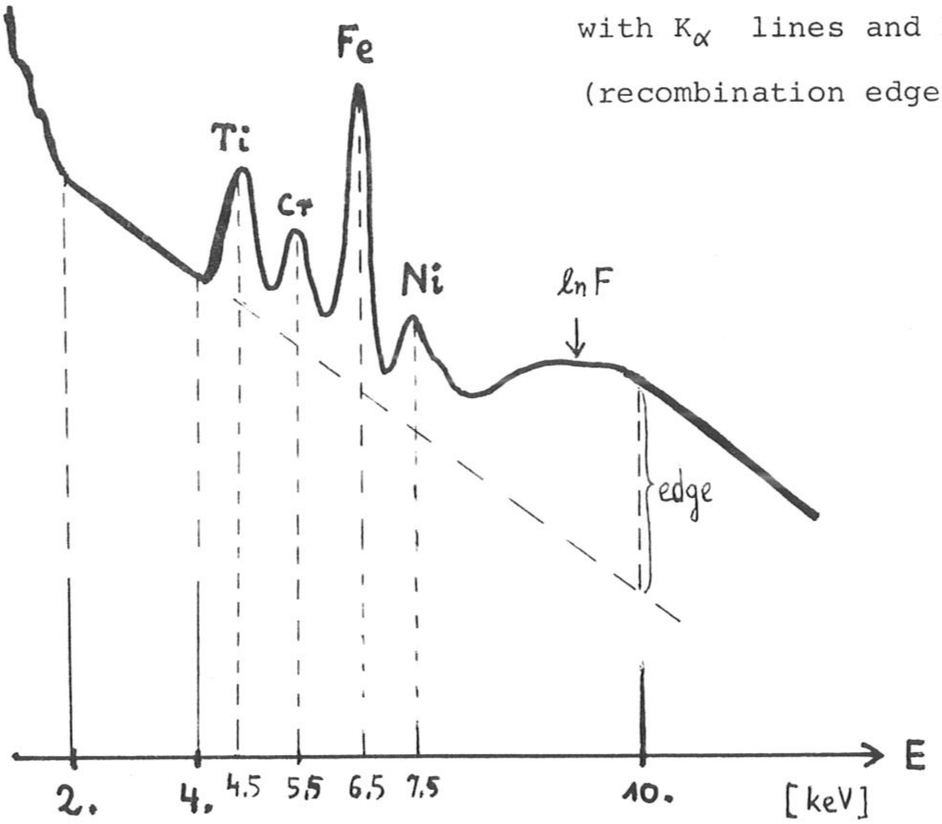


Abb. 4

ln F versus E = hv

with K_α lines and K edge

(recombination edge)

We now outline how α and ß arise from the spectral function U of a clean energy window.

When the OVLAP routine is called the spectral function U(L,J) is given for each probe L at equidistant mesh points, called "reference mesh points"

$$E9(J) = DE9\ J + EO9 \qquad (5.5)$$

see Sec. 14, eq. (14.1). The number of these mesh points is of the order

$$\frac{\text{window length}}{\text{channel width}} \approx \frac{2.\text{keV}}{0.1 \text{ keV}} \approx 20 \qquad (5.6)$$

and may possibly be as high as 100.

From these 10 to 100 U values two parameters, namely α and ß, have to be determined. For this purpose few mesh points with relatively exact U values are more suitable than many mesh points with relatively large statistical error fluctuations because the Abel inversion methods take less computing time the fewer mesh points there are present and work the better the more exactly U is given. We therefore smooth the spectral function U first of all. For this purpose we read in smoothing intervals

$$\text{EL(M)} \leq \text{E} \leq \text{ER(M)} \qquad (5.7)$$

whose centres are located roughly at EID(M); see Sec. 15, eq. (15.1). The GLATT smoothing routine produces from all U(L,J) in the smoothing interval M a mean value

$$\text{ULG(L,M)} = \ln \text{U} \quad \text{at EID(M)} . \qquad (5.7a)$$

The way in which this is done is described in Sec. 15. The ALPBET subroutine then yields the parameters α and ß from the smoothed ULG (see Sec. 18).

We offer various methods which the user can call by choosing the parameter NABEL. The ITERAT subroutine starts from eq. (4.5) and uses eq. (4.16) for A_Z. The method also works when, for example, T_e is not of the profile type at all.

In order to outline the next method, we give the following definitions:

$\alpha_p = \alpha$ calculated by the ITERAT subroutine,

$\beta_p = \beta$ calculated by the ITERAT subroutine

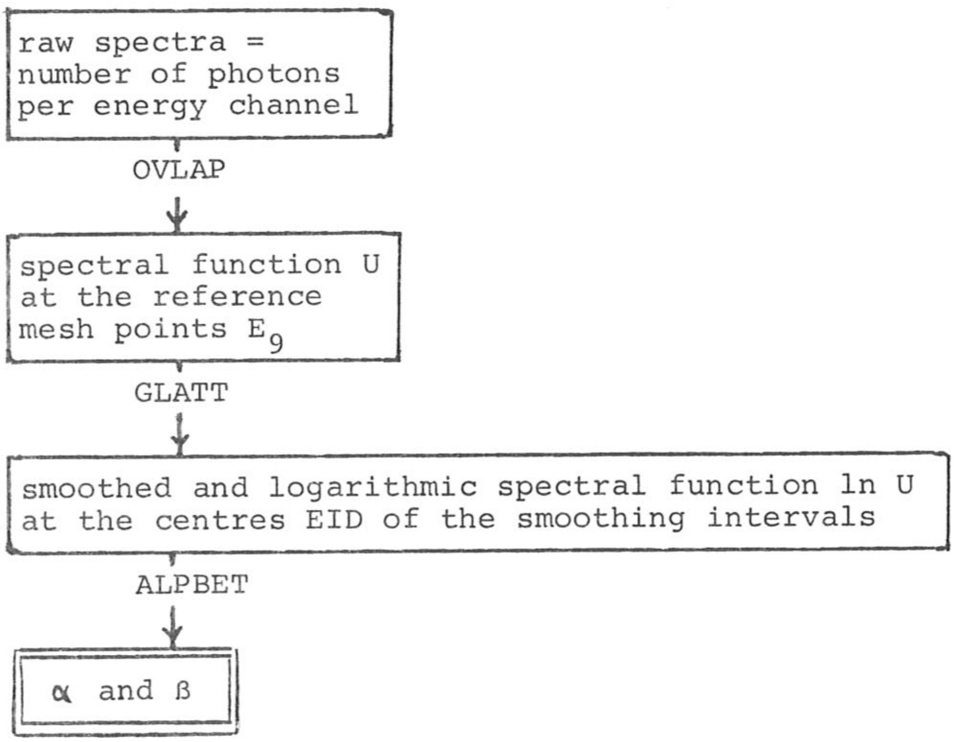
$F_p = \exp\left[\alpha_p + \beta_p E\right]$

$$U_p = 2a\, F_p \sqrt{(1-\hat{p}^2)/A_Z} \quad A_Z \text{ according to eq. (4.16)},$$

$$D = U - U_p \quad . \qquad (5.8)$$

If, for example, the user chooses NABEL = 2, the Abel inversion for D is performed by the ABEL subroutine; the result is G; and then we set $F = F_p + G$. α and β are then determined from F by a least square fit from eq. (4.2).

The other two methods dispense with the ITERAT routine and differ only in the choice of the interpolation function for U. Finally, we trace the path from the experimental data to α and β in the form of a diagram:



6. POSITIONS

In this program the positions p are read in, i.e. they have to be given. The reader who considers this obvious can skip this section. We can, however, test whether any given positions are reasonable because the positions are related to the angles of sight of the probes, which are known very exactly.

The probes are arranged in such a way that their lines of sight intersect at one point, the aperture B (see Fig. 5).

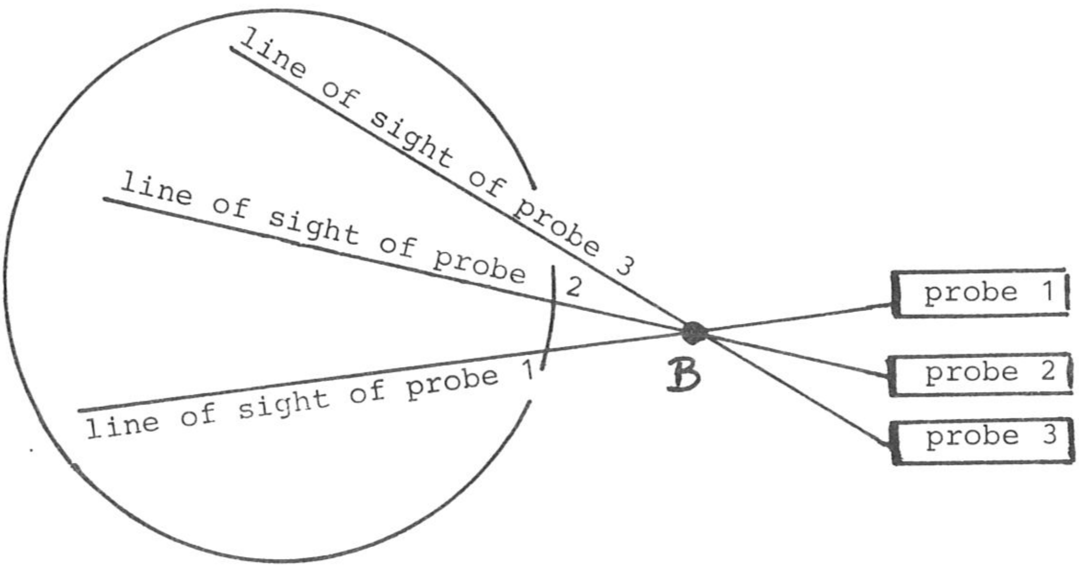


Fig. 5
Plasma cross-section, aperture B
three probes and their lines of sight.

The aperture B corresponds to aperture 1 in Fig. 1 and is common to all probes and detectors.

We now arbitrarily give an origin O of coordinates inside the vessel. The plasma centre M then has relative to O the coordinates x and y, the straight line OB being the x axis. In Fig. 6 the line of sight of the probe L is drawn. It passes the plasma centre M at a distance p_L and forms the angle ϕ_L with the x axis. We refer to ϕ_L as the angle of sight of the probe.

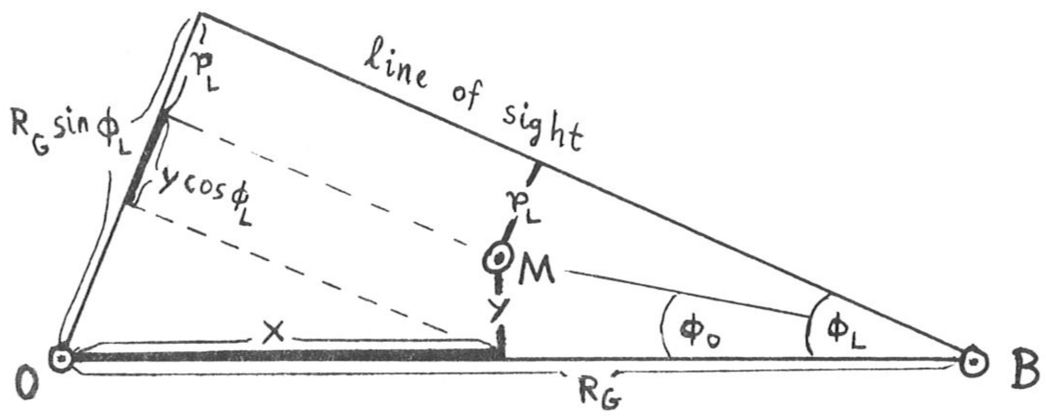


Figure 6 shows
the aperture B,
the line of sight of the probe L with angle of sight ϕ_L,
the plasma centre M, the position p_L and
the plasma shift x, y
with reference to an arbitrary point O inside the vessel;
OB = R_G.

The drawing plane of Fig. 6 is the same as that of Fig. 1 at the beginning of Sec. 2.

From the geometry it follows (see Fig. 6) that

$$p_L = (R_G - x) \sin \phi_L - y \cos \phi_L \qquad (6.1)$$

If we define

$$\tan \phi_o = y/(R_G - x) \qquad (6.2)$$

$$p_o = (R_G - x) \cos \phi_o \qquad (6.3)$$

it then follows that

$$p_L = p_o \sin (\phi_L - \phi_o) \qquad (6.4)$$

This relation can be used for testing because in ASDEX there are five probes (L = 1, 2, 3, 4 and 5) whose positions are expressed in eq. (6.4) by just two poorly known quantities, namely x, y or p_o, ϕ_o.

We now investigate whether the positions can be taken from the experimental data ULG to afford the user the possibility of replacing the reading in of the positions by calculation in a suitable subroutine.

The parameter p_o = BM, the distance of the plasma centre from the aperture is indeterminable because a plasma with small p_o yields exactly the same X-ray spectra as a plasma with large p_o if the other parameters are appropriately chosen: a giant may look just like a dwarf standing closer.

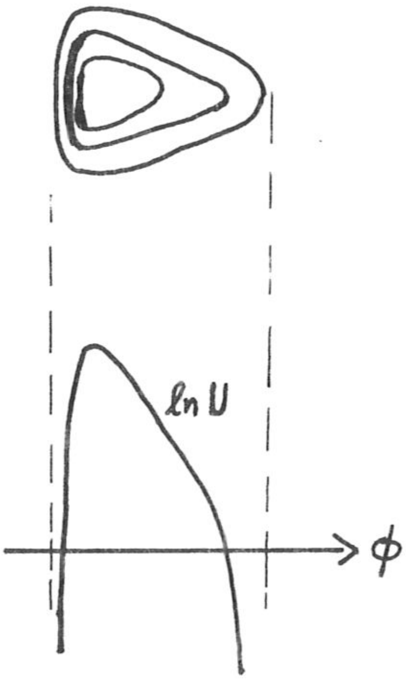
To determine ϕ_o we use the fact that for $E \approx h\nu \gtrsim 2\ kT_e$ can mostly be approximately represented by a Gaussian function, and ln U by a parabola:

$$\ln U = a_o + a_2(\emptyset-\emptyset_o)^2 \qquad (6.5)$$

$$[\ln U]_L = a_o + a_2(\emptyset_L-\emptyset_o)^2 \qquad (6.5a)$$

Thus, when ln U is present at at least three different values of L, then $\emptyset_o$ is the extremum of this parabola. This is only valid, however, when the temperature is approximately of the profile type; if, on the other hand, the temperature has, for example, a crater and two extrema, ln U also has two extrema and is not even approximately parabolic.

Another difficulty is that the plasma is not always of circular cross-section. It is true that the case U(p) = U(-p) cannot be distinguished from a circularly symmetric plasma because only one aperture B is available; cf. Ref. /3/, Sec. 4 on quasi-circularly symmetric emission.



But with D-shaped plasmas the case illustrated alongside, in which ln U strongly deviates from the parabolic shape (6.5), can also occur. Finally, it should be noted that the positions depend on the motion of the plasma and hence on the time, and hence have to be recalculated or read in for every time step.

7. X-RADIATION AND PLASMA PARAMETERS

Here we list the equations describing the relation between the X-ray emissivity F and the plasma parameters T_e, n_e, n_i, etc., the determination of these from the X-ray spectra being the objective of our programs. According to Ref. /1/ it holds that

$$\text{Emissivity } F = F_C + F_L \quad (\text{dimension: cm}^{-3}\ \text{s}^{-1}) \qquad (7.1)$$

F_C = continuum component

F_L = line component

$$F_C = S\, e^{-x} \qquad (7.2)$$

$$x = E/kT_e \qquad (7.3)$$

$$E = h\nu = \text{quantum energy} \qquad (7.4)$$

$$S = S_H\, \zeta \qquad (7.5)$$

$$S_H = F_a\, n_e^2 / \sqrt{kT_e} \qquad (7.6)$$

$$F_a = 3.03\ 10^{-15} \text{ if } T_e \text{ in keV and } n_e \text{ in cm}^{-3} \qquad (7.7)$$

$$\zeta = \sum_i \frac{n_i}{n_e} \left(Z_{iff}^2\, f_{ff}^{(i)} + R_{fb}^{(i)} \right) \qquad (7.8)$$

n_e = electron density

T_e = electron temperature

i = ion species index = nucleus charge

n_i = density of ions of species i

$Z_{iff} \approx i-2$ to i

$g_{ff}^{(i)}$ = GAUNT factor. From ref. /1/, fig. 4a it follows that

$$g_{ff}^{(1)} = 1.2\ (0.5+x)^{-0.45}\ T_e^{-0.07-0.01x} \qquad \text{(hydrogen)}$$

$$g_{ff}^{(8)} = 1.38\ (0.5+x)^{-0.16}\ T_e^{0.35} \qquad \text{(oxygen)}$$

$$g_{ff}^{(i)} = 1.2 \qquad \text{for } i \geq 22$$

$R_{fb}^{(i)}$ = recombination component; see sec. 8 .

8. RECOMBINATION RADIATION

According to eqs. (1) and (3) from Ref. /1/ the recombination term from eq. (7.8) is

$$R_{fb}^{(i)} = \sum_{J=1}^{i} \frac{n_{iJ}}{n_i} g_{fb} Z_{iJ}^2 \left[\frac{\xi}{n^3} x_o e^{x_o} + \sum_{v=1} \frac{2}{n+v} x_v e^{x_v} \right] \qquad (8.1)$$

where

$$x_o = \chi_{iJ} / T_e \qquad = x_{o,iJ} \qquad (8.2)$$

$$x_v = Z_{iJ}^2 \chi_H / \left[(n+v)^2 T_e \right] = x_{v,iJ} \qquad (8.3)$$

i = ion species index, e.g. i = 26 stands for Fe,

$Z_{iJ}=J$ = ionization stage index = ion charge <u>before</u> recombination,

n = principale quantum number of the ground state,

ξ = number of electrons missing in the ground state.

In the example: $i = 26$ (8.3)

$J = 20$

$i = 26$ denotes Fe and

$J = 20$ means that before recombination there are 26 - 20

= 6 electrons present. Of these 6 electrons there are

2 electrons in the K shell ($n = 1$)

4 electrons in the L shell ($n = 2$).

The K shell is completely populated ($\xi = 0$);

the L shell is not completely populated till it has 8 electrons; for complete population there are thus $\xi = 8 - 4 = 4$ electrons missing, see fig. 7.

From $i = 26$ and $J = 20$ it thus follows that $\xi = 4$ and $n = 2$.

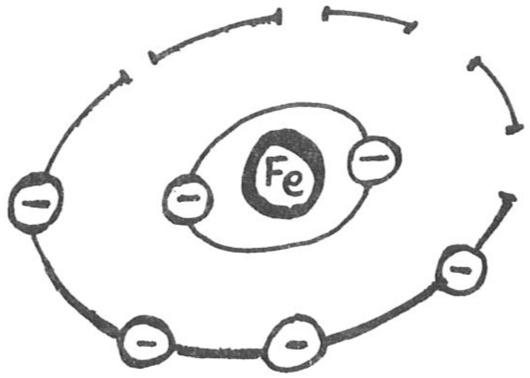


Fig. (7)

i = 26 n = 2

J = 20 ξ = 4

example (8.3)

The other notations are:

χ_{iJ} = energy required to wrest an electron from the J - 1 times ionized ion,

χ_H = 13.6 eV = ionization energy of the hydrogen,

n_{iJ} = density of the ions of species i and charge J.

It should be noted that in Ref. /1/, eq. (3) the ion charge (i.e. our J) is denoted by i and the species index (i.e. our i) is completely omitted.

Equation (8.1) requires explanation. $R_{fb}^{(i)}$ is a function of E = hv and T_e. The latter appears in the denominator of x_v (see eqs. (8.2)) and x_0 ; furthermore, the partial densities n_{iJ}/n_i are functions of T_e; see, for example, Fig. 9.

