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SPECTRAL LINE SHAPE CODE FOR MULTIELECTRON EMITTERS

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INTRODUCTION

This report describes a computer code providing theoretical line profiles of multielectron radiators in plasmas. The line profiles are calculated for a selected spectral range, in the presence of natural broadening, doppler and stark effect. The model used for the description of stark effect assumes that the plasma and atomic structure parameters are such that the static ion microfield approximation and the model of a binary collision electronic operator are valid. Whereas an electronic collision operator can usually safely be used, neglecting ion motion requires that the width of the line is much larger than the typical fluctuation frequency of the ion microfield (ion plasma frequency). A careful check for the validity of this approximation has to be done for hot and dense plasma conditions. Breakdown of the static approximation occur especially for hydrogenic emitters . For multielectron emitters a large validity domain of the static ion approximation is usually found. In this static ion model, an average is performed over a static microfield distribution. For this quantity, the APEX model is used, which allows for calculations in the coupled plasma domain.

The code accepts atomic data from a standard atomic structure code. The atomic data selected all belong to levels associated with an allowed transition whose frequency falls in the selected spectral range. An interface with the user then offers two possibilities for the control of the calculation. The default choice, intended for the casual user, only requires the input of the ion species, the plasma conditions and a frequency range where the line shapes have to be calculated. In case too many levels should be selected for a profile calculation on a given computer, the code suggests a set of atomic levels for which the calculation is possible.

Optionally, the choice of the atomic levels retained in the calculation entirely depends on the user. Typically this option is intended for the user interested in how the structure of the line is modified by the stark effect. The effect of forbidden components or of a reduction of the number of atomic levels contributing to the line shape may then easily be studied. This reduction of the atomic system may be obtained by

selecting or rejecting one by one the levels contributing to the line shapes belonging to the selected frequency range. In the following, we present the formalism and describe the principal numerical techniques used in the code. We emphasize the description of a technique based on the diagonalization of the emitters evolution operator taken for a set of sampled ion microfields. This technique allows a drastic reduction of the computer time needed to obtain the line shape of a complex atomic structure.

I BACKGROUND THEORY AND METHOD

The starting concept of a spectral line profile calculation may be one electric dipole correlation function, proportional to something like

$$Tr\left\{\vec{d}\,.\left\langle\left[\vec{d}(t)\,,\,\rho_0\right]\right\rangle_{av}\right\} \qquad (1)$$

ρ_0 is the initial state density matrix and $<...>_{av}$ means that the emitter is submitted to a perturbation process responsible for relaxation and line-width. The trace in expression (1) is over emitter states. This hamiltonian formalism may be replaced by a liouvillian one, useful for the numerical application of the theory (see appendix I for notation and conventions). The previous trace may be written as a scalar product in the liouville space

$$Tr\{...\} \rightarrow <<\vec{d}|<U(t)>_{av}\,.\,\vec{D}|\rho_0>> \qquad (2)$$

U(t) is the liouville (or tetradic) evolution operator and $\vec{D}$ the liouville dipole operator.

The central difficulty lies in the calculation of $<U(t)>_{av}$. For stark profiles in plasmas, the basic model assumes static ions and impact electrons. Within this framework, any calculation needs several approximations in order to save computer time and provide an accurate numerical representation of the theory.

The ionic emitter is modelised by a finite quantum system and a set of atomic data. The larger is the system, the larger are the matrices involved in the scalar product (2). In consequence, the first

approximation needed is to select, in a data-base, the smallest quantum system required for a given physical problem by the frequency region and the plasmas conditions.

The next approximation concerns the choice of a phenomenological rule to represent the homogeneous line width. The corresponding damping rates, principally due to electron-impact collisions and spontaneous emission rates, are accounted for with non hermitian terms introduced in the evolution operator equation.

The third step is related to the static ionic perturbation. The interaction operator is written in the dipole approximation. It is represented with time independent terms introduced in the evolution operator equation. The required final average is calculated by mean of a weighted sum of single external electric field profiles.

The development of theory and programming follows these three basic steps. It provides a code accounting for static stark effect, able to calculate the emission profile of an arbitrary atomic structure found in a hot plasma

Background algebra

The evolution operator $U_q(t)$ has the form

$$U_q(t) = e^{-i(L_q - i\Phi)t} \qquad (3)$$

where L_q is the liouville operator of the quantum system of interest, perturbed by a static external electric field q. The diagonal elements of this operator are filled with atomic frequencies, and the non diagonal terms with the stark perturbing terms. Φ is the non-hermitian diagonal operator which includes all the phenomenological informations about electronic and natural relaxation.