The x_v are step functions of E = hv, e.g.

$$x_o = \begin{cases} \chi_{iJ}/T_e & E > \chi_{iJ} \\ 0 & E < \chi_{iJ} \end{cases} \qquad (8.4)$$

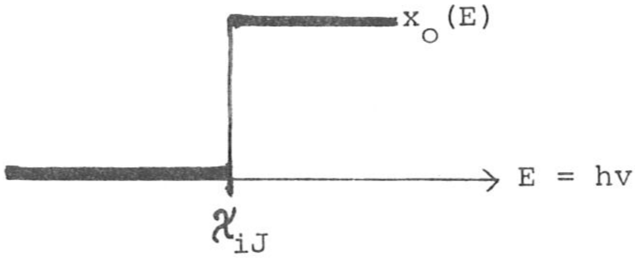


Fig. 8

x_o versus E

$R_{fb}^{(i)}$ is mostly composed from a number of step functions of type (8.4); hence the stair-step-like appearance in, for example, Fig. 11.

For the GAUNT factor we set

$$g_{fb}^{(i)} = 1 \quad . \tag{8.5}$$

9. $R_{fb}^{(26)}$ (IRON)

Here we give a detailed calculation of $R_{fb}^{(i)}$ for iron (i = 26). In the interval

$$0.5 \text{ keV} \leq h\nu \leq 10. \text{keV} \quad (9.1)$$

it holds that $g_{fb} = 1$ independently of E (9.2)

with an inaccuracy of approximately 10 % (cf. Ref. /1/, Fig. 4b).

According to Ref. / / the ionization potentials for iron are at the energies χ_{iJ} (in keV):

J	χ_{iJ}	v = 1	v = 2
26	9.3	2.3	1.02
25	8.8	2.1	0.94
24	2.04	0.87	
23	1.95	0.80	
22	1.80		
21	1.69		
20	1.58		
19	1.45		
18	1.35		
17	1.26		
16	0.49		

Table 1

The 3rd and 4th columns contain $x_v\ T_e = Z_{iJ}^2 \chi_H/n+v)^2$

where

$Z_{iJ} = J$

$\chi_H = 0.0136$ keV

n=1 for J = 25 oder 26

n=2 for $17 \leq J \leq 24$.

The partial densities are plotted in Ref. /2/, Fig. 6. This figure is reproduced in Fig. 9.

Let

$$A_J = n_{iJ}/n_i \qquad (9.3)$$

One then has

$$R_{fb}^{(i)} = \sum_{J=1}^{i} g_{fb}\, Z_{iJ}^2 \frac{n_{iJ}}{n_i} \left[\frac{\xi}{n^3}\; x_o \; e^{x_o} + \sum_{v=1}^{\infty} \frac{2}{n+v}\; x_v \; e^{x_v} \right]$$

$$\begin{aligned} R_{fb}^{(26)} = \; & 1 \cdot 26^2\, A_{26} \left[2 \; \frac{9.3}{T_e} \exp(\frac{9.3}{T_e}) + 1 \; \frac{2.3}{T_e} \exp(\frac{2.3}{T_e}) + .. \right] \\ & + 25^2\, A_{25} \left[1 \; \frac{8.8}{T_e} \exp(\frac{8.8}{T_e}) + 1 \; \frac{2.1}{T_e} \exp(\frac{2.1}{T_e}) + .. \right] \\ & + 24^2\, A_{24} \left[1 \; \frac{2.04}{T_e} \exp(\frac{2.04}{T_e}) + \frac{2}{3} \; \frac{0.87}{T_e} \exp(\frac{0.87}{T_e}) + .. \right] \\ & + 23^2\, A_{23} \left[\frac{7}{8} \; \frac{1.95}{T_e} \exp(\frac{1.95}{T_e}) + \frac{2}{3} \; \frac{0.8}{T_e} \exp(\frac{0.8}{T_e}) + .. \right] \\ & + 22^2\, A_{22} \left[\frac{6}{8} \; \frac{1.8}{T_e} \exp(\frac{1.8}{T_e}) + .. \right] \\ & + \ldots \end{aligned}$$

This summation is arranged according to descending ionization potentials. For this purpose we define

$T_{9.3}$ (read "term with ionization potential 9.3 keV"),

$$T_{9.3} = 26^2\, A_{26}\; 2\; \frac{9.3}{T_e} \exp(\frac{9.3}{T_e}) \qquad (9.5)$$

$$T_{2.3} = 26^2\, A_{26}\; 1\; \frac{2.3}{T_e} \exp(\frac{2.3}{T_e})$$

$$T_{8.8} = 25^2\, A_{25}\; 1\; \frac{8.8}{T_e} \exp(\frac{8.8}{T_e})$$

According to eq. (8.4) it then holds that

$$R_{fb}^{(26)} = T_{9.3} + T_{8.8} + T_{2.3} + T_{2.1} + T_{2.04} + .. \quad \text{for } E > 9.3$$

$$R_{fb}^{(26)} = T_{8.8} + T_{2.3} + T_{2.1} + T_{2.04} + .. \quad \text{for } 8.8 < E < 9.3$$

$$R_{fb}^{(26)} = T_{2.3} + T_{2.1} + T_{2.04} + .. \quad \text{for } 2.3 < E < 8.8$$

$$R_{fb}^{(26)} = T_{2.1} + T_{2.04} + .. \quad \text{for } 2.1 < E < 2.3$$

....

The numerical results obtained by programming this equation can be described by the following approximation formula with about 10 to 20 % inaccuracy:

$$R_{fb}^{(26)} = 5800.\ T_e^{2.5} / (1.+ T_e^{2.9}) \qquad E > 9.3 \qquad (9.7a)$$

$$R_{fb}^{(26)} = 5700.\ T_e^{2.5} / (1.+T_e^{3.88}) \qquad 2.3 < E < 8.8 \qquad (9.7b)$$

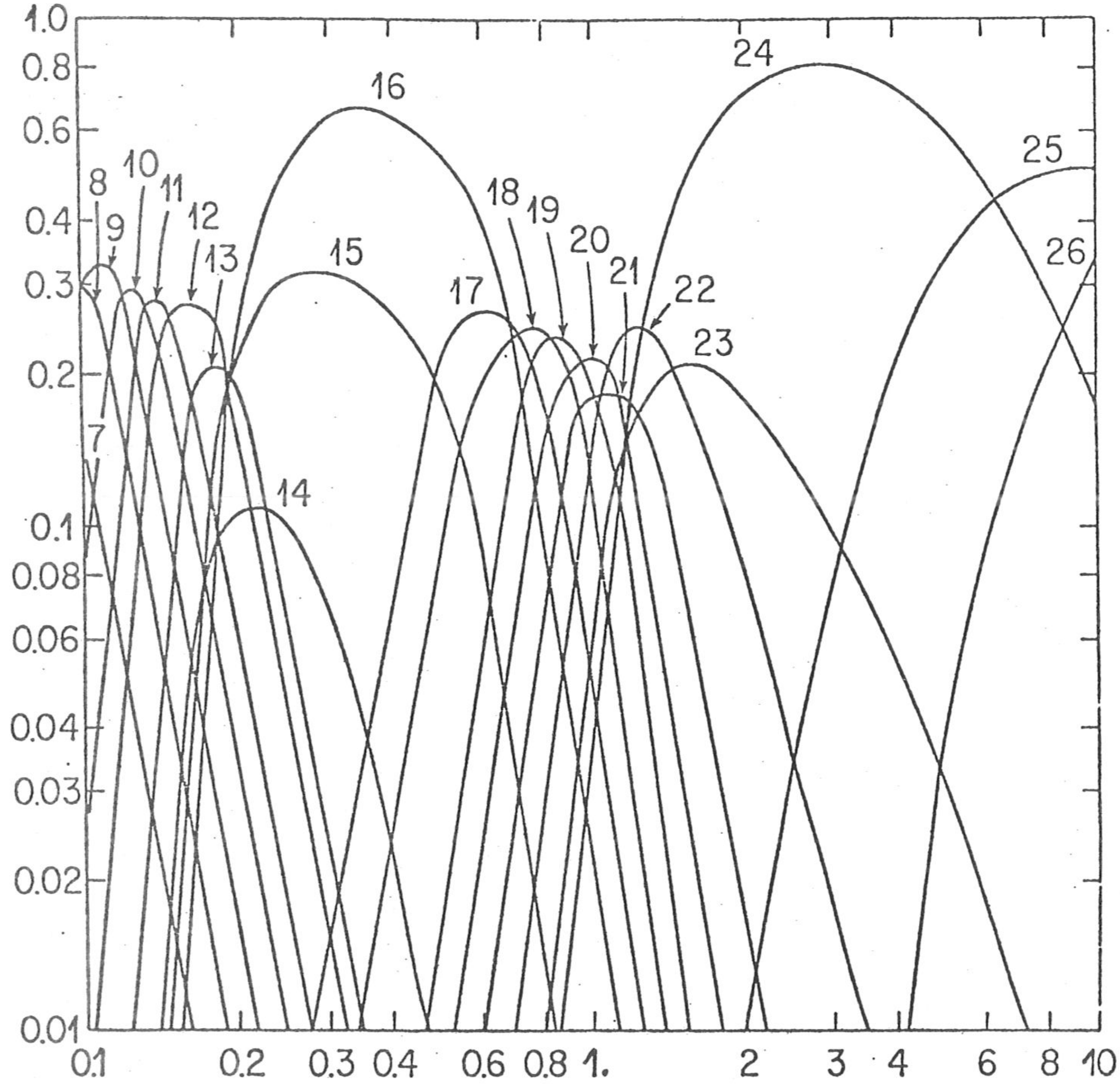


Fig. 9

n_{iJ}/n_i versus T_e in corona equilibrium; for i = 26 (Fe); reproduction of Ref. /2/, Fig. 6.

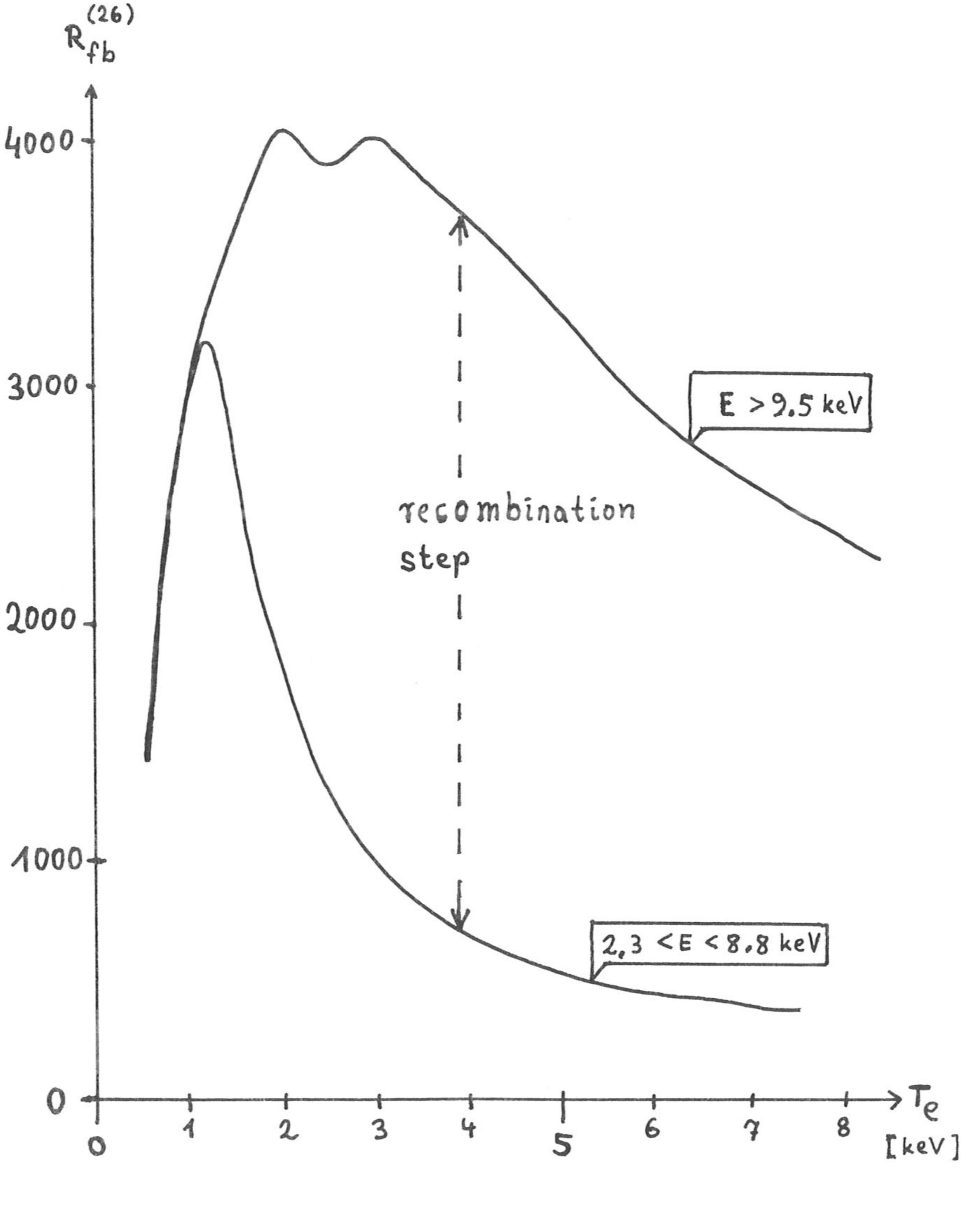


Fig. 10

$R_{fb}^{(26)}$ versus T_e

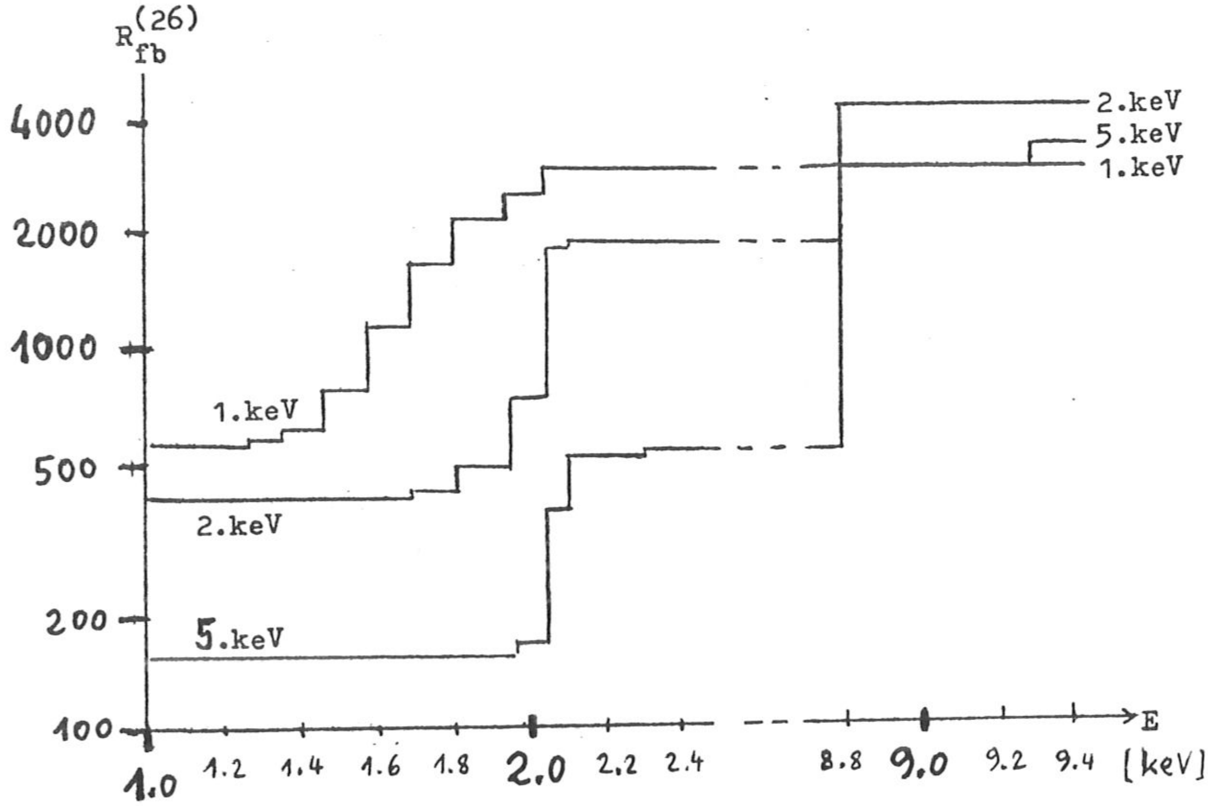


Fig. 11

$R_{fb}^{(26)}$ versus E = hv

for three different temperatures:

kT_e = 1.keV ; 2.keV and 5 keV

The interval $2.1 \leq E \leq 8.8$ is free of steps; consequently, $R_{fb}^{(26)}$ is independent of E in this interval.

In the interval $4 \leq E \leq 8$ keV, however, we have the K_α lines of Ti, Cr, Fe, Ni. Consequently, the interval

$$2.1 \leq E \leq 4.\text{keV}$$

is left over for the energy window No. 1.

There are no steps for $E \geq 9.2$ keV, and so

$$E \geq 9.2 \text{ keV}$$

is the energy window No. 2.

Appendix to Sec. 6

Calculation of $R_{fb}^{(26)}$ for $8.8 < E < 9.3$ keV

$$R_{fb}^{(i)} = \sum_{J=1}^{i} J^2 \quad A_J \quad \frac{\xi}{n^3} \quad x_o \quad e^{x_o}$$ cf. (9.4)

(9.8a)

T_e	J	J^2	A_J	$\frac{\xi}{n^3}$	x_o	e^{x_o}		T	
2.	25	625	0.01	1	4.4	81.45		2240	
	24	576	.70	1	1.02	2.77		1128	$R_{fb} = \sum T = 3650$
	23	529	.18	.875	0.98	2.66		217	
	22	484	.08	.75	0.9	2.46		64	
.7	22	484	0.01	0.75	2.57	13.08		122	
	21	441	.03	.625	2.43	11.34		236	
	20	400	.07	.5	2.28	9.83		318	
	19	381	.21	.375	2.07	7.94		493	$R_{fb} = \sum T = 1540$
	18	324	.24	.25	1.93	6.88		258	
	17	289	.25	.125	1.8	6.05		98	
	16	256	.22	.3	0.7	2.01		23	
5.	25	625	0.34	1	1.76	5.81		2173	
		625	0.34	1	0.42	1.52	*	136	
		625	0.34	.667	0.19	1.21	*	33	$R_{fb} = \sum T = 2600$
	24	576	0.59	1	0.41	1.50		210	
		576	.59	.667	0.17	1.19	*	46	
	23	529	0.03	.875	0.39	1.47		8	

* This terms come from $\sum_{v=1}$; in this case we write x_v instead of x_o in the 6. column.

This shows that although the partial density of Fe(25) at $T_e = 2$ keV is only 1 %, Fe(25) makes the largest contribution to R_{fb}.

At high temperatures ($T_e > 3$ keV) one should not neglect $\sum_{v=1}$.

Comparing (for T_e = 5 keV) the following three values

$$R_{fb} \; (E = h\nu > 8.8) = 2600$$
$$R_{fb} \; (E = h\nu < 8.8) = 400 \; \underline{\text{with}} \; \sum_{v=1}$$
$$R_{fb} \; (E = h\nu < 8.8) = 200 \; \underline{\text{without}} \; \sum_{v=1}$$

it is seen that R_{fb} "left" of the step at 8.8 keV is enhanced by the $\sum_{v=1}$-terms by a factor of at least 2.

<u>Error sources</u>

1) In eq. (8.1) the definition of ξ as the number of electrons missing in the n shell is only an approximation.

2) The ionization potentials χ_{iJ} are not very well known; the data differ by up to 0.5 keV. This can lead to errors of over 30 % in calculating R_{fb}; see example (9.8a) for T_e = 2 keV; contribution J = 25.

3) The assumption of corona equilibrium is not satisfied. For example, J = 25 ions diffuse from hot plasma regions to colder ones without first recombining. The consequence is explained in an example:

<u>Example:</u> In a plasma boundary layer of T_e = 1 keV the density of J = 25 ions is 0.1 %, i.e.
A_{25} = 0.001. One then has

$$\begin{aligned} R_{fb}^{(26)} &= J^2 \; A_J \; x_o \; e^{x_o} \\ &= 625 \; 0.001 \; 8.8 \; e^{8.8} \qquad (9.8d) \\ &= 36000. \end{aligned}$$

i.e. about ten times as large as would be expected from corona equilibrium. We therefore expect in the hot plasma centre a normal recombination step such as is shown in Fig. 10, but in the cool boundary layer a pronounced recombination step. To represent this in Fig. 10, one would have to top curve $E > 9.5$ at $T_e \approx 1$ keV with a peak several meters high.

4) According to D. Düchs one requires for calculating the partial densities in Fig. 9 coefficients which are not accurately known. The error is:

for the ionization coefficient $\approx$ factor 2

for the recombination coefficient factor 5.

10. $R_{fb}^{(i)}$ FOR STRIPPED NUCLEI

At plasma temperatures of $T_e > 0.8$ keV oxygen is almost completely stripped of its electrons. The plasma consists almost exclusively of stripped nuclei. In such a case one has

$$n_{iJ} = \begin{cases} n_i & \text{if } J = i \\ 0 & \text{if } J < i \end{cases} \tag{10.1}$$

From eq. (8.1) it then follows that

$$R_{fb}^{(i)} = 2\, i^2\, x_o\, e^{x_o} \tag{10.2}$$

with

$$x_o = \chi_{ii}/T_e \tag{10.3}$$

$$\begin{aligned} \chi_{ii} &= i^2\, 0.0136 \text{ keV} \\ &= 0.49 \text{ for carbon } (i = 6), \\ &= 0.87 \text{ for oxygen } (i = 8). \end{aligned} \tag{10.4}$$

There are only recombination steps below 1 keV; consequently, $R_{fb}^{(i)}$ is independent of $E = h\nu$ if $i \leq 8$.

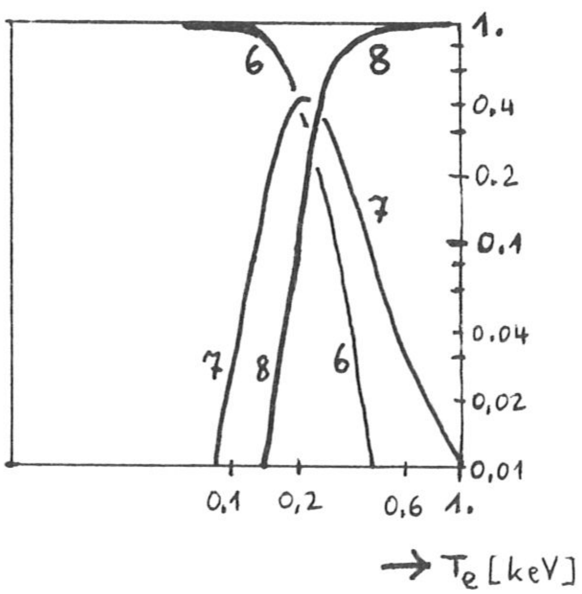


Fig. 11

$\frac{n_{iJ}}{n_i}$ versus T_e

in corona equilibrium

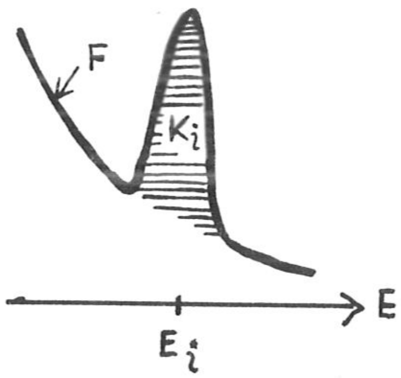
for i = 8.

Reproduction of Ref. /2/, Fig. 4.

11. K_α LINE RADIATION

The metals Ti, Cr, Fe and Ni, which we consider in this report, have their K_α lines in the range 4 keV < hv < 8 keV. Let E_i be the energy at which the ion species i has its K_α line. We then define

$$K_i = \int F_L \, dE = n_e \, n_i \langle \sigma v \rangle \, E_i \qquad (11.1)$$



where the integral is taken over the line; K_i is thus the hatched region in Fig. (12). σ is the cross section for K_α emission.

Fig. 12
F versus E = hv and K_i

$\langle \sigma v \rangle$ is taken from Ref. /4/, Fig. 10, which we reproduce in Fig. 13.

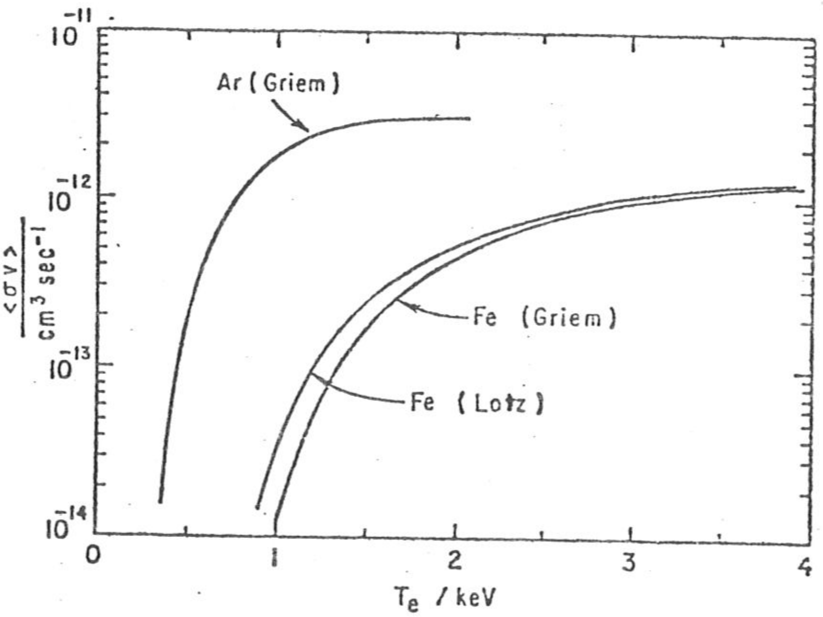


Fig. 13
$\langle \sigma v \rangle$ for K_α emission versus T_e

These curves can be approximated by the following formulae:

$$\langle \sigma v \rangle = \begin{cases} 2\ 10^{-12} \exp(-4.4\ T_e^{-1.7}) \text{ for Fe} & (8.2a) \\ 4\ 10^{-12} \exp(-0.8\ T_e^{-1.7}) \text{ for Ar} & (8.2b) \end{cases}$$

S. von Goeler considers the values shown in Fig. 13 to be too small: at the bottom left by a factor of about 2 or 3, and at the right by about 20 %. We, therefore, choose for our program rather arbitrarily

$$\langle \sigma v \rangle = 10^{-13}\ a \exp\left[- \frac{x}{1. + \frac{a}{x^2}} \right] \text{cm}^3\ \text{s}^{-1} \qquad (11.3)$$

where

$$x = \begin{cases} 2.5\ /\ T_e \text{ for Ar} \\ 5.2\ /\ T_e \text{ for Fe} \end{cases} \qquad (11.4)$$

$$a = \begin{cases} 35. \text{ for Ar} \\ 14. \text{ for Fe} \end{cases} . \qquad (11.5)$$

We require $\langle \sigma v \rangle$ not only for Fe and Ar, but also for other elements, e.g. titanium. For this purpose we arbitrarily generalize eqs. (11.4) and (11.5) as follows:

$$x = 0.0077\ i^2\ /\ T_e\ (\text{keV}) \qquad (11.6)$$

$$a = 4.8\ 10^4\ i^{-2.5} \qquad (11.7)$$

where

$$i = \begin{cases} 18 \text{ for Ar} \\ 26 \text{ for Fe} \end{cases} = \text{ordinal number,}$$

see IMPUR routine . The coefficient 0.0077 i^2 denotes approximately (in keV) the excitation energy for dielectronic K_α emission, which occurs primarily at low temperatures of 1 to 2 keV.

12. STRUCTURE OF ONESHOT PROGRAM

As the name ONESHOT suggests, the program is designed to determine a number of plasma parameters from the data of one shot - although it is also possible to superpose the results of several shots, e.g. by adding up raw spectra of different shots, averaging, introducing more than five probes, i.e. probes No. 1 to 5 yield results from shot No. 1, probes No. 6 to 10 results from shot No. 2, etc. This is not dealt with here.

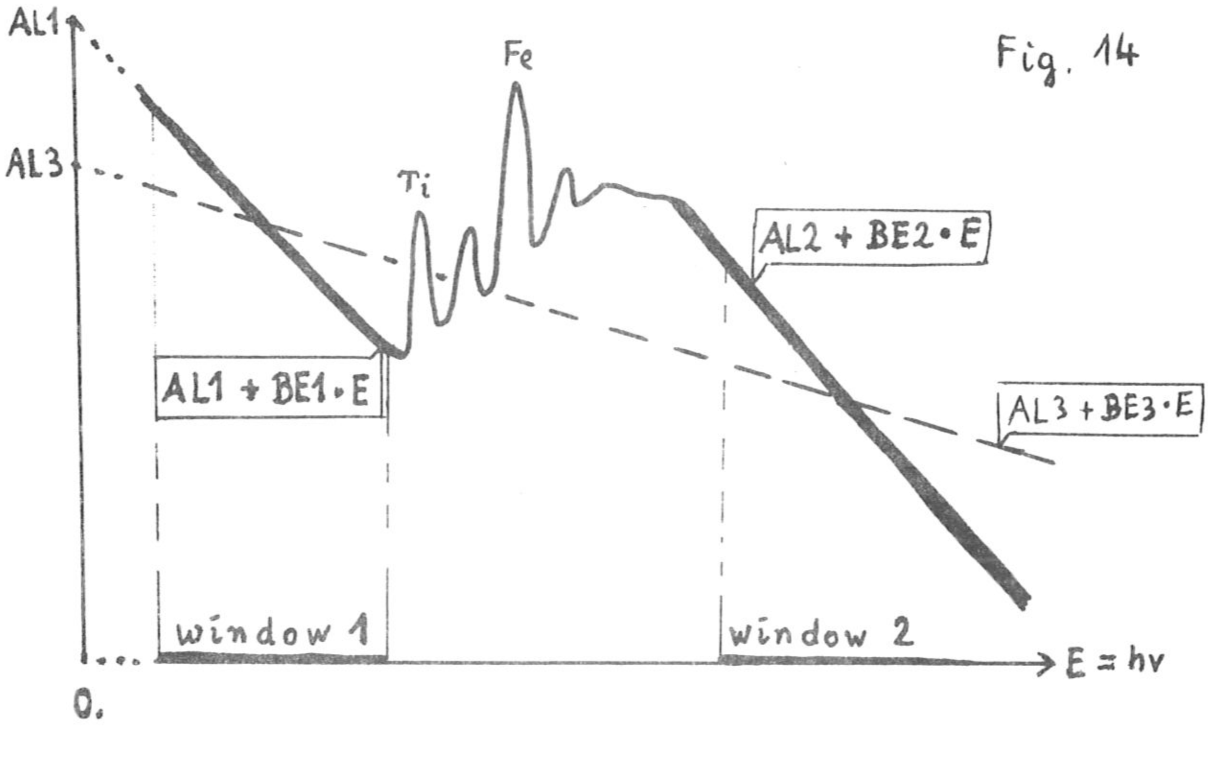
The plasma parameters determined with ONESHOT are:

Electron temperature	TE(L) ;
Ion densities	N1(L) ; N8(L) ; N22(L) ; N24(L) ; N26(L) ; N28(L) ;
ζ factors	Z1(L) ; Z2(L) ;
and	AL1(L); AL2(L); AL3(L) ; BE1(L); BE2(L); BE3(L);

The notations are as follows:

- N1(L) the hydrogen density at $r = p_L$
- N8(L) the oxygen density (Z = 8)
- N22(L) the titanium density (Z = 22), etc.

To explain AL1, AL2, AL3, BE1, BE2, BE3, we reproduce Fig. 4:



Here the recombination step is grossly exaggerated to make the principle clear:

In energy window 1 one has F = AL1 + BE1 E; (12.1)

in energy window 2 one has F = AL2 + BE2 E;

if a straight line is drawn through the F values from the two energy windows, one obtains

$$F = AL3 + BE3\ E.$$

Input data

The input data are stored in the AMOS segment DATA; an example is shown below. The meanings of these parameters are presented in the form of a list. Columns 2 and 3 list the line number and numerical value of the respective parameter in the example[x]; column 4 states the section in which the parameter is introduced or more accurately described.

Para-meter	Line	Value	Sec.	Meaning
IMAX	100	3	13	No. of detectors in a probe
LMA	100	4	18	No. of probes + 1
M_1	100	3		No. of smoothing intervals in window 1
MS	100	6	15	No. of all smoothing intervals
NABEL	100	0	18	For choosing the Abel inversion method
NGLA	100	0	15	For choosing the smoothing method
NMAX	100	4	2	No. of observation time intervals
DE9	100	.27	14	Channel width of reference scale in keV
EO9	100	O.	14	Zero displacement
T(N)	200	0...	2	Observation times in sec
EL(M) ER(M)	300	1.4..	15	Smoothing intervals in keV

x on page 53

The lines 400 - 1200[x] are read in the BLENDE subroutine. The latter is called in the main program in the DO-3 loop a total of IMAX·Lm1 times; in our example[x] we have LM1=LMA-1=3 and IMAX=3; there therefore have to be 3 x 3 = 9 lines available. In our example the filter parameter A has the value 1317 and the filter thickness D has the value 0.00075.

A and D only occur in the combination A·D; consequently, A·D is not changed when A is divided by 1000, and D multiplied by 1000, thus making A and D of the order 1 and therefore allowing them to be read in with F format (see BLENDE, statement No. 3300).

As an example we treat line 700, which contains the data of detector I = 1 of probe L = 2

Parameter	Value	Sec.	Meaning
IMAX(I,L)	19	13	No. of energy channels of detector I, L
A	1.317	13	Filter parameter
B	3.276	13	Filter parameter
D	0.75	13	Filter thickness
DE(I,L)	0.45	2	Channel width of detector I, L in keV
EO(I,L)	0.04	2	Zero displacement
X_1	100.	3	Aperture position in cm; see Fig. 2
X_2	2.	3	" " " "
R_1	.1	3	Aperture radius in cm; see Fig. 2
R_2	.017	3	" " " "
R_3	.11	13	Sensitivity radius of detector

In our example[x] the time loop, i.e. the DO-6 loop of the main program, starts from line 1300. First we read in:

[x] on page 53

Parameter	Line	Value	Sec.	Meaning
Ne(L)	1300	10. ..		Electron density
P(L)	1400	0. ..	5	Aperture position (L=1,2,3) and plasma radius (L=4)

Then the raw spectra are read in the OVLAP subroutine. The latter is located in the DO-4 loop of the main program, the loop running from 1 to LM1; the READ command for the raw spectra in the OVLAP routine is located in the DO-5 loop, which runs from 1 to IMAX. For each time step we thus have to read in LM1·IMAX = 9 raw spectra; for the 1st time step (N = 1) these are lines 1500 - 2300.

In our example we manage with one line per raw spectrum. The reason is the choice JMAX = 19 in lines 400 - 1200, and that there is room in one line for 24 integers. If, for example, we had chosen JMAX = 27, we should need 2 lines per raw spectrum.

In line 2400 we have the electron density for the next time step - and the game starts all over again.

Sample input data

```
 100    3   4   3   6   0   0   4 .27 0.
 200  0.     .1     .2     .3
 300  1.4    2.6    2.0    3.6    2.8    4.2    6.     7.2    6.8    8.3    8.      9.
 400    19 1.317 3.276 0.75   0.57   0.13   100.   2.     .1     .01    .11
 500    19 1.317 3.276 20.    0.55   0.05   100.   2.     .1     .016   .11
 600    19 1.317 3.276 200.   0.53   0.     100.   2.     .1     .04    .11
 700    19 1.317 3.276 0.75   0.45   0.04   100.   2.     .1     .017   .11
 800    19 1.317 3.276 20.    0.51   0.09   100.   2.     .1     .03    .11
 900    19 1.317 3.276 200.   0.52   0.26   100.   2.     .1     .09    .11
1000    19 1.317 3.276 0.75   0.57   0.06   100.   0.2    .1     .08    .11
1100    19 1.317 3.276 5.     0.48   0.15   100.   0.2    .1     .2     .11
1200    19 1.317 3.276 50.    0.51   0.     100.   0.2    .1     1.     .11
1300  10.    6.     2.     0.
1400  0.     .4     .7     1.
1500    5  28  18  11   6   4   2   5   1   1
1600            1   5   8   7   5   8   2   2   1   3   1
1700                            1   5   8   4   4   9   5   2   2   1   1   1
1800       25  26  16   9   5   3   2   1   3
1900                5   7   6   5   5   5   1   1   2
2000                        1   2   7   5   3   2   7   1   1   1
2100   10  88  32  10   3   1
2200        9  73  56  27  12   5   2   2   1
2300                6  48  65  45  34  21   5   2   3
```

Main program (MAINPR)

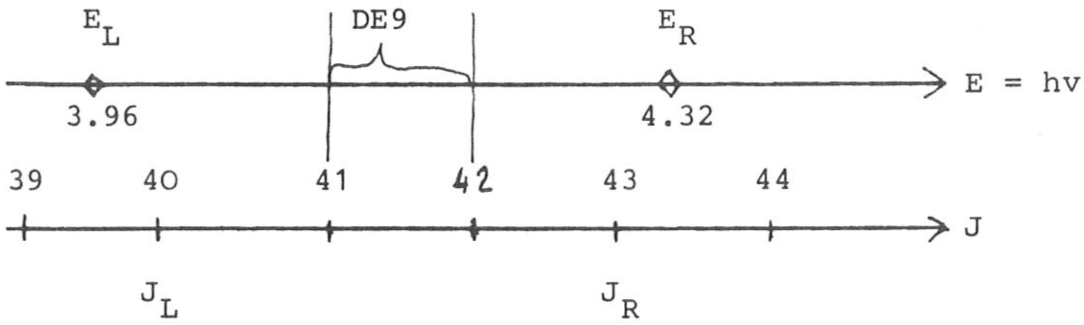
The main program includes read-in and print-out of the input data and conversion of the smoothing intervals in the DO-2 loop:

In Sec. 15 the smoothing intervals are not required in keV but in units of the channel width DE9. Conversion is done as follows:

$$JL = (EL - EO9) / DE9 + 1$$
$$JR = (ER - EO9) / DE9 \qquad (12.2)$$

so that the JL, JR interval is somewhat shorter than the corresponding EL, ER interval. This is illustrated by an example with EO9 = 0 , DE9 = 0.1 in fig. 15 :

Fig. 15



The energy window parameter M1 decides which M intervals belong to energy window 1:

The intervals $1 \leq M \leq M1$ belong to energy window 1

The intervals $M1 + 1 \leq M \leq MS$ belong to energy window 2.

<u>The program flow</u>

After read-in of the filter, aperture and other parameters in MAINPR statement No. 1200 etc. and in BLENDE routine the time independent component U_o (see eq. (2.3)) of the normalization factor is calculated in the BLENDE routine. Then the time (DO-6) loop commences:

The raw spectra are read in normalized and superposed in the OVLAP routine, yielding the spectral function U(L, J); the SESNIC routine computes the parameters collected at the beginning of this section.

Altogether, the following subroutines are required:

Routine	Input	Output	Description
BLENDE	aperture and filter parameters	U_o	Sec. 2; 3; 13
OVLAP	U_o; raw spectra	U(L,J)	Sec. 2; 14
GLATT	U(L,J); JL(M); JR(M)	ULG(L,M);EID(M)	Sec. 15
SESNIC	U; ULG	TE; N26 etc.	Sec. 23
ALPBET	ULG	AL; BE	Sec. 18
ABEL	U	F	Sec. 19
AZRUT	C, H, x	AZ	eq. (4.16a-e)
ITERAT	ULG	ALP; BET	Sec. 17
LSTSQ	i.e. E; ln U	α ; ß	Sec. 16
SORTIR	Q(L)	MA(L)	Sec. 20
IMPUR	U; TE; i.e.Z=26	i.e.N26; P26	Sec. 21
METAL	TE	ZME_1; ZME_2	Sec. 22

In addition, most routines require the positions P_L.

We now discuss the COMMON blocks and the meaning of the variables stored in them.