The following notation, g_i, $i=1,..,n_g$ and e_j, $j=1,...,n_e$ will be used for the ground and the excited states of the selected quantum system. The distinction between radiative dipoles associated with the $\langle g_i|\vec{d}|e_j\rangle$ matrix elements and stark dipoles associated with the $\langle g_i|\vec{d}|g_j\rangle$ or $\langle e_i|\vec{d}|e_j\rangle$ terms is introduced. This distinction will be emphasized in the code description.

A first usual simplification is now introduced because, due to the no quenching approximation (no stark $\langle g_i|\vec{d}|e_j\rangle$ terms), $U_q(t)$ is block diagonal:

$$U_q(t) = \begin{bmatrix} [gg] & & & \\ & [ge] & & \\ & & [eg] & \\ & & & [ee] \end{bmatrix} \qquad (4)$$

Furthermore, with the hypothesis that $\langle e_i|\rho_0|e_i\rangle=1$ for every e_i, it can be seen that the contribution of the microfield strength q to the trace (2) is:

$$S_q(t) = \ll\vec{d}|U_q(t)|\vec{d}\gg \qquad (5)$$

where $U_q(t)$ is now restricted to the $|e.g\gg$ subspace.

The spectral intensity of the emitted radiation is proportional to the one sided fourier transform of S_q, averaged over microfield states with the density of probability w(q).

$$I(\omega) \approx \frac{1}{\pi} \mathrm{Re} \int w(q) \int_0^{\infty} e^{i\omega t} S_q(t)\, dt\, dq \qquad (6)$$

The line shape results from a competition between inhomogeneous and homogeneous broadening. Due to degeneracy removal, stark effect breaks each initial line in many stark components on which natural and electronic relaxation work like a noise filter. This may be used to replace the microfield average integral with a weighted sum of n_q terms:

$$I(\omega) = \sum_{q=1}^{n_q} W_q I_q(\omega) \qquad (7)$$

the data set W_q being chosen to optimize computer time and give an accurate representation of the theory.

At this point there are two possible ways to proceed, either perform the fourier transform and then invert the resulting matrix, or calculate

and fourier transform $e^{-i(L_q - i\Phi)t}$. The last way will be preferred because it allows to save much more computer time.

To apply this method, the basic idea is to look for the basis in which L_q-iΦ is diagonal. In such a basis, states $|k>>$ are eigen vector of L_q-iΦ with complex eigenvalue $z_k=x_k+i.y_k$. If M_q is the similarity transformation matrix, we may write the radiated intensity for the emitter population in an electric microfield strength q :

$$I_q(\omega) \approx \frac{1}{\pi} \mathrm{Re} \ll\vec{d}| M_q \int_0^{\infty} e^{i\omega t} e^{-i M_q^{-1} (L_q - i\Phi) M_q t} M_q^{-1} dt |\vec{d}\gg \qquad (8)$$

The fourier transformation of this expression is easily performed

$$I_q(\omega) \approx -\frac{1}{\pi} \mathrm{Im} \ll\vec{d}| M_q \begin{bmatrix} \frac{1}{\omega - z_1} & & \\ & \ddots & \\ & & \frac{1}{\omega - z_n} \end{bmatrix} M_q^{-1} |\vec{d}\gg \qquad (9)$$

It appears now that all the information lies in the coefficient of a sum

$$I_q(\omega) = \sum_k \frac{\beta_k(\omega - x_k) + \alpha_k y_k}{(\omega - x_k)^2 + y_k^2} \qquad (10)$$

The previous expressions for $I_q(\omega)$ shows that the coefficients can be calculated separately for each k. A complete profile will be associated with $n_q x n_g x n_e x 4$ coefficients.

A very useful approximation may be used to simplify all the previous algebra. L_q is a real and symmetric matrix which can be diagonalized more easily than L_q-iΦ. For a real symmetric matrix, an orthogonal similarity transformation M_q exists such that $L'_q=M_q{}^t L_q M_q$ is diagonal with M_q real and $M_q{}^t=M_q{}^{-1}$ (superscript t means transposed). The corresponding hypothesis requires that the homogeneous width does not prevail when the new basis is looked for. This hypothesis is generally valid in hot and dense plasmas because the inhomogeneous stark structure is in many cases more larger than the homogeneous width. However each case has to

be carefully examined. If this approximation holds, one simply rotates the relaxation operator Φ and keeps out its diagonal part

$$\Phi'_{ij} = (M_q^t \Phi M_q)_{ij} \delta_{ij}$$

(M_q real implies that Φ_{ij} is real). The scalar product becomes

$$\ll \vec{d} | M_q e^{-i(L'_q - i\Phi')t} M_q^t | \vec{d} \gg \qquad (11)$$

Without imaginary coefficients, the profile spectra is a sum of lorentzian components, each one being defined by three quantities: amplitude, frequency and width. In the code, an option will be proposed to the user between an exact diagonalization of a complex matrix, or a fast diagonalization driven by the liouvillian real symmetric part.