1) Blank COMMON (blk)

		Sec.	
EID	smoothing interval centres	15	Fig. 17
GEW	weighting factors	15	eq. (15.5a)
P	L=1,..LM1: probe positions L=LMA : plasma radius	2 4	Fig.1;Sec.6
PLOG	$= \ln (1-\hat{p}^2)$	17	
U	spectral function at the reference grid points (14.1)		
ULG	ln U at EID	15	Fig. 17
DE9 EO9	reference grid points	14	eq.(14.1)
JMAX9	number of reference grid points	=JR(MS)	
LM1	number of probes		
LMA	= LM1 + 1		
M_1	number of M grid points in the energy window 1		
M_S	number of M grid points in the energy windows 1 + 2 ; M grid point = smoothing interval centre		

2) COMMON /BLE/

		Sec.	
DE(I,L)=	channel width of detector No. 1 of probe No. L	2 13	Fig. 1b
EO(I,L)=	zero displacement	2	Fig. 1b
UO	normalization factor	2	eq.(2.5-6)
JMAX(I,L)	number of energy channels for detector I, probe L		

3) COMMON /OVL/

T(N)	observation times t(N)	2	eq.(2.5)
DTN	= T(N) - T(N-1)		
IMAX	= number of detectors of a probe		

4) COMMON /GLA/

JL(M) JR(M)	smoothing interval No. M	15 12	Fig. 17 Fig. 15

COMMON /ALB/

5) FP profile F, UP profile U — see Sec.5, just before eq. (5.8)

6) COMMON /ITE/

ALP $= \alpha_p$, BET $= \beta_p$ — see Sec. 5, just before eq. (5.8)

C, H — profile numbers; eqs. (4.14) to (4.16)

7) COMMON /IMP/

NE(L), TE(L) — electron density, temperature at $r = p_L$

8) COMMON /MET/

$P22 = \frac{N22}{NE}$ = partial density of titanium (Z = 22); similar to the rest

9) COMMON /SES/ — Sec.

AL1 = α in energy window 1		
AL2 = α in energy window 2	12	Fig. 14
AL3 = α in energy windows 1+2		
BE3 = β in energy windows 1+2		
N8 = oxygen density in energy window 1		
D8 = oxygen density in energy window 2		
analogous: N1 and D1 for hydrogen		
N22 = titanium density (Z = 22); analogous: N24, N26, N28		
Z1 = ζ factor in energy window 1		
Z2 = ζ factor in energy window 2		

S1, S2, S3, T1, T2, T3 are not needed in the present version. The parameters listed in COMMON /SES/ only feature in the SESNIC routine. We have collected them in a COMMON block in case later users write an input/output routine in which COMMON/SES/ would appear.

Precision parameters

The routines of this program contain inquiries with "built-in parameters". An example of such a parameter is the number 0.1 in the test IF(RL. LE.01) .. in the OVLAP routine, ISN 0061, which is discussed in detail at the end of Sec. 14. The user may now want to replace the number 0.1 by another and do the same in other test statements. We therefore present at the end of this section a list of all test statements containing built-in parameters:

Routine	Statement	Discussion
BLENDE	ISN 0026	If hv $\leq$ 0.1 , then set U = 0
BLENDE	ISN 0029	If FILTER $\geq$ 13. , then set U = 0
OVLAP	ISN 0061	If R $\leq$ 0.1 , then set U = 0 (Sec. 14)
LSTSQ	ISN 0010	In eq. (16.2) sum terms are ignored,
LSTSQ	ISN 0012	if G $\leq$ 0.001 or V $\leq$ -700
LSTSQ	ISN 0021	If D $\leq 10^{-6}$, absurd values are set for α and ß
SESNIC	ISN 0030	If $ß_1 \leq$ -0.001, then set N_g = 0 (or if $T_e \geq$ 1.MeV or negative)
ABEL	ISN 0022-28	Sec. 18 and 19
ALPBET	ISN 0034	If ULG $\leq$ -100. then set D=U=0
ALPBET	ISN 0061	} If MC $\leq$ 1 then set α , ß absurd
ITERAT	ISN 0037	}
ITERAT	ISN 0052	If LC $\leq$ 1 , then set H=C=2 (see Sec. 17, Fig.22).
ITERAT	ISN 0056	" H $\leq$ 0. , " " H = 2
ITERAT	ISN 0058	" C $\leq$ 0. ; " " C = 2 ; step profile not permitted

13. BLENDE SUBROUTINE

The BLENDE[x] subroutine is for calculating the time independent normalization factor U_o from Sec. 2, eqs. (2.2) - (2.5). In the ASDEX experiment there are five probes with three detectors each. In our program each detector therefore has a probe index L and a detector index I:

The probe index L goes from 1 to LM1 (in ASDEX LM1 = 5);
the detector " I goes from 1 to IMA (in ASDEX IMA = 3).

Those characteristics of a detector which are also used outside the BLENDE routine (mostly in OVLAP) are therefore given the indices I and L. The characteristics of a detector are :

aperture radii	R_1 and R_2
aperture positions	x_1 and x_2 (see Sec.3, Fig.2),
sensitivity radius	x_3
filter constants	a, b, d
energy channel width	DE
zero displacement	EO
number of energy channels	JMAX.

These parameters are read in statement ISN 0005.

---

[x] BLENDE (German) = aperture (English)

The first part of the routine is for calculating DSDO = $\Delta S \Delta \Omega$ according to eq. (3.10). Here the following change was made compared with Sec. 3: the detector has a finite sensitivity radius x_3.

If $x_3 \gg x_2$, then eq. (3.10) is valid.
If $x_3 \ll x_2$, then x_3 has to be substituted for x_2 in eq. (3.10).
If $x_3 \approx x_2$, we interpolate, see ISN 0016.

The second part of the routine consists of the DO-5 loop. The loop index JI counts the energy channels of the detector; EN is the energy in the centre of the energy channel JI. We set $U_o = 0$ if the energy is too small (EN $\leq$ 0.1) or if the filter function is too large (FILTER $>$ 13). In the normal case (statement ISN 0031) eq. (2.3) is valid.

Finally, we discuss the filter function. From the filter constants a, b, d we form

$$\text{FILTER} = \mu(E)\ d \tag{13.2}$$

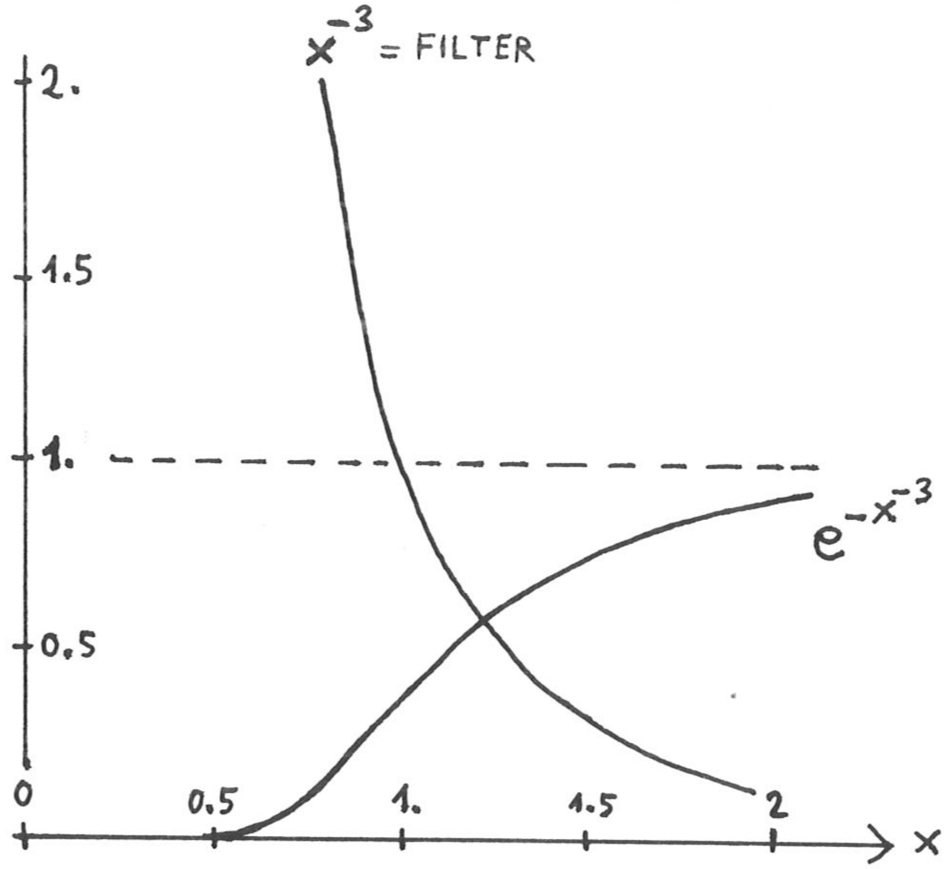
$$\mu(E) = a\ E^{-b} \tag{13.3}$$

where $E = h\nu$.

For most materials one has $b \approx 3$; for this special case we therefore plot FILTER versus $x = E(d \cdot a)^{-1/3}$ in Fig. 16 .

Fig. 16

Filtering for
$b = 3$,
$E = x \sqrt[3]{d \cdot a}$



14. OVLAP SUBROUTINE

The OVLAP subroutine is used for

1) reading in the raw spectra (in statement ISN 0013),
2) normalization (statement ISN 0016),
3) superposing the normalized spectra (ISN 0038, ISN 0063).

The user reads in the numbers DE9 and EO9 in the main program, and from these one forms the energy mesh points (ISN 0018)

$$E9(J) = DE9\ J + EO9 \qquad (14.1)$$

This energy scale is called the reference scale. The purpose of OVLAP is to calculate the spectral function U(L,J) = $U(p_L;\ E9)$ according to eq. (2.4). Before describing the program, we define the necessary concepts "energy channel", "channel width" and "zero displacement".

A detector can be schematically described by energy mesh points

$$E_I(J_I) = DE_I\ J_I + EO_I \qquad (14.2)$$

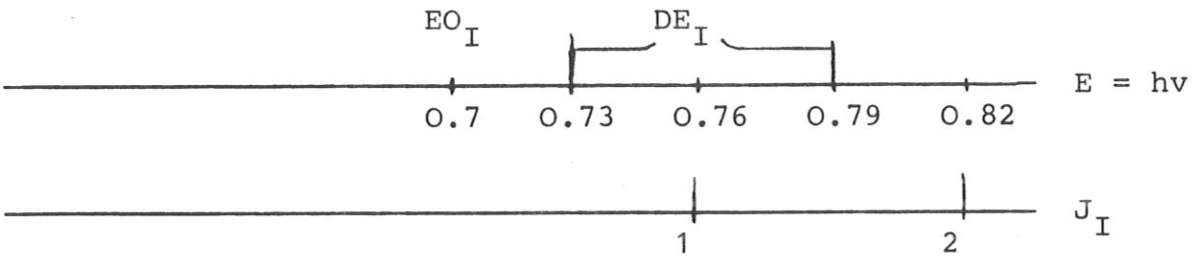
located in the centre of intervals of length DE_I.
These intervals are called "energy channels",
the interval length DE_I is called "channel width", and
the quantity EO_I is called "zero displacement".
When a quantum with an energy in the interval

$$E_I(J_I) - 0.5\ DE_I \leq h\nu \leq E_I(J_I) + 0.5\ DE_I$$

enters the detector, the counter with the number J_I is advanced by 1. We illustrate the situation with an example: let

$$EO_I = 0.7 \text{ keV}$$
$$DE_I = 0.06 \text{ keV} \quad .$$

The first energy channel is then located in the interval $0.73 \leq E \leq 0.79$ keV. A quantum with the energy 0.71 is not recorded. A quantum with the energy 0.74 is recorded as a quantum in the energy channel $J_I = 1$, causing the raw spectrum $R_I(J_I = 1)$ to be increased by 1.



We now describe the program.

The OVLAP routine gets the parameters DE9 and EO9 via the unlabeled COMMON, and the zero displacements EO(I,L) and channel widths DE(I,L) of the detectors via COMMON /BLE/; here L = probe index and I = detector index.

The raw spectra are read in the DO-5 loop and normalized; the result is UB(I,J). The index L is not needed at this point because it appears in the argument list of OVLAP.

Superpositioning of the normalized spectra according to eq. (2.4) takes place in the DO-7 loop. In this loop we form

$$S_R = \text{denominator of eq. (2.4)} = \sum_{I=1}^{IMAX} R^{(I)}, \qquad (14.3)$$

$$S_U = \text{numerator of eq. (2.4)} = \sum R^{(I)} \; U_B^{(I)}$$

at the reference energy E9. For this purpose we require $R^{(I)}$ and $U_B^{(I)}$ at E9. For this purpose we look for the channel number J_I for which

$$E_I(J_I) \leq E9 \leq E_I(J_I+1)$$

is valid. The solution is

$$J_I = \frac{E9 - EO_I}{DE_I} \qquad \text{(statement ISN 0025).}$$

We then check whether J_I is reasonable. This is done by means of the IF-statements ISN 0028-32: J_I is <u>not</u> reasonable and therefore does not make any contribution to S_R and S_U if

1) J_I does not occur among the channel numbers of detector I, <u>or</u>

2) R = 0 for J_I <u>and</u> J_I + 1.

If J_I is reasonable, a linear interpolation is performed:

$$RI = R^{(I)}(E9) = VL\ R_{JI} + VR\ R_{JI+1} \qquad \text{(ISN 0037).}$$

The quantity R_L calculated in ISN 0060 is the raw spectrum at E9 and according to sec. 2 the inaccuracy in calculating the spectral function U is about $1/R_L$. Therefore it is tested in statement ISN 0061, whether R_L is sufficiently large. In ISN 0061 we compare R_L with 0.1; in this case practically every quantum is taken into account, but it may also lead to large statistical errors. If the user does not need the rare high--energy quanta, but good statistics instead, he may replace the number 0.1 by a larger one.

15. GLATT SUBROUTINE

In the GLATT subroutine we smooth the spectral function within the clean energy windows. For this purpose we read in several smoothing intervals (see Sec. 12, eq. (12.2)) and determine ULG = ln U in the centre EID(M) of these smoothing intervals. This is done because for application in the ALPBET routine U or ln U should be available with a good degree of accuracy at a few mesh points. After OVLAP (MAINPR, statement ISN 0043) is called, however, the spectral function U(L,J) is present at very many mesh points, viz. the reference mesh points (14.1), and is subject to large statistical errors.

Such a smoothing interval is shown in Fig. 17.

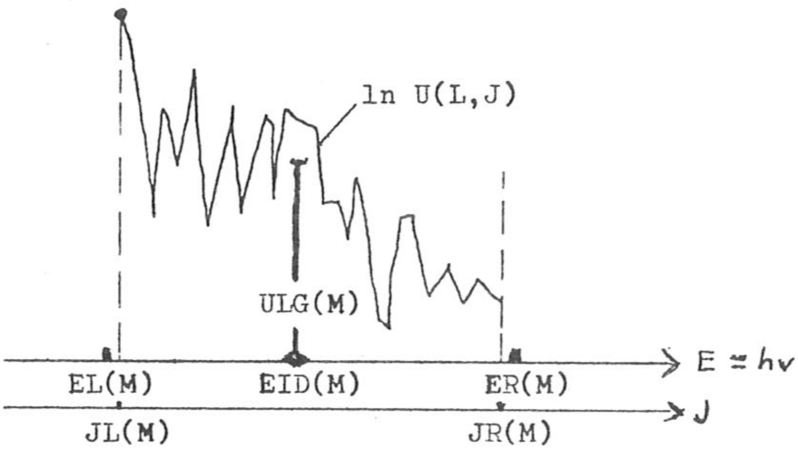


Fig. 17

The spectral function U(L,J) at the reference mesh points E9 = DE9 J + EO9 within the smoothing interval JL(M) $\leq$ J $\leq$ JR(M).

The GLATT routine works as follows:

<u>Given:</u> U(L,J) ; DE9 ; EO9 ; JL(M) ; JR(M)

J=1, .. JMAX9 energy channels,
L=1, .. LMA-1 probe positions
M=1, .. MS smoothing intervals.

<u>Required:</u> ULG = ln U at EID(M),

where EID(M) = 0.5 DE9 [JL(M) + JR(M)] + EO9. (15.1)

<u>Method:</u> The GLATT routine should only be used within clean energy windows, where

$\ln F = \alpha + \beta E$, see (5.4)

is valid. Substituting this equation in eq. (4.16), it is seen that, if the smoothing intervals are properly chosen (in window 1 approx. up to 1 keV long, in window 2 in Fig. 4 up to 4 keV long), ln U is also a linear function of E:

$$\ln U = \alpha_8^{(M)} + \beta_8^{(M)} E \qquad (15.2)$$

where unlike eq. (5.4), of course, the coefficients α_8 and β_8 may be different from one smoothing interval to the next and therefore have the index M.

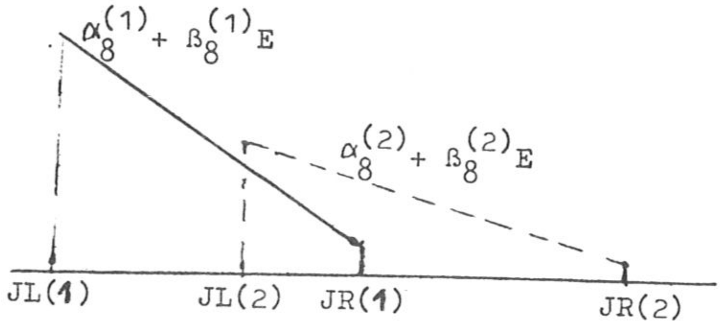


Fig. 18

Clean energy window with two smoothing intervals.

From eq. (15.2) it follows that at EID(M):

ULG = arithmetic average value of ln U(L,J);

U = geometric average value of U(L,J).

But this way of taking the average value raises problems when so few quanta are available that one gets U(L,J) = 0 at a few mesh points. An example is given in Fig. 19.

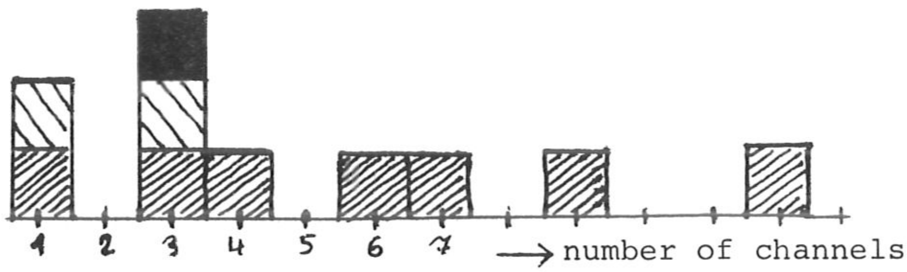


Fig. 19

Distribution of 10 quanta on 12 energy channels.

We offer two methods of taking the average value, which the user can select by the choice of the parameter NGLA:

NGLA = 0 We take the geometric average value from the arithmetic average value of U(L,J) by means of the correction factor (15.4). For this purpose we determine β_8 in Appendix A (eq. (15.8)) and use it to form

$$z = \beta_8 (E_8 - E_9), \qquad (15.3)$$

which is the dimensionless length of the smoothing interval. The index M has been omitted. By means of z one can calculate the ratio of the arithmetic to the geometric mean: it holds that

(see Appendix B)

$$\frac{\text{arithmet. aver.}}{\text{geomet. aver.}} = \frac{e^{0.5z} - e^{-0.5z}}{z} \tag{15.4}$$

$$1 + \frac{z^2}{24}\left[1. + \frac{z^2}{80}\left(1. + \frac{z^2}{168}\right)\right].$$

The advantage of this method is that it also works if a large number of U = 0 mesh points is present, and, furthermore, requires only two transcendental functions to produce ULG, viz. the root in eq. (15.8f) and the logarithm for obtaining ln U.

NGLA $\geq$ 2 The influence of the U = 0 mesh points are taken into account by a correction term:

$$ULG = \frac{1}{SU} \sum_{J=JL}^{JR}{}' \ln U(L,J) + \ln \frac{SU}{KM} \tag{15.5}$$

where

KM = JR - JL + 1 = number of all mesh points,

SU = number of mesh points with U $\neq$ 0.

Summation is only performed over those J for which U(L,J) $\neq$ 0 is valid, hence the prime at the summation symbol. The method NGLA $\geq$ 2 requires much more computing time than method NGLA = 0 because when, for example, SU = 20, the logarithm is called 20 times to produce ULG. An advantage of the method NGLA $\geq$ 2 is the stronger smoothing, which is discussed in Appendix A for a particular example.

For subsequent least squares fitting the mesh points EID(M); ULG(L,M) are given the weighting GEW(L,M) = SU. (15.5a)

APPENDIX A

Calculation of β_8

From the U(L,J) of the interval (15.1) we perform the two summations

$$S_o = \sum_{J=JL}^{JR} U(L,J)$$

$$S_1 = \sum_{J=JL}^{JR} U(L,J)\ E$$

where $E = DE9\ J + E09$,

We now consider S_o and S_1 as approximations for the integrals

$$S_o = \frac{1}{DE9} \int_{E_8}^{E_9} dE\ \ U \tag{15.6a}$$

and

$$S_1 = \frac{1}{DE9} \int_{E_8}^{E_9} dE\ U\ E \tag{15.6b}$$

where

$$E_8 = DE9\ (JL - 0.5) + E09 \tag{15.7a}$$

$$E_9 = DE9\ (JR + 0.5) + E09\ . \tag{15.7b}$$

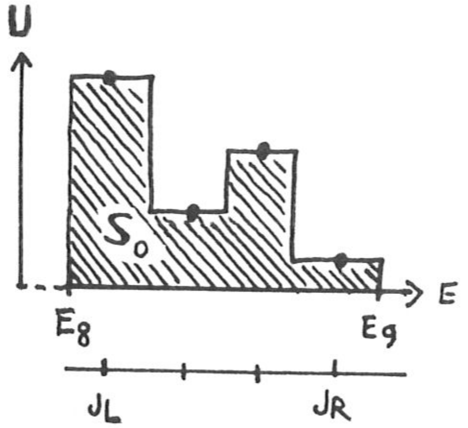


Fig. 19a

U versus E;
S_o (hatched area),
E_8 and E_9

Substituting U prop. $\exp(\beta_8 E)$ (15.2)

in eq. (15.6) and defining $Q = S_1/S_o$

$C = (Q-E_9)/(E_8-Q)$

$F = \beta_8 \; (E_8-Q)$ (15.8)

one obtains the transcendental equation

$$\exp\left[(1+C)F\right] = \frac{1+CF}{1-F}$$

for the dimensionless unknown F; the solution is approximated by

$$F \approx \frac{C-1}{C - C^2 \Big/ \sqrt{1.-0.8\,C + 8.6\,C^2 - 0.8\,C^3 + C^4}} \quad (15.8f)$$

The inaccuracy of the approximation (15.8) is approx. 1 %, and it applicable for all β_8.

Finally, we discuss the advantages and disadvantages of the two methods. Method (15.4 + 8) or NGLA = 0 is recommended when there are a large number of U = 0 mesh points present. The disadvantage of using an approximation formula is more of a theoretical nature. Much more important in practice is what happens when there are "wild points", i.e. mesh points with U values which for some reason become too large. We use both methods in the following example:

	J	U	
JL=1	1	1	
JR=7	2	1	
$ß_8=0$	3	1	
KM=7	4	100	← wild point
SU=7	5	1	
SO=106	6	1	
	7	1	

NGLA = 0 $\qquad$ $ULG = \ln \left[S_o / K_M \right]$

$$= \ln(106/7) = 2.7$$

NGLA ≥ 2 $\qquad$ $ULG = \frac{1}{SU} \sum \ln U$

$$= \frac{1}{7} \ln 100 = 0.66$$

Wild points are thus more strongly damped by eq. (15.5) than by eq. (15.4). With "ordinary" errors, on the other hand, this effect is not very pronounced: substituting U(J=4) = 2 in the above example yields

ULG = 0.13 for NGLA = 0
ULG = 0.10 for NGLA = 3.

If it is to be feared that the spectrum of the clean, or rather presumably clean, energy windows will be distorted by wild points, method NGLA ≥ 2 is to be recommended instead.

APPENDIX B

Relation between the arithmetic and the geometric averaged value of the spectral function U in the smoothing interval.

Introducing the dimension-less variables

$$x = -\,\beta_8(E-E_8)$$

and

$$z = \beta_8(E_8-E_9)$$

one has $U = e^{-x}$ (normalized to 1 at $E = E_8$).

The arithmetic averaged value is

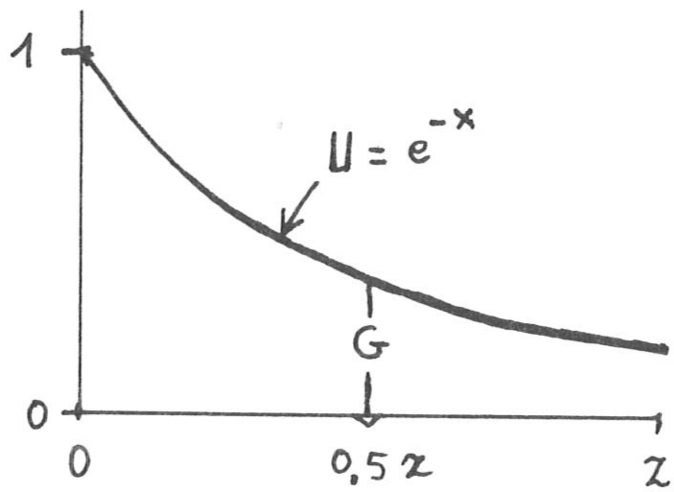
$$A = \frac{1}{z}\int_0^z dx\; U = \frac{1}{z}\left[1.- e^{-z}\right].$$

The geometric averaged value is

$$G = \exp\left\{\frac{1}{z}\int_0^z dx\; \ln U\right\} = e^{-0.5z}$$

and, consequently,

$$\frac{A}{G} = \frac{e^{0.5z} - e^{-0.5z}}{z}$$



16. LSTSQ SUBROUTINE

We are given pairs of values E_J; V_J and their weighting G_J. The purpose of the LSTSQ subroutine is to calculate two numbers α, β so that

$$V_J = \quad + \beta E_J \tag{16.1}$$

is satisfied as well as possible or that the square of the error

$$S = \sum_{J=1}^{JMA} G_J \left[\alpha + \beta E_J - V_J \right]^2 \tag{16.2}$$

becomes minimal. The system of equations

$$\frac{\partial S}{\partial \alpha} = \frac{\partial S}{\partial \beta} = 0 \tag{16.3}$$

can be reduced to the form

$$A_{11}\alpha + A_{12}\beta = B_1 \qquad (16.3a)$$
$$A_{12}\alpha + A_{22}\beta = B_2 \qquad b)$$

where

$$A_{11} = \sum G_J \qquad (16.4a)$$
$$A_{12} = \sum G_J E_J \qquad b)$$
$$A_{22} = \sum G_J E_J^2 \qquad c)$$
$$B_1 = \sum G_J V_J \qquad d)$$
$$B_2 = \sum G_J V_J E_J \qquad e)$$

IF-statements

If $V < -700.$, the respective sum term is not taken into account. When this is applied to $V = \ln U$ the "trivial" cases $U = 0$ are not counted.

If the determinant is $D = 0$, absurd values $\alpha = -444$ and $\beta = 222$ are set.

17. ITERAT SUBROUTINE

The ITERAT subroutine calculates the quantities α and β and the emissivity F for a given spectral function U. It performs Abel inversion by means of eq. (4.16), A_Z being calculated on the assumption that S and kT_e are of the profile type (eqs. 4.14 and 4.15). Since this assumption need not always be correct, we do not call the result α, β but α_p, β_p.

Given:

Energy mesh points	E = EID(M),	M = ML, MR
Probe positions	p_L = P(L) ,	L = 1, LMA
Spectral function	ln U= ULG(L,M);	

Required:

α_p = ALP

β_p = BET

F_p = FP(L,M)

U_p = UP(L,M).

Method:

It is assumed that the energy mesh points are located in a clean energy window so that eq. (5.4) is valid.

The basis equation is eq. (4.5) in the form

$$\alpha_p(r) + \beta_p(r)\ E = W \qquad (17.1)$$

where

$$W = \ln U - \ln \left\{ 2a \sqrt{\frac{1-\hat{p}^2}{A_Z}} \right\} \qquad (17.2)$$

The idea is now to choose α_p and β_p for fixed r such that eq. (17.1) is satisfied as well as possible (see Fig. 20).

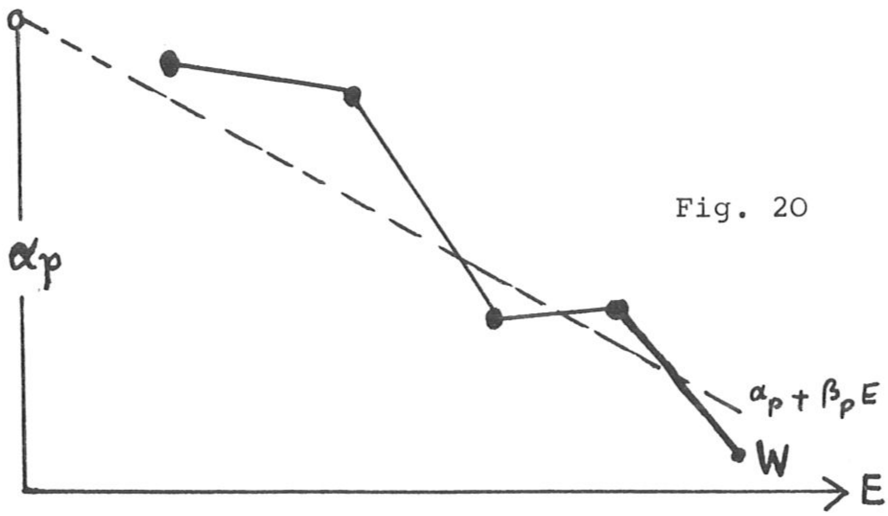


Fig. 20

To determine AZ we use eq. (4.16a-e), i.e. we assume that the quantities S and T_e are of the profile type (eq. (4.14)-(4.15)). If S and T are not of the profile type, there are errors which experience shows to be small because W only depends logarithmically on AZ. Another difficulty is that the variational problem (eqs.(17.1)-(17.2)) is not linear because W depends on α_p and β_p via A_Z. Under these circumstances we calculate α and β by the following iteration method:

Let $\left.\begin{array}{l}\alpha_n = \alpha_p \\ \beta_n = \beta_p\end{array}\right\}$ after the n-th iteration step;

we then make the ansatz

$$\alpha_{n+1} + \beta_{n+1}E = W(\alpha_n;\beta_n;E;..) \tag{17.3}$$

and determine α_{n+1} and β_{n+1} so that eq. (17.3) is satisfied as well as possible (least square fit; see Sec. 16 on LSTSQ routine). Here α_n and β_n and hence W are known from the previous iteration step. As already mentioned above, the left-hand side of eq. (17.1) depends much more strongly on α_p, β_p than the right-hand side W; the method therefore already converges after 2 to 3 iteration steps.

To calculate A_Z, we need the profile numbers C and H. These are determined by a least squares fit from the rearranged equations (4.14)-(4.15):

$$\alpha_n(r) = \ln S_o + C \ln(1.-\hat{r}^2) \tag{17.4}$$

$$-\ln(-\beta_n(r)) = \ln T_o + H \ln(1.-\hat{r}^2) \tag{17.5}$$

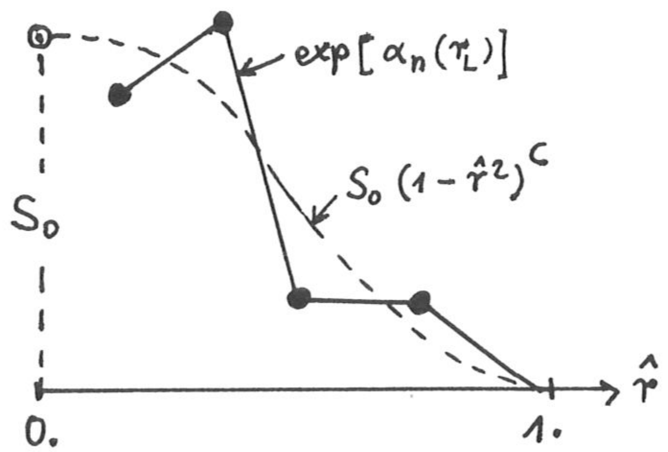


Fig. 21

Determination of the profile number C

We start the method by arbitrarily giving

$$C = H = 2\ , \quad \beta_{n=0} = -1. \tag{17.6}$$

Each iteration step consists of the parts given in the table below:

Table III

Calculation of	according to equation:	routine:	parameters necessary:		line
AZ	(4.16a-e)	AZRUT	C, H, ß	x	I
W	(17.2)		AZ, ln U		II
α_{n+1}; β_{n+1}	(17.3)	LSTSQ	W		III
S_o; $C\|_{n+1}$	(17.4)	LSTSQ	α_{n+1}		IV
T_o; $H\|_{n+1}$	(17.5)	LSTSQ	β_{n+1}		V

Line III is a least squares fit in the E direction: α_{n+1} and β_{n+1} are chosen for fixed $r=p_L$ so that eq. (17.3) is satisfied as well as possible. Lines IV and V are least square fits in the r or p direction: S_o and C are chosen such that eq. (17.4) is satisfied as well as possible. The analogy is as follows:

In line III W is approximated by a linear function of E and in line IV α_{n+1} is approximated by a linear function of $\ln(1-\hat{r}^2)$. We have thus determined α_p and β_p from U. This also yields F_p from eq. (5.4) (see DO-8 loop at the end of ITERAT) and U_p from eqs. (4.16) and (4.3).

Furthermore, an error square

$$ER = \frac{1}{SU} \sum_{L,M} \left[\frac{\ln UP - ULG}{ULG}\right]^2 \qquad (17.7)$$

is formed rather arbitrarily at the end of the DO-8 loop, SU being the number of sum terms.

Meaning of variables appearing in ITERAT

ML ≤ M ≤ MR energy mesh points used for calculating α_p, β_p

$$\left.\begin{array}{l} ALP = \alpha_p \\ BET = \beta_p \\ FP = F_p \\ UP = U_p \\ ULG = \ln U \\ P = p \end{array}\right\} \text{from Sec. 5}$$

C, H profile numbers from eqs. (4.14) - (4.16)

LMA = number of p mesh points (probes and plasma radius)

MS = number of EID " " (smoothing intervals)

GE, GEW, G weighting factors for the least square fit (see Sec. 16)

PLOG(L) = $\ln(1.-\hat{p}_L^2)$

AL = ALP $= \alpha_p$

TL(L) = $\ln\left[-1/\beta_L\right]$ From this the profile number H is determined in statement ISN 0054 by a least square fit.

W see eq. (17.2).

Structure

The first lines up to the DO-1 loop describe the start of the iteration method (eq. (17.6)). In addition, the quantities TL and AL are given absurd values so that they are defined if for any reason the mesh point has to be missed later. Later we also have the same basic structure in most DO loops:

1) Weighting factor made zero
2) Absurd value for the variable (e.g. W or TL)
3) Test: if, for example, ULG absurd, then GO TO CONTINUE
4) ULG reasonable: then calculate the variable.

The DO-6 loop contains the iteration scheme described in Table III; the result is ALP(L), BET(L), C and H. The ULG are supplied together with the weighting factors GEW by the calling program; G is calculated in statement ISN 0033 from the GEW.

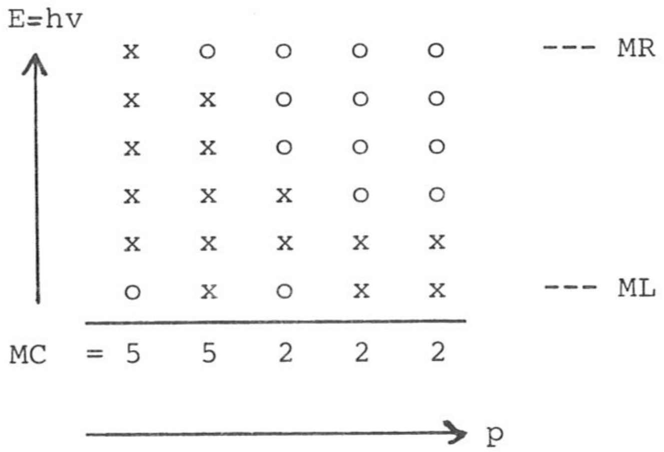
Our next task is to discuss the meaning of the variables LC and MC. For this purpose we have to know that in the high-energy regime there are many "trivial" mesh points, i.e. pairs of numbers L, M for which

$$U(L,M) = 0 \qquad \text{or} \qquad ULG(L,M) = -711$$

is valid. This is because the quantum density decreases as $\exp(-\frac{h\nu}{kT_e})$ for high energies $h\nu$. But trivial mesh points may also exist for very low energies if the filters are too impermeable. On the whole, there is then, in principle, a distribution of the trivial (o) and non-trivial (x) mesh points, as shown in Fig. 22.

Fig. 22

Distribution of trivial (o) and non-trivial (x) mesh points in the p-E plane



MC denotes the number of non-trivial mesh points of a column. IF - statement ISN 0037 means: ALP and BET are only calculated when MC $\geq$ 2; this condition is met in our example (Fig.22) in all five columns. LC denotes the number of columns for which ALP and BET are calculated; in the example in Fig. 22 one thus has LC = 5. The if statement ISN 0052 means: C and H are only calculated when LC $\geq$ 2. Otherwise C = H = 2 is set. In the case of Fig. 22 one has LC = 5.

18. ALPBET SUBROUTINE

The ALPBET subroutine calculates the quantities α and β.

Given:

Energy mesh points	E = EID(M)	, M = ML, MR
probe positions	p = P(L)	, L = 1, LMA-1
Plasma radius	a = P(LMA)	
Spectral function	$\ln U$ = ULG(L,M)	

Required: $\alpha(p_L)$ = AL(L)
$\beta(p_L)$ = BE(L)

The variable NABEL specifies the method used:

NABEL = 0 Use of ITERAT routine. We set

$\alpha = \alpha_p$ AL = ALP

$\beta = \beta_p$ BE = BET

and thus consider the α_p and β_p yielded by ITERAT in Sec. 5 to be the best approximations for α and β.

NABEL = 2 Use of ITERAT and ABEL routines. In addition to α_p and β_p ITERAT yields U_p and F_p (see ITERAT, DO-8 loop); for the difference D = U - U we do the ABEL inversion in the ABEL routine. The result is G. We form

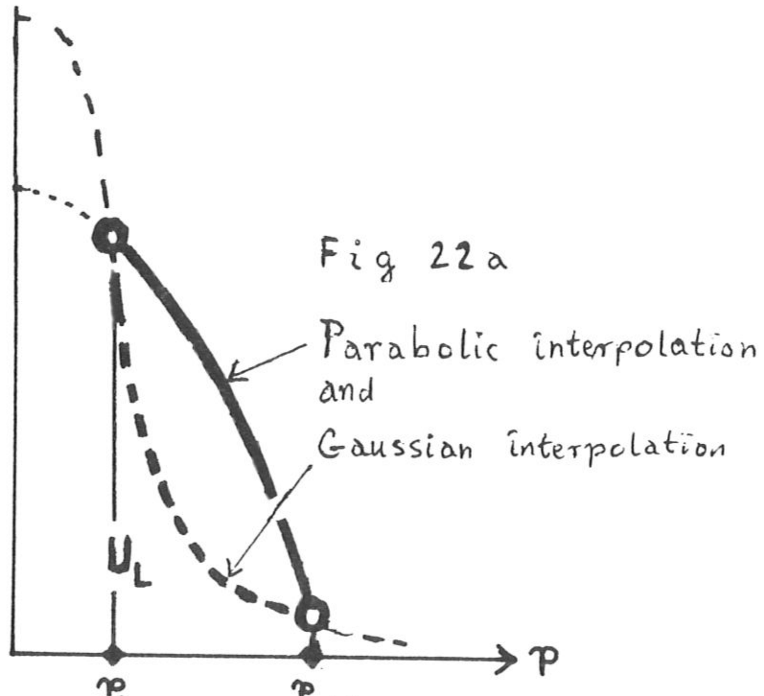
$$F = F_p + G \, . \qquad \text{etc., see Sec. 5.}$$

NABEL $\geq$ 3 We skip ITERAT and calculate F solely by means of ABEL. To allow this, se set $U_p = 0$ in the DO-3 loop.

NABEL = 4 In the ABEL routine Gaussian interpolation is used - if possible.

NABEL = 6 In the ABEL routine only parabolic interpolation is used.

In the DO-9 loop F is put in log form. In the DO-11 loop α and ß are calculated by a least squares fit according to eq. (5.4). If the parameter JWRITE $\geq$ 2 is chosen, intermediate results are printed out.