Background atomic physic

The profile spectra calculations need the input of atomic data, and other external plasma parameters like the temperature, the electronic density and the microfield distribution. In the following, it will be understood that the plasma conditions are consistent with the static-ion and impact-electron model.

Obviously, the atomic data must provide all the quantities required to calculate the terms involved in the scalar product, like for instance liouville and electric dipole operators, collisional and spontaneous rates.

Subset selection

The first step listed in the above paragraph, consists in selecting within a data-base, a subset of levels. In the following the hierarchy between states, levels and configurations is used, and respectively noted $|\gamma,J,M>$, $|\gamma,J>$ and $|\gamma>$.

First, the subset is selected to be relevant with a particular frequency interval $[\omega_a,\omega_b]$. All the levels associated with an allowed transition whose frequency belongs to $[\omega_a,\omega_b]$, plus all the levels linked to the previous ones by an allowed transition, must be selected. In practice, other criterions are applied in order to reduce the quantum systems to a tractable size. Further informations about this selection and the strategy chosen to overcome the difficulty arising from too large

relevant systems, will be given in chapter II. At the present a system is supposed to be selected. It consists in a subset of "ground" levels and a subset of "excited" levels. Inside both of these subset links (stark transitions) exist. The links existing between ground and excited levels are the radiative transitions.

Atomic input data and damping terms

The minimum information required to calculate the profile spectrum associated with a given system will be, for each level, a label, the energy, the quantum number J and the spontaneous-emission damping rate, and for each transition, the lower and upper label of the two connected levels and the oscillator strength.

The liouville matrix elements are filled according to

$$L = \frac{1}{h} (H \otimes I^{d} - I \otimes H^{d})$$

(superscript d means dual space operator, see appendix II)

In the relevant liouville subspace, generated with the |e,g>> basis, the matrix elements of the real symmetric operator L_q are

$$\begin{aligned} &\langle\langle e_i,g_j|L_q|e_i,g_j\rangle\rangle = \omega_{ij} \\ &\langle\langle e_i,g_j|L_q|e_i,g_k\rangle\rangle = \langle g_j|d|g_k\rangle q \\ &\langle\langle e_i,g_j|L_q|e_k,g_j\rangle\rangle = -\langle e_j|d|e_k\rangle q \end{aligned} \qquad (12)$$

where q is the local static electric field, ω_{ij} the energy of the radiative transition e_i-g_j. The electric dipole matrix elements are obtained from well known expressions (see Cowan).

In usual notations the electric dipole matrix elements is related to the reduced radial matrix element by:

$$\langle \gamma JM|\, d_\alpha|\gamma' J'M'\rangle = (-1)^{J-M} \begin{pmatrix} J & 1 & J' \\ -M & \alpha & M' \end{pmatrix} \langle \gamma J||\mathbf{P}^{(1)}||\gamma' J'\rangle \qquad (13)$$

In the 3-J symbol, $\alpha=0,\pm1$ corresponds to the three components of the electric dipole d_z , $d^{\pm}=d_x \pm d_y$ The dipole strength S and the oscillator strength f_{ij} are given by:

$$S = |\langle \gamma J || \mathbf{P}^{(1)} || \gamma J' \rangle|^2$$

and

$$f_{ij} = \frac{E_i - E_j}{3(2J'+1)} S \qquad (14)$$

In high density, high temperature plasmas, spontaneous emission may contribute to the line width because the transition probability scales as z^4 where z is the emitter charge seen from the valence electron. From upper state $|\gamma' J' M'\rangle$ to lower level $|\gamma J\rangle$ the transition probability coefficient is:

$$A = \frac{2.0261\ 10^{-6}}{2J'+1} \left(\frac{1}{\lambda}\right)^3 S \ \text{sec}^{-1} \qquad (15)$$

The total spontaneous damping rate for a given state, results from a sum over all lower levels. As already pointed out this is accounted for in the formalism with a non hermitian coefficient in the diagonal term of the liouvillian. For a $|e_i\ g_j\rangle$ state it will be

$$\omega_{ij} - i\frac{1}{2}(A_i + A_j) \qquad (16)$$

These rates are considered as external atomic inputs, i.e. they are calculated before reducing the database to a subsystem, because in small systems, the sum over lower states would give an incorrect value.