19. SUBROUTINE ABEL

The ABEL subroutine is used to perform ABEL inversion, i.e.

Given:

Positions p_L, Mesh points r_K $\Big\}$ $K = L = 1,2,..N$

and $U_L = U(p_L)$;

Required: $F_K = F(r_K)$ for $r_K = p_K$.

The formal solution to Abel's integral equation (4.5) is

$$F(r) = -\frac{1}{\pi}\int_r^a \frac{dp}{\sqrt{p^2-r^2}}\,\frac{dU}{dp}$$

It follows that

$$F_K = -\frac{1}{\pi}\sum_{L=K}^{N-1}\int_{r_L}^{r_{L+1}} \frac{dp}{\sqrt{p^2-r^2}}\,\frac{dU}{dp} \quad . \qquad (19.1)$$

In the ABEL subroutine we provide two interpolation ansatzes for U:

1) If

$$\left.\begin{array}{ll} & U_L > U_{L+1} > 0 \\ \text{and} & \text{NABEL} = 4 \end{array}\right\} \qquad (19.2)$$

is satisfied, we use Gaussian interpolation:

$$\ln U = B_L - C_L p^2 \quad \text{for} \quad p_L \le p \le p_{L+1} \qquad (19.3)$$

It follows that

$$F_K = \frac{1}{\pi} \sum_{L=K}^{N-1} \sqrt{C_L} \exp(B_L - C_L r^2) \left[\operatorname{erf} \sqrt{C_L (p^2 - r^2)} \right]_{p_L}^{p_{L+1}}$$

where

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z dx\, e^{-x^2} \qquad (19.4)$$

In the program we use, instead of erf, the complementary function

$$\operatorname{erfc}(z) = 1.- \operatorname{erf}(z). \qquad (19.5)$$

2) If condition (19.2) is not satisfied, we use the parabolic interpretation:

$$U = Q_o + Q_L p^2 \quad \text{for} \quad p_L \leq p \leq p_{L+1} \qquad (19.6)$$

It follows that

$$F_K = + \frac{2}{\pi} \sum_{L=K}^{N-1} Q_L \left[\sqrt{p_L^2 - r_K^2} - \sqrt{p_{L+1}^2 - r_K^2} \right] \qquad (19.7)$$

In both cases (Gaussian and parabolic interpolation) it is assumed that

$$U_N = F_N = 0 \qquad (19.8).$$

As can be seen from Sec. 6, negative positions can also occur, e.g. when some of the lines of sight of the probes pass the plasma centre on the right and some on the left. The few mesh points that we have are thus distributed over an interval

$$-1. \leq \hat{p} \leq +1$$

As circular symmetry was assumed in eq. (4.1), U only depends on U via p^2; we therefore sort the mesh points according to increasing p_L^2 by calling the SORTIR routine, which yields an index function

$$J = MA(L)$$

with the following property:

$$QS(L+1) > QS(L)$$

with $$QS(L) = Q(J) = p_J^2 \; .$$

In the DO-7 loop at the end of the ABEL routine the sequence originally presented is restored.

The variable NG denotes the number of non-trivial mesh points. A mesh point is said to be "trivial" when U = 0 there. Trivial mesh points are particularly abundant for high quantum energies, especially for relatively large positions p. If there is only one non-trivial mesh point, no statement is possible by means of F; because we had set F = 0 in the DO-1 loop we can give RETURN in this case (statement ISN 0017).

The variable NABEL selects the interpolation method:

NABEL ≤ 4 if at all possible, Gaussian interpolation (eq. (19.3) - (19.5))

NABEL ≥ 5 parabolic interpolation (eq. (19.6)-(19.7)).

20. SORTIR SUBROUTINE

SORTIR orders the components Q(L) of a vector according to magnitude. The notations are as follows:

LMA = number of components of the vector Q;

M(L)= an index function with the property

$$Q(M(I)) > Q(M(K)) \quad \text{if} \quad I > K . \tag{20.1}$$

First we consider an example:

$$\text{LMA=3} \qquad \begin{matrix} Q(1) = 23. \\ Q(2) = 67. \\ Q(3) = 34 \end{matrix} \qquad \text{Then} \qquad \begin{matrix} M(1) = 1 \\ M(2) = 3 \\ M(3) = 2 \end{matrix} \tag{20.2}$$

The SORTIR routine is for calculating the index function M(L). For this purpose we start in statement ISN 0006 with an arbitrary function,

$$M(L) = L.$$

If we find a pair of indices I, K for which condition (20.1) is not satisfied, we set

$$M(I)_{neu} = M(K)_{alt} \tag{20.3}$$

and

$$M(K)_{neu} = M(I)_{alt} .$$

21. IMPUR SUBROUTINE

The IMPUR subroutine calculates for the metal impurity with nucleus charge number Z and K_α - line at EI the ion density NI and the ratio PI = NI/NE according to the formulae of Sec.11.

Given:

Spectral function	U(L,J) ; DE9 ; EO9
Electron density	NE(L)
Electron temperature	TE(L)
Atomic number	Z
K_α energy	EI

Required:

Ion density NI(L) and $PI(L) = \frac{NI(L)}{NE(L)}$

Method:

First we determine the continuum component according to the principle in Fig. 23a: it is assumed that in the intervals

$$JLI-N < J \leq JLI \quad (21.1)$$

and

$$JRE+N > J \geq JRE \quad (21.2)$$

we have $U = U_C$ (21.3)

i.e. there is no line radiation present. The mean values of U in these intervals are U_L and U_R respectively.

From these we take the mean value

$$U_C = \sqrt{U_L U_R}. \quad (21.4)$$

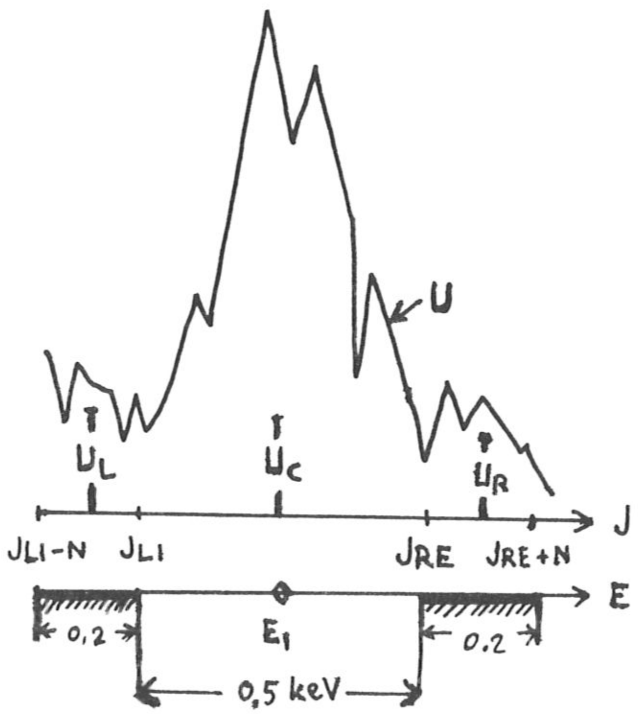


Fig. 23a

Here we have assumed

$$DE9(JRE-JLI) = 0.8 \text{ keV} \tag{21.5}$$

as a measure of the extent of the K_α spectrum and

$$DE9\ N = 0.2 \text{ keV} \tag{21.6}$$

for the line-free boundary continuum.

We now form

$$UK = \int dE\ (U - UC),$$

$$UK = DE9 \sum_J \left[U(L,J) - UC\right] \tag{21.7}$$

It is allowed to take for the continuum component UC the mean value from eq. (21.4) because UC is approximately a linear function of E. UK and K from Sec. 11 are related by Abel's integral equation:

$$UK = 2\int_p^a \frac{dr\ r\ K}{\sqrt{r^2 - p^2}} \tag{21.8}$$

Depending on the choice of NABEL (see Sec. 18), K is calculated from UK either by ABEL inversion (CALL ABEL) or from AZ by means of eq. (4.3) (CALL AZRUT). As soon as K is known, the formulae from Sec. 11 are used in the DO-9 loop to calculate the impurity density.

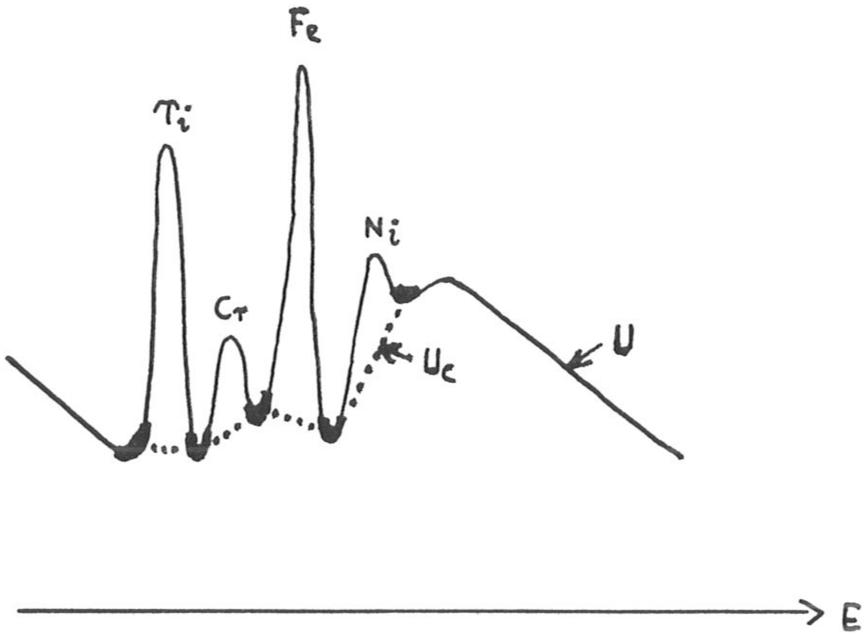


Fig. 24

Schematic representation of U and U_C versus E if the IMPUR routine is called four times to determine the densities of Ti, Cr, Fe and Ni. The dashed line represents the continuum component U_C.

22. METAL SUBROUTINE

The METAL subroutine calculates for a given temperature the contribution of the metals Ti, Cr, Fe and Ni to the ζ factor (eq. 7.8). According to Sec. 5, Fig. 4, we have two clean energy windows in which R_{fb} can assume various values. These values were calculated for iron in eq. (9.7). We repeat eq.(9.7) here in the form

$$RFE1 = 5700\ T_e^{2.5} / (1.+T_e^{3.88})$$ for energy window 1 $2. < E < 4.$ keV

$$RFE2 = 5800\ T_e^{2.5} / (1.+ T_e^{2.9})$$ for energy window 2 $E > 10.$keV

For the other metals there are no curves like those in Fig. 9 for the partial densities of the individual ionization stages. Calculation is therefore not yet possible; the same values are taken for Ti, Cr, and Ni as for Fe.

The second part of the routine is concerned with the contributions of the individual metals. For example, according to eq. (7.8)

$$ZFE1 = \frac{n_i}{n_e}\left[Z_{iff}^2\ g_{ff}^{(i)} + R_{fb}^{(i)}\right] \qquad (22.2)$$

$$= P26(J)\left[600. + RFE1\right] \qquad (22.3)$$

is the contribution of iron to the ζ factor in the energy window 1. Here we have roughly estimated

$$Z_{iff}^2\ g_{ff}^{(i)} \approx 600. \qquad (22.4)$$

which according to Fig. 9 is probably best satisfied at 3 keV. The contributions of the other metals were similarly estimated.

The partial densities (e.g. P26) were calculated in the IMPUR routine before calling the METAL routine.

23. SESNIC SUBROUTINE

The SESNIC subroutine determines the plasma parameters from the spectral function U; see beginning of Sec. 12. The spectral function U(L,J) is obtained at the reference mesh points

$$E9(J) = DE9 + EO9$$

from Sec. 14, eq. (14.1). From it we obtain the smoothed ULG = ln U at the centres EID(M) of the smoothing intervals by calling the GLATT routine . By calling the ALPBET routine we then get the plasma parameters AL1 ... BE3, the meanings of which are shown in Sec. 12, Fig. 14. The DO-3 loop contains a temperature definition

$$T_e = - 1/BE3 \ , \qquad \text{ISN 0016}$$

which we use because it is calculated from all available energy mesh points. It is not clear, however, whether this is the best temperature definition; perhaps only energy window 1 should be enlisted, i.e. $T_e = -1/BE1$ should be used, if, for example, BE2 is distorted by any effects (e.g. runaway electrons).

After the DO-3 loop the IMPUR routine determines the density of the metal ions Ti, Cr, Fe, Ni. For this purpose we require the electron density, which is stored therefore in COMMON /IMP/. The DO-6 loop now following is essentially for calculating the density of the oxygen ions. At the beginning the temperature TEMP is somewhat differently defined than in the DO-3 loop.

Furthermore we have

according to eq. (7.6) $SH = 3 \times 10^{11}\ n_e^2 / \ T_e$ ISN 0036

and according to eq. (7.5) $Z_1 = \exp(\alpha_1)/SH$ ISN 0037

and, similarly, for window 2 $Z_2 = \exp(\alpha_2)/SH$ ISN 0038

Z1 is the ζ factor in the energy window 1;

Z2 is the ζ factor in the energy window 2.

The METAL routine then yields the contribution of the metals Ti, Cr, Fe, Ni to the ζ factor. As was shown in Sec. 9 for the example of Fe, the ζ factor in the energy window 1 is smaller than in energy window 2. The METAL routine therefore yields

ZME1 = metal contribution to the ζ factor in the energy window 1

and ZME2 = metal contribution to the ζ factor in the energy window 2.

While ZME may be about 5 to 10 for 1 to 2 o/oo Fe, the contribution of hydrogen to the ζ factor is equal to the Gaunt factor and is of the order 0.5. The Gaunt factor depends on x (see eq. (7.10)); but we do not deal with this here. For each energy window we calculate with a mean x: for energy window 1 we set x_1 = 3/TEMP because E = 3 keV is about the centre of energy window 1. Ignoring the x dependence of the Gaunt factor can distort the temperature by up to 10 %. Furthermore,

Z81 is the contribution of oxygen to the ζ factor in energy window 1

and Z82 is the contribution of oxygen to the ζ factor in energy window 2.

RO is the recombination term according to Sec. 10 (ISN 0052). Strictly speaking, the statements for Z81 and Z82 should include the Gaunt factor for the hydrogen multiplied by the (unknown) partial density of the hydrogen. This has been neglected for convenience because either there are no impurities present and the partial density is then 1, or there are impurities and the error in determining ζ is mostly larger than the Gaunt factor g_H itself.

R_1 in ISN 0025 is the partial density of the hydrogen without taking oxygen into account. Here we have rather arbitrarily set the ion charge number of the metal ions equal to the nucleus charge number - 2; this means that the metal ions are predominantly in a helium-like state.

We now conclude by considering the accuracy of the data and parameters calculated in SESNIC and elsewhere. α and ß are reliable to a certain extent, i.e. AL1 ... BE3; the error for data with mean noise level is in T_e a few % and in S approximately 20 % or 10 %.

The metal ions are determined from the line integrals; the inaccuracy of these is, say, 20 %. Furthermore, $\langle\sigma v\rangle$ from Sec. 11 appears in the calculation; $\langle\sigma v\rangle$ is inaccurate by a factor of about 2 (see Fig. 13). Consequently, the metal ion density is only known to within a factor of 2. With 1 to 2 o/oo metal the metal component ZME of the ζ factor is of the order of 5 to 10 according to Sec. 9, i.e. much larger than the hydrogen component. It may now very well be that the ζ factor calculated from α according to $\zeta = \exp(\alpha)/SH$ is smaller than ZME. This is because so little is known about the constants in $\langle \sigma v \rangle$ and also in the METAL routine. Since α and ß are reliable to a certain extent, and at least the order of magnitude of n_i is known - if i = 22, 24, 26, 28 - no faith should be put in the oxygen calculation performed in this section until the constants in Secs. 11 and 22 are known exactly and reliably to within a few %.

AKNOWLEDGEMENTS

The author wishes to thank D.Düchs, S.v.Goeler and S.Sesnic for helpful discussions.

REFERENCES

/1/ S. v.GOELER, Nucl.Fus. 15 (1975), p. 301 ff.

/2/ D. DÜCHS et al., Nucl.Fus. 17, 3 (1977), p. 579, Fig. 4
p. 581, Fig. 6

/3/ F. POHL, IPP 6/173 (1978)