The last preliminary calculation is devoted to the electronic collisional operator. For radiative transitions the electronic damping process requires the same stark transitions and the same level set as the ion static perturbation.The $\vec{d}.\vec{d}$ operator evaluated in both lower-level set and upper-level set, is the principal ingredient used to calculate the electronic damping rate. In addition, strong collision correction terms are introduced as discussed in the appendix II.

Final average and output information

As previously seen, the microfield average will be performed by mean of a weighted sum over a small number of terms. In some cases the homogeneous width dominates and the average is useless. In the general

case, a discrete distribution is designed to fit the static distribution The discrete field strengths are picked out in order to have a nearly equal weight W_q, i.e. each field represents the same fraction of the total distribution.

Reexamining expression 9 and 10, it can be seen that

$$\frac{\beta_k(\omega-x_k)+\alpha_k y_k}{(\omega-x_k)^2+y_k^2} = -\frac{1}{\pi}\,\mathrm{Im}\sum_{ij}\vec{d}_i\,M_{q_{ik}}\frac{1}{\omega-z_k}M_{q_{kj}}^{-1}\,.\vec{d}_j \quad (17)$$

This resonance term multiplied by the weight W_q will contribute to the final line profile. The corresponding information is enclosed in the four coefficients $W_q\alpha_k$, $W_q\beta_k$, y_k and z_k The final profile then simply appears as a sum of the resonance functions over q which labels the microfield strength and k which labels the liouville space basis

$$f_q(\omega) = W_q\frac{\beta_k(\omega-x_k)+\alpha_k y_k}{(\omega-x_k)^2+y_k^2} \quad (18)$$

In the next chapter it will be seen that the whole information may be considered in some cases as redundant and may be reduced to give a smaller output file without a heavy loss of precision.

Some additional modifications may are performed on the final line profile to take account of the doppler and apparatus profiles. These effects are easily included using a convolution.

II CODE DESCRIPTION

II.1 Foreword

The code has been developed under the following constraints:

i) Computer time saving

The code has been developed and works on a microVAX II computer. Typical computer time may be a few hours for the whole n=3 to n=5 profile, for the lithium-like case. This ensures fast calculations if a super computer is employed.

ii) User-friendliness

The code and special related routines designed to help the casual user to pick out a quantum system in a huge data file, have been conceived to work interactively, with the exception of a heavy calculation program which is preferably run as a batch job.

iii) Ability to work for any multi-electron emitter and for any plasma conditions

At present, the code works with the only requirements that an atomic data-base exists and may be read, and that the external routine (apex) provides the microfield distribution. However, the reliability of the model will be carefully discussed for exotic conditions.

iv) Accurate results in the context of l.t.e., ion static approximation and electron impact collision model

The basic model is clearly defined, but, as mentioned earlier, many further approximations are needed to perform each calculation. The code is written to control each step with the ability to switch on or switch off any approximation when it is introduced. This rule has been carefully applied for static stark effect.

II.2 CODE ORGANISATION

The code is divided in three parts labeled for convenience BEGIN, STARK and PROFILE. Each module needs input files and provides output files used as input by the next step. This structure has been adopted to isolate the core calculation (module STARK). The two others modules are devoted to set, in interactive mode, all the parameters needed to perform a complete calculation, from the database to the final profile.

Before to be started, the code may require some tunings. Array dimensions must be optimized in accordance with the computer and with the emitter structure. Particularly, the maximum size of the matrices to be diagonalized may be adjusted in order to obtain a good balance between speed and precision. These parameters are enclosed in include files (extended fortran) to propagate easily any change in the whole routine package, when it is compiled.

If a new emitter is considered, the whole routine package has to be linked with one specific module capable to read the database and fill

correctly the level names list. Usually a specific reading module may work for emitters with the same atomic structure.

i) BEGIN

The task performed by begin is the preparation of the whole data needed to specify the plasma conditions and the frequency range in which the spectrum profile has to be evaluated.

The first screen appearing when BEGIN is started is a sequence of ten numbers or names, labeled with character strings, and used in BEGIN to identify each number or name. For instance the following list, included in the input file **data.txt**, may appear:

1	iotype	lilike12.dat	name of the data-base
2	atomw	12	atomic mass
3	z	4	ion charge seen from the valence electron
4	zp	0	perturber charge if different from emitter
5	dens	8.e17	electronic density
6	temp	120000	temperature
7	da	10.489	lower bound of the frequency interval (ev)
8	db	10.688	upper bound of the frequency interval
9	datout	data.out	name of the output file
10	nmc	15	number of the sampled microfields

If necessary each value and each name in column three may be changed. This is simply done by answering to questions asked by BEGIN to the user. When this step is ended the program extracts from the supplied database (**lilike12.dat** for instance) a preliminary subset of states

It is agreed that in a database there are two distinct data sets: a level set, containing at least label, energy and J for each level, and a transition set containing, for each transition, two labels for the two levels connected, and the oscillator strength .

The conditions for a state to be selected are that it is linked to an other state by a dipole transition whose energy belongs to the interval [da,db], or it is linked by a dipole transition with a state of the previous type. In fact, only the most active transitions are selected in order to obtain a relevant system. For each transition an approximate stark shift is evaluated in the reading module, with the following algorithm

$$s = \left| \Delta - \sqrt{\Delta^2 + q^2} \right|$$

where $\Delta=0.5|E_i-E_j|$ is the half energy for the transition i-j, and $q^2=(1/307.5)f_{ij}.\Delta\lambda_{ij}$ is the magnitude of the dipole perturbing term for a microfield strength fixed to 1, (f_{ij} is the oscillator strength and $\Delta\lambda_{ij}$ the wave length expressed in angström). Statistical weight and 3j symbols are not included in the evaluation of the shift. In the following set-identification modules these coefficients are ranked to keep transitions up to 1/p of the largest one, p being an adjustable parameter.

Next, the program offers the possibility to the user to drop out some further levels if necessary. To show the usefulness of this possibility an example will be given with the line shape calculation between levels with the same principal quantum number n. In this case the previous selection may keep levels and transitions connected to others n-numbers which are irrelevant taking account of the population of higher energy levels and line-intensity arguments.

The following question asked to the user, concerns the possible creation of a datafile of nmc representative coordinates of the static microfield distribution. In case of positive answer the APEX program will be run and provides both the full distribution and a sampling of it.

The BEGIN module yields three output datafiles

1-**samfld.** filled with the sampled data microfield values

2-**data.txt** the modified file

3-**miscel.** which contains the data and the names enclosed in **data.txt** and two arrays of integers used to code the selected levels and transitions. In the case of levels, the index 1 (or 2) means lower (or upper) level selected. For transitions the index 1 (or 2) means selected stark (or radiative) transition.

ii) STARK

samfld., **miscel.** and **lilike12.dat** (more generally the character string enclosed in iotype) are the three input datafiles needed by to run STARK

The first task carried out by STARK (after reading the three datafiles and calculating the spontaneous emission rates) is the set selection according to the index arrays inclosed in **miscel.** If the system size is consistent with the tunable parameters mentioned in the above introduction, the execution of module STARK will continue. In the

opposite case the program cuts down the too large systems and defines a radiative subsystem for each radiative transition. In this case, some radiative transitions belonging to the preliminary set may are re-affected to become stark transition. This is specially useful when radiative transitions between two levels with the same principal quantum number are considered. In this case the no quenching approximation is always preserved because the only link between upper and lower state is the radiative transition used to build a subsystem.

In any case, a quantum system is associated with the following data arrays :

levels: level-name /parity /**energy** /principal quantum-number /**spontaneous emission-rate** /J-quantum number /**statistical weight**

transitions: **lower-level label /upper-level label /oscillator strength**/wave length.

where the basic arrays are written with bold characters, and the others are used to facilitate the atomic physic manipulations.

These atomic physic data are all that is needed to prepare the diagonalization module and execute a profile calculation. The tasks listed below prepare the filling of the matrix to be diagonalized

1- state counting
2- evaluation of the electric dipole matrix elements
3- collisional electronic operator calculation
4- evaluation of the hamiltonian diagonal terms

The core calculation is then executed and provides the necessary informations for the profiles. As mentioned in the previous chapter, two options are proposed, either an exact diagonalization of the complex evolution matrix or an approximate evaluation based on the diagonalization of the real symmetric part alone. For each microfield strength the routines (**sfawc** or **sfawr**) fills in an array with $4 \times ng \times ne$ data corresponding to the frequency, amplitude (real and imaginary parts) and width. This information may be either fully written in an output data-file or reduced in order to provide more tractable outputs. In this later case, an adjustable parameter is used to cut the frequency interval into a grid. Then, if two resonances belong to the same box, their amplitudes a_i (proportional to the area under each lorentzian) are added and the widths w_i summed according to

$$w = \frac{a_1 x w_1 + a_2 x w_2}{a_1 + a_2}$$

This process may cause some inaccuracy and must be controlled. Finally STARK outputs the compressed (or not) information in a datafile with the name fixed in the program BEGIN.

iii) PROFILE

The task devoted to PROFILE is simply to transform the information about the frequency, amplitude and width into the coordinates of a profile function ready to be drawn.