/4/ S. v.GOELER, Varenna Como (Italy); Course on Diagnostics for Fusion Experiments, 4.-16. Sept. 1978, Soft X-ray Measurements.

```
             C TOKOMAK X-RAYS , SEGMENT  M A I N P R
ISN 0002           REAL*4   NE
ISN 0003           DIMENSION   EL(12) , ER(12)
ISN 0004           COMMON  EID(47), GEW(5,12), P(6), PLOG(47), U(5,301), ULG(5,12)
                  1     ,  DE9, E09, JMAX9, LM1, LMA, M1, MS
ISN 0005           COMMON /GLA/  JL(12), JR(12)
ISN 0006           COMMON /OVL/  T(20), DTN, IMAX
ISN 0007           COMMON /IMP/   NE(5) , TE(5)
ISN 0008        10 PRINT 98
ISN 0009           PRINT 90
ISN 0010           PRINT 91
ISN 0011           READ  710,  IMAX, LMA, M1, MS, NABEL, NGLA, NMAX, DE9, E09
ISN 0012           PRINT 709,  IMAX, LMA, M1, MS, NABEL, NGLA, NMAX, DE9, E09
ISN 0013           PRINT 94
ISN 0014           READ  112,   ( T(N), N=1,NMAX)
ISN 0015           PRINT 110,   ( T(N), N=1,NMAX)
ISN 0016           PRINT 93
ISN 0017           READ  112,   ( EL(M), ER(M), M=1,MS)
ISN 0018           PRINT 110,   ( EL(M), ER(M), M=1,MS)
ISN 0019           DO 2      M=1,MS
ISN 0020               JL(M) = (EL(M) -E09) / DE9  +  1
ISN 0021               JR(M) = (ER(M) -E09) / DE9
ISN 0022         2    EID(M) = 0.5* DE9*( JL(M) + JR(M)) + E09
ISN 0023               JMAX9 = JR(MS)
ISN 0024           PRINT 89
ISN 0025           PRINT 92
ISN 0026                          LM1 = LMA - 1
ISN 0027           DO 3      L=1,LM1
ISN 0028           PRINT 100,   L
ISN 0029           DO 3       I=1,IMAX
ISN 0030           CALL BLENDE ( I , L )
ISN 0031         3 CONTINUE
ISN 0032           DO 6       N=2,NMAX
ISN 0033           PRINT 202,    N, T(N-1) , T(N)
ISN 0034                  DTN = T(N) - T(N-1)
ISN 0035           PRINT 99
ISN 0036           READ  112,  ( NE(L), L=1,LM1)
ISN 0037           PRINT 110,  ( NE(L), L=1,LM1)
ISN 0038           PRINT 95
ISN 0039           READ  112,    ( P(L), L=1,LMA)
ISN 0040           PRINT 112,    ( P(L), L=1,LMA)
ISN 0041           DO 4      L=1,LM1
ISN 0042              PLOG(L) = ALOG( 1.- ( P(L)/P(LMA))**2)
ISN 0043         4 CALL OVLAP ( L , N )
ISN 0044           CALL SESNIC ( NGLA , NABEL )
ISN 0045         6 CONTINUE
ISN 0046           GO TO 10
ISN 0047        89 FORMAT(/33H   FILTER- UND BLENDEN-PARAMETER:)
ISN 0048        90 FORMAT(/32H === H A U P T P R O G R A M ===)
ISN 0049        91 FORMAT(/70H    IMAX     LMA      M1       MS     NGLA    NABEL    NMAX
                  1    DE9      E09)
ISN 0050        92 FORMAT(/113H           I      L    JMA       A        B         D        D
                  1E       E0       X1      X2      R1       R2       R3       DSOO)
ISN 0051        93 FORMAT(/76H    EL     M=1 ER          EL     M=2 ER          EL     M=3 E
                  1R        EL    M=4  ER)
ISN 0052        94 FORMAT(/6H     T)
ISN 0053        95 FORMAT(/6H     PH)
ISN 0054        98 FORMAT (1H1)
ISN 0055        99 FORMAT(/38H    NE     ELECTRON DENSITY 10**13 CM-3)
ISN 0056       100 FORMAT ( 100X , 10H          L=,I1)
ISN 0057       110 FORMAT ( F6.1 , 10F10.1)
ISN 0058       112 FORMAT ( 12F6.1)
ISN 0059       202 FORMAT(/16H       TIME     N=,I2,12H      T(N-1)=,1PE9.2
                  1                               ,12H        T(N)=,1PE9.2)
ISN 0060       709 FORMAT ( 7I8 ,  5F8.2)
ISN 0061       710 FORMAT ( 7I4 ,  5F4.1)
ISN 0062           END
```

```
ISN 0002          SUBROUTINE BLENDE ( I , L )
ISN 0003          COMMON /BLE/  DE(3,5) ,E0(3,5) , U0(3,5,301), JMAX(3,5)
ISN 0004          COMMON /OVL/  T(20), DTN, IMAX
ISN 0005          READ 213,  JMAX(I,L), A,B,D, DE(I,L), E0(I,L), X1, X2, R1, R2, R3
            C
            C X1 = ABSTAND DER BLENDE 1 VOM DETEKTOR ; DAHER  X2 << X1
            C
ISN 0006              S1 = 3.1416 * R1**2
ISN 0007              S2 = 3.1416 * R2**2
ISN 0008              S3 = 3.1416 * R3**2
ISN 0009              R4 = X1* (R2 -R1)/(X1 -X2)  +  R1
ISN 0010              R5 = X1* (R2 +R1)/(X1 -X2)  -  R1
ISN 0011              D2 = (X1 -X2)**2
ISN 0012          IF ( R3. LE. R4)      GO TO 34
ISN 0014          IF ( R3. GE. R5)      GO TO 35
ISN 0016              SD = S3/X1**2 *(R5-R3)/(R5-R4) + S2/D2 *(R3-R4)/(R5-R4)
ISN 0017          GO TO 1
ISN 0018       34     SD = S3/X1**2
ISN 0019          GO TO 1
ISN 0020       35     SD = S2/D2
ISN 0021        1                                    DSDO = S1 * SD
ISN 0022                 JMA = JMAX(I,L)
ISN 0023          DO 5      JI=1,JMA
ISN 0024          U0(I,L,JI) = 0.
ISN 0025                 EN = JI * DE(I,L) + E0(I,L)
ISN 0026          IF ( EN. LE. 0.1)         GO TO 5
ISN 0028              FILTER = D*A / EN**B
ISN 0029          IF (FILTER. GE. 13.)      GO TO 5
ISN 0031          U0(I,L,JI) = 12.5664 * EN *EXP(FILTER) / (DE(I,L) * DSDO)
ISN 0032        5 CONTINUE
ISN 0033          PRINT 310, I,L,JMA, A,B,D, DE(I,L),E0(I,L), X1,X2, R1,R2,R3, DSDO
ISN 0034          RETURN
ISN 0035      310 FORMAT ( I12,2I6, 2F8.3, 5F8.2, 3F8.3, 1P2E10.2)
ISN 0036      213 FORMAT ( I4 , 11F6.3)
ISN 0037          END
```

```
ISN 0002          SUBROUTINE SORTIR ( Q, M, LMA)
ISN 0003          DIMENSION   Q(6), M(6)
ISN 0004                 LM1 = LMA - 1
ISN 0005          DO 2       L=1,LMA
ISN 0006        2        M(L) = L
ISN 0007          DO 4       L=1,LM1
ISN 0008                   I = L
ISN 0009          DO 3       K=L,LMA
ISN 0010                 MK = M(K)
ISN 0011                 MI = M(I)
ISN 0012          IF ( Q(MK). LT. Q(MI))        I=K
ISN 0014        3 CONTINUE
ISN 0015                 ML = M(L)
ISN 0016               M(L) = M(I)
ISN 0017               M(I) = ML
ISN 0018        4 CONTINUE
ISN 0019          RETURN
ISN 0020          END
```

```
ISN 0002          SUBROUTINE CVLAP ( L , N )
ISN 0003          INTEGER*2      R(3,256) , R1J , R2J , R3J
ISN 0004          REAL*4      NWNG
ISN 0005          DIMENSION            UB(3,256)
ISN 0006          COMMON  EID(47), GEW(5,12), P(6), PLOG(47), U(5,301), ULG(5,12)
                1      ,  DE9, E09, JMAX9, LM1, LMA, M1, MS
ISN 0007          COMMON /BLE/  DE(3,5) ,E0(3,5) , U0(3,5,301), JMAX(3,5)
ISN 0008          COMMON /GLA/  JL(12), JR(12)
ISN 0009          COMMON /OVL/  T(20), DTN, IMAX
ISN 0010             JWRITE = 6
ISN 0011          DO 5        I=1,IMAX
ISN 0012                JMA = JMAX(I,L)
ISN 0013          READ 130,   ( R(I,J) , J=1,JMA)
ISN 0014               NWNG = 1.
ISN 0015          DO 5        J=1,JMA
ISN 0016        5   UB(I,J) = U0(I,L,J) * R(I,J) * NWNG / DTN
ISN 0017          DO 7        J=1,JMAX9
ISN 0018                  E9 = DE9 *J + E09
ISN 0019                  SQ = 0.
ISN 0020                  SR = 0.
ISN 0021                  SU = 0.
ISN 0022          DO 6        I=1,IMAX
ISN 0023                 E0I = E0(I,L)
ISN 0024                 DEI = DE(I,L)
ISN 0025                  JI = (E9 - E0I) / DEI
ISN 0026                 JMA = JMAX(I,L)
ISN 0027                 JM1 = JMA - 1
ISN 0028          IF ( JI. GE. JM1)                              GO TO 6
ISN 0030          IF ( JI. LE. 0)                                GO TO 6
ISN 0032          IF ( R(I,JI). LE. 0. AND. R(I,JI+1). LE. 0.)    GO TO 6
ISN 0034                  EI = DEI *JI + E0I
ISN 0035                  VR = (E9 -EI) / DEI
ISN 0036                  VL = 1. - VR
ISN 0037                 RI =              R(I,JI) *VL +  R(I,JI+1) *VR
ISN 0038                  SU = SU + RI* (UB(I,JI) *VL + UB(I,JI+1) *VR)
ISN 0039                  SR = SR + RI
ISN 0040                  SQ = SQ + RI**2
ISN 0041          IF (JWRITE. LE. 7)  GO TO 6
ISN 0043          IF ( L. NE. 1)      GO TO 6
ISN 0045          IF ( N. NE. 2)      GO TO 6
ISN 0047          IF ( J. GE. 8)      GO TO 6
ISN 0049          PRINT 90
ISN 0050          PRINT 81
ISN 0051          PRINT 712,   I, J, JI, L, R(I,JI), R(I,JI+1), DEI, DE9, E0I, E09
                1     ,RI, SQ, SR, VL, VR, SU, UB(I,JI), UB(I,JI+1)
ISN 0052       81 FORMAT(/127H           I  J JI  L  R          DEI      DE9      E0I
                1 E09       RI        SQ        SR        VL        VR        SU  UB(I,JI)
                2   JI+1)
ISN 0053      712 FORMAT ( I10, 5I3, F10.2, 8F8.2, 1P3E10.3)
ISN 0054        6 CONTINUE
ISN 0055             U(L,J) = 0.
ISN 0056          IF ( SR. LE. 0.)      GO TO 7
ISN 0058          IF ( SU. LE. 0.)      GO TO 7
ISN 0060                  RL = SQ / SR
ISN 0061          IF ( RL. LE. 0.1)      GC TO 7
ISN 0063             U(L,J) = SU / SR
ISN 0064        7 CONTINUE
            C PRINT
ISN 0065          IF ( JWRITE. LE. 5)       GO TO 80
ISN 0067          PRINT 101,    N ,L
ISN 0068          PRINT 91
ISN 0069          DO 79         J=1,JMAX9
ISN 0070                 R1J = 0.
ISN 0071                 R2J = 0
ISN 0072                 R3J = 0
ISN 0073                UB1J = 0.
ISN 0074                UB2J = 0.
ISN 0075                UB3J = 0.
ISN 0076                  E1 = DE(1,L) *J   +  E0(1,L)
ISN 0077                  E2 = DE(2,L) *J   +  E0(2,L)
ISN 0078                  E3 = DE(3,L) *J   +  E0(3,L)
ISN 0079                  E9 = DE9      *J   +  E09
ISN 0080          IF ( J. GT. JMAX(1,L))       GO TO 71
ISN 0082                 R1J = R(1,J)
ISN 0083                UB1J = UB(1,J)
ISN 0084       71 IF ( J. GT. JMAX(2,L))       GO TO 72
ISN 0086                 R2J = R(2,J)
ISN 0087                UB2J = UB(2,J)
ISN 0088       72 IF ( J. GT. JMAX(3,L))       GO TO 79
ISN 0090                 R3J = R(3,J)
ISN 0091                UB3J = UB(3,J)
ISN 0092       79 PRINT 606,  N,J, R1J, E1, UB1J, R2J, E2, UB2J, R3J, E3, UB3J, E9
                1             , U(L,J)
ISN 0093       90 FORMAT(/15H === O V L A P/)
ISN 0094       91 FORMAT(/122H        N         J      R(1,J)      E1   UB(1,J)    R(
                12,J)       E2   UB(2,J)     R(3,J)       E3   UB(3,J)       E9     U(J,
                2N))
ISN 0095      101 FORMAT(/21H == O V L A P ==    N=,I2, 4H  L=,I1)
ISN 0096      130 FORMAT ( 24I3)
ISN 0097      606 FORMAT ( 3I10 , F8.2 , 1PE10.2 , I10 , 0PF8.2 , 1PE10.2
                1     ,     I10,0PF8.2 , 1PE10.2 ,        0PF8.2 , 1PE10.2)
ISN 0098       80 RETURN
ISN 0099          END
```

```
ISN 0002          SUBROUTINE SESNIC ( NGLA , NABEL )
ISN 0003          REAL*4   N1, N8, N22, N24, N26, N28, NE
ISN 0004          DIMENSION  E(47), G(47), V(47), ZME1(5), ZME2(5)
ISN 0005          COMMON  EID(47), GEW(5,12), P(6), PLOG(47), U(5,301), ULG(5,12)
                 1     ,  DE9, E09, JMAX9, LM1, LMA, M1, MS
ISN 0006          COMMON /SES/  AL1(5), BE1(5), N1(5) , N24(5), S1(5), T1(5), Z1(5)
                 1           , AL2(5), BE2(5), N8(5) , N26(5), S2(5), T2(5), Z2(5)
                 2           , AL3(5), BE3(5), N22(5), N28(5), S3(5), T3(5)
                 3                             , D1(5) , D8(5)
ISN 0007          COMMON /MET/   P1(5), P8(5), P22(5), P24(5), P26(5), P28(5)
ISN 0008          COMMON /IMP/   NE(5) , TE(5)
ISN 0009          DO 1      L=1,LM1
ISN 0010        1 CALL GLATT ( L , NGLA )
ISN 0011                                                M2 = M1 + 1
ISN 0012          CALL ALPBET( AL1 , BE1 , 1 , M1 , NABEL)
ISN 0013          CALL ALPBET( AL2 , BE2 , M2, MS , NABEL)
ISN 0014          CALL ALPBET( AL3 , BE3 , 1 , MS , NABEL)
ISN 0015          DO 3       L=1,LM1
ISN 0016               TE(L) = - 1./ BE3(L)
ISN 0017        3 CONTINUE
ISN 0018          CALL IMPUR ( 4.5 , N22 , P22 , 22. , NABEL)
ISN 0019          CALL IMPUR ( 5.5 , N24 , P24 , 24. , NABEL)
ISN 0020          CALL IMPUR ( 6.5 , N26 , P26 , 26. , NABEL)
ISN 0021          CALL IMPUR ( 7.5 , N28 , P28 , 28. , NABEL)
ISN 0022          DO 6       L=1,LM1
ISN 0023               Z1(L) = - 11.
ISN 0024               Z2(L) = - 22.
ISN 0025                  R1 = 1.- 20.*P22(L) - 22.*P24(L) - 24.*P26(L) - 26.*P28(L)
ISN 0026               P8(L) = 0.
ISN 0027               D8(L) = 0.
ISN 0028               N8(L) = 0.
ISN 0029               P1(L) = R1
ISN 0030          IF ( BE1(L). GE. -0.001)       GO TO 5
ISN 0032                TEMP = - 1. / BE1(L)
ISN 0033          IF ( BE2(L). GE. -0.001)       GO TO 4
ISN 0035                TEMP = - 2. / ( BE1(L) + BE2(L))
ISN 0036        4          SH = 3.03E+11 * NE(L)**2 / SQRT( TEMP)
ISN 0037               Z1(L) = EXP( AL1(L)) / SH
ISN 0038               Z2(L) = EXP( AL2(L)) / SH
ISN 0039          CALL METAL ( TEMP , ZME1(L), ZME2(L), L )
ISN 0040                  X1 = 3. / TEMP
ISN 0041                  X2 =11. / TEMP
ISN 0042                 GH1 = 1.2  * (0.5 + X1)**(-0.45) * TEMP**(-0.07 -0.01* X1)
ISN 0043                 GH2 = 1.2  * (0.5 + X2)**(-0.45) * TEMP**(-0.07 -0.01* X2)
ISN 0044                 Z81 = Z1(L) - ZME1(L) - GH1
ISN 0045                 Z82 = Z2(L) - ZME2(L) - GH2
ISN 0046                 P12 = R1
ISN 0047          IF ( Z81. LE. 0.)       GO TO 5
ISN 0049          IF ( Z82. LE. 0.)       GO TO 5
ISN 0051                  X0 = 0.87 / TEMP
ISN 0052                  R0 = 128.* X0 * EXP( X0)
ISN 0053                 G01 = 1.38 * (0.5 + X1)**(-0.16  * TEMP**0.35)
ISN 0054                 G02 = 1.38 * (0.5 + X2)**(-0.16  * TEMP**0;35)
ISN 0055               P8(L) = Z81 / (64.*G01 + R0)
ISN 0056                 P82 = Z82 / (64.*G02 + R0)
ISN 0057               P1(L) = R1 - 8.*P8(L)
ISN 0058                 P12 = R1 - 8.*P82
ISN 0059               N8(L) = P8(L) * NE(L)
ISN 0060               D8(L) = P82   * NE(L)
ISN 0061        5      N1(L) = P1(L) * NE(L)
ISN 0062               D1(L) = P12   * NE(L)
ISN 0063        6      TE(L) = TEMP
               C PRINT
ISN 0064          PRINT 98
ISN 0065          PRINT 90
ISN 0066          PRINT 83
ISN 0067          PRINT 113,    ( P(L) , L=1,LMA)
ISN 0068          PRINT 84
ISN 0069          PRINT 113,    (TE(L) , L=1,LM1)
ISN 0070          PRINT 85
ISN 0071          PRINT 113,    (NE(L) , L=1,LM1)
ISN 0072          PRINT 87
ISN 0073          PRINT 901,    ( N1(L), L=1,LM1)
ISN 0074          PRINT 901,    ( D1(L), L=1,LM1)
ISN 0075          PRINT 908,    ( N8(L), L=1,LM1)
ISN 0076          PRINT 908,    ( D8(L), L=1,LM1)
ISN 0077          PRINT 908,    ( D8(L), L=1,LM1)
ISN 0078          PRINT 922,    (N22(L), L=1,LM1)
ISN 0079          PRINT 924,    (N24(L), L=1,LM1)
ISN 0080          PRINT 926,    (N26(L), L=1,LM1)
ISN 0081          PRINT 928,    (N28(L), L=1,LM1)
ISN 0082          PRINT 89
ISN 0083          DO 11       M=1,MS
ISN 0084       11 PRINT 110,      EID(M), ( ULG(L,M) , L=1,LM1)
```

```
ISN 0085          PRINT 91
ISN 0086          PRINT 113,   (AL1(L), L=1,LM1)
ISN 0087          PRINT 113,   (AL2(L), L=1,LM1)
ISN 0088          PRINT 113,   (AL3(L), L=1,LM1)
ISN 0089          PRINT 92
ISN 0090          PRINT 113,   (BE1(L), L=1,LM1)
ISN 0091          PRINT 113,   (BE2(L), L=1,LM1)
ISN 0092          PRINT 113,   (BE3(L), L=1,LM1)
ISN 0093          PRINT 93
ISN 0094          PRINT 113,   ( Z1(L), L=1,LM1)
ISN 0095          PRINT 113,   ( Z2(L), L=1,LM1)
ISN 0096          PRINT 94
ISN 0097          PRINT 113,   (ZME1(L), L=1,LM1)
ISN 0098          PRINT 113,   (ZME2(L), L=1,LM1)
ISN 0099          RETURN
ISN 0100       83 FORMAT(/50H                    P    POSITIONS                    )
ISN 0101       84 FORMAT(/50H                    TE   ELECTRON TEMPERATURE         )
ISN 0102       85 FORMAT(/50H                    NE   ELECTRON DENSITY             )
ISN 0103       87 FORMAT(/50H                    NI   ION DENSITIES  (10**13 CM-3))
ISN 0104       89 FORMAT(/38H           EID         ULG              )
ISN 0105       90 FORMAT(/18H ===== S E S N I C)
ISN 0106       91 FORMAT(/42H                    AL                    )
ISN 0107       92 FORMAT(/42H                    BE                    )
ISN 0108       93 FORMAT(/42H                    Z   ZETA-FACTOR       )
ISN 0109       94 FORMAT(/50H                    ZME  ZETA-FACTOR, METAL PART      )
ISN 0110       98 FORMAT( 1H1)
ISN 0111      110 FORMAT( 12F10.3)
ISN 0112      113 FORMAT( F20.3 , 10F10.3)
ISN 0113      901 FORMAT( 10H         1 ,10F10.3)
ISN 0114      908 FORMAT( 10H         8 ,10F10.3)
ISN 0115      922 FORMAT( 10H        22 ,10F10.3)
ISN 0116      924 FORMAT( 10H        24 ,10F10.3)
ISN 0117      926 FORMAT( 10H        26 ,10F10.3)
ISN 0118      928 FORMAT( 10H        28 ,10F10.3)
ISN 0119          END
```

```
ISN 0002          SUBROUTINE METAL ( TEMP, ZME1, ZME2, L)