The program is designed to choose interactively the following options:

1- enter names of the input and output files

2- choose output data in eV or in angström

3- use doppler convolution

4- define new bounds for the frequency range

5- enter the apparatus-function widths for a lorentzian, a gaussian or both.

As mentioned in the previous chapter, the basic profile can be seen as a sum of lorentzians of different intensity, resonance frequency and width. This representation is correct in the center of the lines but overestimates the far wings which asymptotically decrease like $\omega^{-5/2}$ instead of ω^{-2} In order to correct this discrepancy two functions are used. Following the notations of (17) the center of the lines stay unchanged and the wings are represented with

$$\frac{d^{5/2}(a+xd)y^{3/2}}{(d^2+1)|\omega-x|^{5/2}}$$

where d is an adjustable parameter (5 seems to be a quite good value) such that dy (y is the half width at half maximum) is the detuning where the wings begin.

In order to take account of doppler broadening, fast fourier transform routines are used to convolve the whole profile with a

gaussian function. This method, commented in the code, just imposes some special rules to define the working arrays

In case of broadening due to apparatus function the user can either add a constant width to each basic resonance or increase the doppler width and convolve with the whole profile. These two options may are used simultaneously, they correspond respectively to a lorentzian or a gaussian apparatus function.

At the end of execution PROFILE write two columns for the profile coordinates in the datafile whose name is involved in datout. The computer default format is used

iv) OTHER ROUTINES

Both BEGIN and STARK programs make use of a subroutine called DATAR, especially written for each ion species and whose task is to extract the information from a database. and built up the full name of levels. In the present code, the DATAR subroutines use formats able to read the two provided databases one for the lithium-like case and the other for the neon-like case. As mentioned earlier these DATAR subroutines are the only specific part involved in the code. Modifying this part may open the code to other database or ion species

In order to help the user to choose an atomic system a program named SHOSET has been written. This program extracts the information from the database as does BEGIN and provides an output datafile (**printset.**) involving the list of the selected radiative subsystem and the corresponding transitions.

II.3 EXAMPLE OF STUDIES

In this chapter a detailed explanation of the way to use the code on a VAX computer is given by going through two complete examples of execution. The first uses a database for the oxygen lithium-like case and concens radiative transitions between different principal quantum numbers n. The second shows radiative transitions between levels with the same n for the selenium neon-like case. A complete execution involve, as seen in the previous chapter, the following steps:

1-<u>TUNING</u>: adjustment of the parameters involved in the include files, compiling and linking

2- BEGIN: choice of the system and of the physical conditions. Running of BEGIN to prepare the calculation.
3-STARK: calculation.
4-PROFILE: processing the results by running PROFILE to have an x,y output ready to draw

A Oxygen lithium-like case

1- TUNING

The first task to do is the tuning of the code by modifying the parameters involved in the include files. For example the length of the character strings of level names is preferably set to be as short as possible. See below the include file **bascom.inc**

```
c---------common     block     include---------------------------
c          character spar*1,sname*15     ! neon-like
           character spar*1,sname*5       !lithium-like
           common/basdatc/spar(lsup),sname(lsup)
             common/basdat/energ(lsup),fij(ltsup),dlamb(ltsup),
      f       aspo(lsup),nquant(lsup),quantj(lsup),jwth(lsup),
     f      itt(ltsup),jtt(ltsup)
```

One then has to set correctly the parameters contained in **parameter.inc** listed below

```
c-maximum microfield-states number
          parameter(kmax=100)
c-maximum state number and natural label number
           parameter(ngs=24,nes=30,nees=nes*nes,nggs=ngs*ngs,ns=nes*ngs)
c            parameter(labs=25) !25 for neon-like
          parameter(labs=24)
c-maximum level and transition number
           parameter(lsup=16,ltsup=37)
c-number of points in the output grid
           parameter(igrid=1000)
```

In this example the integers ngs (maximum ground-state number) and nes (maximum excited state number) set the maximum size of the matrix to

be diagonalized which is 720x720, whereas lsup and ltsup fix the the maximum length of the arrays containing the atomic data entering the calculation module. If one of these four parameters is exceeded, the code automatically uses sub-systems compatible with the previous dimensions. For instance, in the lithium like case, the system containing all the n=2 and n=3 states is unchanged, while for n=3 and n=4, the number of states in the configuration n=4 is 32 and subsystems are created.