ISN 0003          COMMON /MET/   P1(5), P8(5), P22(5), P24(5), P26(5), P28(5)
ISN 0004                RTI1 = 5700. * TEMP**2.5 / (1. + TEMP**3.88)
ISN 0005                RTI2 = 5800. * TEMP**2.5 / (1. + TEMP**2.9 )
ISN 0006                RCR1 = 5700. * TEMP**2.5 / (1. + TEMP**3.88)
ISN 0007                RCR2 = 5800. * TEMP**2.5 / (1. + TEMP**2.9 )
ISN 0008                RFE1 = 5700. * TEMP**2.5 / (1. + TEMP**3.88)
ISN 0009                RFE2 = 5800. * TEMP**2.5 / (1. + TEMP**2.9 )
ISN 0010                RNI1 = 5700. * TEMP**2.5 / (1. + TEMP**3.88)
ISN 0011                RNI2 = 5800. * TEMP**2.5 / (1. + TEMP**2.9 )
ISN 0012                ZTI1 = P22(L)  * (500. + RTI1)
ISN 0013                ZTI2 = P22(L)  * (500. + RTI2)
ISN 0014                ZCR1 = P24(L)  * (550. + RCR1)
ISN 0015                ZCR2 = P24(L)  * (550. + RCR2)
ISN 0016                ZFE1 = P26(L)  * (600. + RFE1)
ISN 0017                ZFE2 = P26(L)  * (600. + RFE2)
ISN 0018                ZNI1 = P28(L)  * (620. + RNI1)
ISN 0019                ZNI2 = P28(L)  * (620. + RNI2)
ISN 0020                ZME1 = ZTI1 + ZCR1 + ZFE1 + ZNI1
ISN 0021                ZME2 = ZTI2 + ZCR2 + ZFE2 + ZNI2
ISN 0022          RETURN
ISN 0023          END
```

```
ISN 0002          SUBROUTINE LSTSC ( AL, BE, E, G, V, JMA)
ISN 0003          DIMENSION     E(47) , G(47) , V(47)
ISN 0004                 A11 = 0.
ISN 0005                 A12 = 0.
ISN 0006                 A22 = 0.
ISN 0007                  B1 = 0.
ISN 0008                  B2 = 0.
ISN 0009          DO 4      J=1,JMA
ISN 0010          IF ( G(J). LE. 0.001)     GO TO 4
ISN 0012          IF ( V(J). LE. -700.)     GO TO 4
ISN 0014                 A11 = A11 + G(J)
ISN 0015                 A12 = A12 + G(J) * E(J)
ISN 0016                 A22 = A22 + G(J) * E(J)**2
ISN 0017                  B1 = B1  + G(J) * V(J)
ISN 0018                  B2 = B2  + G(J) * V(J) * E(J)
ISN 0019        4 CONTINUE
ISN 0020                   D = A11 *A22 - A12**2
ISN 0021          IF ( ABS(D). LT. 1.E-6)      GO TO 7
ISN 0023                  BE = (B2 *A11 - B1*A12) / D
ISN 0024                  AL = (B1 *A22 - B2*A12) / D
ISN 0025          RETURN
ISN 0026        7         AL = - 444.
ISN 0027                  BE =   222.
ISN 0028          RETURN
ISN 0029          END
```

```
ISN 0002          SUBROUTINE ALPBET ( AL, BE, ML, MR, NABEL)
ISN 0003          DIMENSION  AL(5), BE(5), D(6), E(47), F(6), FID(5,12),G(47), V(47)
ISN 0004          COMMON  EID(47), GEW(5,12), P(6), PLOG(47), U(5,301), ULG(5,12)
                 1     , DE9, EO9, JMAX9, LM1, LMA, M1, MS
ISN 0005          COMMON /ITE/  ALP(5), BET(5), C, H
ISN 0006          COMMON /ALB/  FP(5,12), UP(5,12)
ISN 0007             JWRITE = 0
ISN 0008          IF (JWRITE. LE. 1)      GO TO 2
ISN 0010          PRINT 90
ISN 0011          PRINT 89
ISN 0012          DO 1        M=ML,MR
ISN 0013        1 PRINT 113,      EID(M), ( ULG(L,M) , L=1,LM1)
ISN 0014        2 DO 3        L=1,LM1
ISN 0015          DO 3        M=ML,MR
ISN 0016             FP(L,M) = 0.
ISN 0017        3    UP(L,M) = 0.
ISN 0018          IF (NABEL. GE. 3)      GO TO 7
ISN 0020          CALL ITERAT ( ML , MR )
ISN 0021          IF ( JWRITE. LE. 1)      GO TO 5
ISN 0023          PRINT 86
ISN 0024          DO  4       M=ML,MR
ISN 0025        4 PRINT 109,    EID(M) , ( FP(L,M) , L=1,LM1)
ISN 0026        5 DO 6        L=1,LM1
ISN 0027              AL(L) = ALP(L)
ISN 0028        6     BE(L) = BET(L)
ISN 0029          IF ( NABEL. LE. 1)      RETURN
ISN 0031        7 DO 9        M=ML,MR
ISN 0032          DO 8        L=1,LM1
ISN 0033              D(L) = 0.
ISN 0034          IF ( ULG(L,M). LE. -100.)      GO TO 8
ISN 0036              D(L) = EXP(ULG(L,M)) - UP(L,M)
ISN 0037        8 CONTINUE
ISN 0038          CALL ABEL ( F, P, D, LMA, NABEL)
ISN 0039          DO 9        L=1,LM1
ISN 0040            FID(L,M) = - 712.
ISN 0041                  FD = F(L) + FP(L,M)
ISN 0042          IF (    FD. LE. 1.E-7)      GO TO 9
ISN 0044            FID(L,M) = ALOG( FD)
ISN 0045        9 CONTINUE
ISN 0046          DO 11       L=1,LM1
ISN 0047                 MC  = 0
ISN 0048                 NS = MR - ML + 1
ISN 0049          DO 10      M=ML,MR
ISN 0050                  N = M  - ML + 1
ISN 0051              E(N) = EID(M)
ISN 0052              G(N) = 0.
ISN 0053              V(N) = FID(L,M)
ISN 0054          IF ( FID(L,M). LE. -100.)      GO TO 10
ISN 0056                 MC  = MC + 1
ISN 0057              G(N) = 1.
ISN 0058       10 CONTINUE
ISN 0059              AL(L) = - 99.
ISN 0060              BE(L) = -555.
ISN 0061          IF ( MC. LE. 1)      GO TO 11
ISN 0063          CALL LSTSQ( ALPHA , BETA , E , G , V , NS)
ISN 0064              AL(L) = ALPHA
ISN 0065              BE(L) = BETA
ISN 0066       11 CONTINUE
ISN 0067          IF ( JWRITE. LE. 1)      RETURN
ISN 0069          PRINT 101,  MC
ISN 0070          PRINT 94
ISN 0071          PRINT 109,  ( AL(L), L=1,LM1)
ISN 0072          PRINT 95
ISN 0073          PRINT 109,  ( BE(L), L=1,LM1)
ISN 0074       86 FORMAT(/38H          EID         FC             )
ISN 0075       89 FORMAT(/38H          EID         ULG            )
ISN 0076       90 FORMAT(/16H === A L P B E T)
ISN 0077       94 FORMAT(/12H        ALPHA)
ISN 0078       95 FORMAT(/12H         BETA)
ISN 0079      101 FORMAT(/12H         MC =,I3)
ISN 0080      109 FORMAT(  F12.2 , 1P10E10.2)
ISN 0081      113 FORMAT( F12.2 , 11F10.2)
ISN 0082          RETURN
ISN 0083          END
```

```
ISN 0002          SUBROUTINE ABEL ( F, P, U, N, NABEL)
ISN 0003          DIMENSION  F(6), FS(6), P(6), Q(6), QS(6), U(6), US(6), MA(6)
ISN 0004          DO 1       L=1,N
ISN 0005               F(L) = 0.
ISN 0006              FS(L) = 0.
ISN 0007       1       Q(L) = P(L)**2
ISN 0008               U(N) = 0.
ISN 0009          CALL SORTIR ( Q, MA, N)
ISN 0010                 NG = 0
ISN 0011          DO 2       L=1,N
ISN 0012                  J = MA(L)
ISN 0013          IF ( ABS( U(J)). GE. 1.E-5)           NG = NG + 1
ISN 0015              US(L) = U(J)
ISN 0016       2      QS(L) = Q(J)
ISN 0017          IF ( NG. LE. 1)          RETURN
ISN 0019          DO 6       K=1,NG
ISN 0020                 SU = 0.
ISN 0021          DO 5       L=K,NG
ISN 0022          IF ( NABEL.   GE.     5)       GO TO 3
ISN 0024          IF ( US(L).   LE. 1.E-8)       GO TO 3
ISN 0026          IF ( US(L+1). LE. 1.E-8)       GO TO 3
ISN 0028          IF ( US(L).   LE. US(L+1))     GO TO 3
ISN 0030                 UL = ALCG( US(L))
ISN 0031                  C = ( UL - ALOG( US(L+1))) / (QS(L+1) - QS(L))
ISN 0032                  B =   UL  +  C* QS(L)
ISN 0033                 WE = SQRT( C)  * EXP( B - C* QS(K))
ISN 0034                 A1 = SQRT( C   * ( QS(L+1) -  QS(K)))
ISN 0035                 A2 = SCRT( C   * ( QS(L)   -  QS(K)))
ISN 0036                 DF = 0.56419 * WE * (ERFC( A2) - ERFC( A1))
ISN 0037          GO TO 5
ISN 0038       3         QL = (US(L+1) - US(L)) / (CS(L+1) - QS(L))
ISN 0039                 W2 = SQRT( QS(L)   - QS(K))
ISN 0040                 W1 = SQRT( CS(L+1) - QS(K))
ISN 0041                 DF = 0.63662 * QL * (W2 -W1)
ISN 0042       5         SU = SU + DF
ISN 0043       6      FS(K) = SU
ISN 0044          DO 7       L=1,N
ISN 0045                  J = MA(L)
ISN 0046       7       F(J) = FS(L)
ISN 0047             JWRITE = 0
ISN 0048          IF (JWRITE. LE. 1)       RETURN
ISN 0050          PRINT 111,  ( U(L), L=1,5) , ( F(L), L=1,5)
ISN 0051      111 FORMAT ( 1P11E10.2)
ISN 0052          RETURN
ISN 0053          END
```

```
ISN 0002          SUBROUTINE AZRUT ( AZ, C, H, X)
ISN 0003                 AA = C+ H*X
ISN 0004                  E = 0.5 + C.46/(1.+H) + 0.03*C
ISN 0005                 XA = 1.8 * X**E * H**2 / (1.+ 0.83*H)
ISN 0006                  Z = H / (1.+ (C+H)/XA)
ISN 0007                 AZ = 1.+ (1.+ 0.273*(AA+1.)/(AA+1.17)) *AA  +  Z
ISN 0008          RETURN
ISN 0009          END
```

```
ISN 0002        SUBROUTINE ITERAT  ( ML , MR )
ISN 0003        DIMENSION    AL(47), E(47), G(47), GE(47), TL(47), W(47)
ISN 0004        COMMON  EID(47), GEW(5,12), P(6), PLOG(47), U(5,301), ULG(5,12)
              1     ,  DE9, E09, JMAX9, LM1, LMA, M1, MS
ISN 0005        COMMON /ITE/  ALP(5), BET(5), C, H
ISN 0006        COMMON /ALB/  FP(5,12), UP(5,12)
ISN 0007                  H = 2.
ISN 0008                  C = 2.
ISN 0009                ALG = 0.693 + ALOG( P(LMA))
ISN 0010        DO 1       L=1,LM1
ISN 0011              TL(L) = - 714.
ISN 0012              AL(L) = - 714.
ISN 0013              GE(L) = 0.
ISN 0014      1      BET(L) = - 1.
ISN 0015        DO 6       IT=1,3
ISN 0016                 LC = 0
ISN 0017        DO 4       L=1,LM1
ISN 0018              GE(L) = 0.
ISN 0019                 MC = 0
ISN 0020                 NS = MR - ML + 1
ISN 0021        DO 2       M=ML,MR
ISN 0022                  N = M  - ML + 1
ISN 0023               E(N) = EID(M)
ISN 0024               W(N) = - 700.
ISN 0025               G(N) = 0.
ISN 0026        IF ( ULG(L,M). LE. -400.)       GO TO 2
ISN 0028                 MC = MC + 1
ISN 0029                  X = - EID(M) * BET(L)
ISN 0030        IF ( X. LE.  0.001)             GO TO 2
ISN 0032        CALL AZRUT ( AZ, C, H, X)
ISN 0033               G(N) = GEW(L,M)
ISN 0034              GE(L) = GE(L) + G(N)
ISN 0035               W(N) = ULG(L,M) + 0.5*( ALOG( AZ) - PLOG(L))  -  ALG
ISN 0036      2 CONTINUE
ISN 0037        IF ( MC. LE. 1)       GO TO 3
ISN 0039                 LC = LC + 1
ISN 0040        CALL LSTSQ ( ALPHA, BETA, E, G, W, NS)
ISN 0041        IF ( BETA. GE. 0.)         GO TO 3
ISN 0043              TL(L) = - ALOG( - BETA)
ISN 0044              AL(L) = ALPHA
ISN 0045             BET(L) = BETA
ISN 0046        GO TO 4
ISN 0047      3      BET(L) =  -44.44
ISN 0048              GE(L) = 0.
ISN 0049      4 CONTINUE
ISN 0050                  C = 2.
ISN 0051                  H = 2.
ISN 0052        IF ( LC. LE. 1)       GO TO 6
ISN 0054        CALL LSTSQ  ( TLOG , H , PLOG , GE, TL , LM1 )
ISN 0055        CALL LSTSQ  ( SLOG , C , PLOG , GE, AL , LM1 )
ISN 0056        IF ( H. LE. 0.)          H = 2.
ISN 0058        IF ( C. LE. 0.)          C = 2.
ISN 0060      6 CONTINUE
ISN 0061        DO 7       L=1,LM1
ISN 0062      7      ALP(L) = AL(L)
ISN 0063                 ER = 0.
ISN 0064                 SU = 0.
ISN 0065        DO 8       M=ML,MR
ISN 0066        DO 8       L=1,LM1
ISN 0067           FP(L,M) = EXP( ALP(L) + BET(L) *EID(M))
ISN 0068                  X = - EID(M) * BET(L)
ISN 0069        CALL AZRUT ( AZ, C, H, X)
ISN 0070           UP(L,M) = 2.* FP(L,M) * SQRT( (1. - (P(L)/P(LMA))**2) / AZ)
              1                  *  P(LMA)
ISN 0071        IF(UP(L,M).          LE. 1.E-5)      GO TO 8
ISN 0073        IF( ABS( ULG(L,M)). LE. 1.E-5)       GO TO 8
ISN 0075                 ER = ER +((ALOG( UP(L,M)) - ULG(L,M))/ ULG(L,M))**2
ISN 0076                 SU = SU + 1.
ISN 0077      8 CONTINUE
ISN 0078             JWRITE = 0
ISN 0079        IF ( JWRITE. LE. 1)       RETURN
ISN 0081              ERROR = - 77.
ISN 0082        IF ( SU. LE. 0)       GO TO 9
ISN 0084              ERROR = ER / SU
ISN 0085      9 PRINT 101,   ERROR
ISN 0086    101 FORMAT(/27H === I T E R A T:   ERROR =,1PE9.2)
ISN 0087        RETURN
ISN 0088        END
```

```
ISN 0002          SUBROUTINE IMPUR ( EI , NI , PI , Z , NABEL)
ISN 0003          REAL*4   K(6) , NI(5) , NE
ISN 0004          DIMENSION    PI(5)  , UK(6)
ISN 0005          COMMON  EID(47), GEW(5,12), P(6), PLOG(47), U(5,301), ULG(5,12)
                 1     ,  DE9, E09, JMAX9, LM1, LMA, M1, MS
ISN 0006          COMMON /ITE/  AL3(5) , BE3(5) , C, H
ISN 0007          COMMON /IMP/   NE(5) , TE(5)
ISN 0008                 JLI = ( EI - 0.4 - E09) / DE9
ISN 0009                 JRE = ( EI + 0.4 - E09) / DE9
ISN 0010                   N = 0.21 / DE9   + 1
ISN 0011              JWRITE = 7
ISN 0012          IF ( JWRITE. LE. 1)      GO TO 1
ISN 0014          PRINT 90
ISN 0015          PRINT 91
ISN 0016        1 DO 4      L=1,LM1
ISN 0017               NI(L) = 0.
ISN 0018               PI(L) = 0.
ISN 0019                  UL = 0.
ISN 0020                  UR = 0.
ISN 0021          DO  2      M=1,N
ISN 0022                 JLN = JLI - M + 1
ISN 0023                 JRN = JRE + N - 1
ISN 0024                  UL = UL + U(L,JLN)
ISN 0025        2         UR = UR + U(L,JRN)
ISN 0026                  UC = SQRT( UL*UR) / FLOAT( N)
ISN 0027                  SU = 0.
ISN 0028          DO 3       J=JLI,JRE
ISN 0029        3         SU = SU          + U(L,J) - UC
ISN 0030               UK(L) = SU * DE9
ISN 0031          IF ( JWRITE. LE. 1)      GO TO 4
ISN 0033                  JM = 0.5*( JLI +JRE)
ISN 0034          PRINT 310, L, JLI, JRE, JM, N,  EI, UL, UR  , UC, UK(L), U(L,JLI)
                 1                                            , U(L,JM)  , U(L,JRE)
ISN 0035        4 CONTINUE
ISN 0036          IF ( NABEL. LE. 2 )    GO TO 6
ISN 0038          CALL ABEL( K, P, UK, LMA, NABEL)
ISN 0039          GO TO 8
ISN 0040        6 DO 7       L=1,LM1
ISN 0041                   X = EI / TE(L)
ISN 0042          CALL AZRUT ( AZ, C, H, X)
ISN 0043                  P2 = 1. - ( P(L) / P(LMA))**2
ISN 0044        7       K(L) = UK(L) * SQRT( AZ / P2) / (2.* P(LMA))
ISN 0045        8 DO 9      L=1,LM1
ISN 0046          IF ( K(L). LE. 0.)           GO TO 9
ISN 0048                  XX = 0.0077 * Z**2 / TE(L)
ISN 0049                   A = 48000. * Z**(-2.5)
ISN 0050                  SV = A* EXP( - XX / (1.+ A/ XX**2))
ISN 0051               NI(L) = K(L) / (NE(L) *SV *EI)                     * 1.E-13
ISN 0052               PI(L) = NI(L) / NE(L)
ISN 0053        9 CONTINUE
ISN 0054          IF ( JWRITE. LE. 1)       RETURN
ISN 0056          PRINT 93
ISN 0057          DO 10      L=1,LM1
ISN 0058                  XX = 0.0077 * Z**2 / TE(L)
ISN 0059                   A = 48000. * Z**(-2.5)
ISN 0060                  SV = A* EXP( - XX / (1.+ A/ XX**2))
ISN 0061       10 PRINT 210,       L, TE(L), K(L), XX, A, SV, NI(L)
ISN 0062          RETURN
ISN 0063       90 FORMAT(/14H === I M P U R)
ISN 0064       91 FORMAT(/99H          L JLI JRE  JM    N      EI        UL        UR
                 1 UC        UK     U(L,JLI)    U(L,JM)  U(L,JRE))
ISN 0065       93 FORMAT(/80H          L          TE         K          XX          A
                 1   SV          NI          PI)
ISN 0066      210 FORMAT( I10, F10.2, 1P10E10.2)
ISN 0067      310 FORMAT( I9, 4I4, F7.2, 1P2E9.2, 1P6E10.2)
ISN 0068          END
```

```
      SUBROUTINE GLATT ( L , NGLA )
      COMMON  EID(47), GEW(5,12), P(6), PLOG(47), U(5,301), ULG(5,12)
     1     ,  DE9, E09, JMAX9, LM1, LMA, M1, MS
      COMMON /GLA/  JL(12), JR(12)
      IF ( NGLA. GE. 2)                    GO TO 3
      DO 2       M=1,MS
        GEW(L,M) = 0.
        ULG(L,M) = - 712.
              J8 = JL(M)
              J9 = JR(M)
          EID(M) = 0.5* DE9* (J8 + J9)  +  E09
              KM = J9 - J8 + 1
              S0 = 0.
              S1 = 0.
              SU = 0.
              E8 = DE9* (J8 -0.5) + E09
              E9 = DE9* (J9 +0.5) + E09
      DO 1       J=J8,J9
      IF ( U(L,J). LE. 1.E-7)       GO TO 1
              SU = SU + 1.
               E = DE9*J + E09
              S0 = S0 + U(L,J)
              S1 = S1 + U(L,J) * E
    1 CONTINUE
      IF ( SU. LE. 2.)            GO TO 2
               Q = S1 / S0
               C = (Q- E9) / (E8 -Q)
              C2 = C**2
               F = (C-1.)/( C- C2/SQRT( 1.- 0.8*C +C2*(8.6 -0.8*C +C2)))
              B8 = F / (Q- E8)
              Z2 = (B8*(E9 -E8))**2
            GEOM = S0 / ((J9-J8+1) *(1.+ 0.04167 *Z2 *(1.+ 0.0125 *Z2)))
        ULG(L,M) = ALOG( GEOM)
        GEW(L,M) = SU
    2 CONTINUE
      RETURN
    3 DO 9       M=1,MS
        GEW(L,M) = 0.
        ULG(L,M) = - 712.
              J8 = JL(M)
              J9 = JR(M)
          EID(M) = 0.5* DE9* (J8 + J9)  +  E09
              KM = J9 - J8 + 1
              SU = 0.
              SV = 0.
      DO 8       J=J8,J9
              UG = U(L,J)
      IF ( UG. LE. 1.E-9)       GO TO 8
              SU = SU + 1.
              SV = SV + ALOG( UG)
    8 CONTINUE
      IF ( SU. LE. 0.)       GO TO 9
        GEW(L,M) = SU
        ULG(L,M) = SV / SU   +  1.1 * ALOG( SU / FLOAT( KM))
    9 CONTINUE
      RETURN
      END
```