The last parameter igrid, sets the size of the frequency interval in which two elementary resonances are considered to have the same frequency (db-da)/igrid. If a very large frequency domain is chosen, this parameter may be increased

In the following include file: **setex.inc**, the role of some of the commented parameters must be emphasized

```
          parameter(nls=100,nts=100,cuts=100.,nsub=20,icut=5)
c_nls/nts: maximum level/transition-number to be read in the data-base
c_cuts: parameter used for the transition-selection operation
c_nsub: maximum transition number in each radiative sub-system
c_icut: icut-1=number of selected stark-transitions
c          character atype*15,sp*1,sn*15   !neon-like
          character atype*15,sp*1,sn*5    !lithium-like
          common/identc/sp(nls),sn(nls)
            common/ident/en(nls),f(nts),dl(nts),xs(nts),as(nls),xsm,
         f      it(nts),jt(nts),idl(nls),idt(nts),nq(nls),jw(nls),qj(nls)
```

nsub: when a subsystem, corresponding to one radiative transition is searched by the code, a maximum of nsub transitions (radiative and stark transitions) are considered.

icut: among the nsub pre-selected transitions the code selects icut1 transitions as stark transitions. The selection uses the parameter cut commented below. A too large value of icut may create conflicts with the parameters set in **parameter.inc**.

cut: the stark transitions are ranked according to an approximate stark-effect coefficient (described in the previous chapter) and then selected up to a value 1/cut of the largest one. In all cases the number of stark transitions is less than icut-1.

After editing the include files, compiling and linking in order to propagate the new parameters through the code the step BEGIN can be executed.

2- BEGIN

The user may have a preview of the atomic data to be processed in the calculation module by listing the file **prinset** created by the routine SHOSET. For example using a database with the name **lilio.dat,** within the frequency range 71.55 to 71.75 eV, one obtains the following list :

label/name/energy

1	2S1:2	0.00000E+00
2	2P1:2	11.950
3	2P3:2	12.020
5	3P1:2	82.590
6	3P3:2	82.610
7	3D3:2	83.650
8	3D5:2	83.650

1,2 stark or rad. transition/names/i,j labels/
coef. for selection/energy eV,angstrom

1	2S1:2	2P1:2	1	2	0.18264E-01	11.9500	1037.60
1	2S1:2	2P3:2	1	3	0.36450E-01	12.0200	1031.90
2	2P1:2	3D3:2	2	7	0.51804E-02	71.7000	172.930
2	2P3:2	3D3:2	3	7	0.51880E-03	71.6300	173.090
1	3P1:2	3D3:2	5	7	0.93426	1.06001	11744.0
1	3P3:2	3D3:2	6	7	0.15551	1.04000	11964.0
2	2P3:2	3D5:2	3	8	0.46883E-02	71.6300	173.080
1	3P3:2	3D5:2	6	8	0.87442	1.04000	11892.0

Running BEGIN produces the following message on the screen

1	iotype	lilio.dat	name of the data-base
2	atomw	16	atomic mass
3	z	6	ion charge seen from the valence electron
4	zp	0	perturber charge if different from emitter
5	dens	2.e19	electronic density
6	temp	200000	temperature

```
 7 da         71.55        lower bound of the frequency interval (eV)
 8 db         71.75        upper bound of the frequency interval
 9 datout     lilio.out    name of the output-file
10 nmc        10           number of sampled micro-fields
modification of these data (n)o (yes default)
```

A carriage return (CR) gives the possibility to modify one of the data involved in the third column. When the data are well adjusted the reply must be "n" After some questions and reply with "y", "n" or CR the user can do a new selection on the previously selected quantum system.

```
 further approximation (y)es (no default)
y
2S1:2 to be kept? (n)o, yes(def.)

2P1:2 to be kept? (n)o, yes(def.)

2P3:2 to be kept? (n)o, yes(def.)

3P1:2 to be kept? (n)o, yes(def.)

3P3:2 to be kept? (n)o, yes(def.)

3D3:2 to be kept? (n)o, yes(def.)

3D5:2 to be kept? (n)o, yes(def.)
```

When this is done all the information is ready to be transferred to the calculation module

3- STARK

By running STARKP1 the user can get results for one microfield (for instance 0 or the mean microfield value) instead of those corresponding to the whole static distribution given by STARKP

The results provided by STARKP1 are written in **lilio.out** as fixed in BEGIN An example for a 0 microfield value is listed below:

```
 16.00000       6.000000       0.0000000E+00  2.0000000E+19   200000.0
 71.55000       71.75000
```

71.62988	0.3167564	0.0000000E+00	2.6789007E-03
71.70035	0.1577151	0.0000000E+00	2.7077985E-03

The two first lines reproduce some of the data chosen in BEGIN, whereas the others lines contain the frequency amplitude and width corresponding to the selected radiative transitions (there are three radiative transitions, but two levels are degenerated as can be seen in **printset**). The results provided by STARKP1 for a microfield value different from 0 or by STARKP obviously contain more than two elementary resonances .

The **lilio.out** files can now be used by PROFILE to process the x y profile data.

4- PROFILE

The folowing list shows an example of dialog with the computer to get a file zz. ready to draw a profile with doppler effect, in the frequency range 71.55 tà 71.75

```
$ run profile
input/data-file name
lilio.out
output/data-file name
zz.
 output in angstrom y(es) (default: output in ev)

 doppler convolution y(es) (no default)
y
 frequency set (ev):a=   71.55000      b=   71.75000
 enter new set a, b (0 0 for the same set)
0  0
 apparatus function (y)es (no default)
y
 enter two apparatus functions, 0 is accepted
 wg: gaussian full width at half maximum in ev
 wl: lorentzian half width at half maximum in eV
1.e-3   0
```

B Selenium neon-like case

This example has been executed with the same general tuning as before (except the length of the level names), and with the following input data

```
 1 iotype   nelise.dat     name of the data-base
 2 atomw    79             atomic mass
 3 z        25             ion charge seen from the valence electron
 4 zp       0                 perturber charge if different from emitter
 5 dens     1.e21          electronic density
 6 temp     1.e7           temperature
 7 da       59.             lower bound of the frequency interval (eV)
 8 db       59.2           upper bound of the frequency interval
 9 datout   neout.         name of the output-file
10 nmc      10             number of sampled micro-fields
```

This case is different from the previous one because all the levels considered belong to the same atomic configuration. The frequency interval leads to the selection of a sub-system which contains one radiative transition (see below the file **printset**.) between 3s and 3p states, whereas the stark coupling links the 3s with the 3p, and the 3p with the 3d states. Here the no quenching approximation implies that the radiative transition is not used for the stark effect (see diagram in Fig 2)

```
   frequency  range/lv/lt/liv/lig
 59.000       59.200       27  100    9    4

        4 = number of ground levels
     rank/name/energy (eV)
           1 2p3s(3:2)(1:2)2    1435.360
           2 2p3p(3:2)(1:2)1    1482.610
           3 2p3p(3:2)(1:2)2    1486.020
           4 2p3p(3:2)(3:2)2    1498.810
           5 2p3p(3:2)(3:2)3    1494.470
           6 2p3d(3:2)(5:2)4    1559.230
radiative  transition    2p3s(3:2)(1:2)2  2p3p(3:2)(3:2)3
```

```
 5  6   64.760      191.45
 1  2   47.250      262.41
 1  3   50.660      244.78
 1  4   63.450      195.43
 1  5   59.110      209.75
label/name/energy
 2  2p3s(3:2)(1:2)2     1435.4
 6  2p3p(3:2)(1:2)1     1482.6
 7  2p3p(3:2)(1:2)2     1486.0
 8  2p3p(3:2)(3:2)3     1494.5
10  2p3p(3:2)(3:2)2      1498.8
18  2p3d(3:2)(5:2)4      1559.2
19  2p3d(3:2)(5:2)2      1559.3
20  2p3d(3:2)(3:2)3      1559.4
22  2p3d(3:2)(5:2)3      1564.8
1,2 stark or rad. transition/names/i,j labels/
coef. for selection/energy eV,angstrom
1  2p3s(3:2)(1:2)2  2p3p(3:2)(1:2)1    2    6   0.78392E-03  47.2500      262.414
1  2p3s(3:2)(1:2)2  2p3p(3:2)(1:2)2    2    7   0.63133E-03  50.6600      244.782
2  2p3s(3:2)(1:2)2  2p3p(3:2)(3:2)3    2    8   0.15755E-02  59.1100      209.754
1  2p3s(3:2)(1:2)2  2p3p(3:2)(3:2)2    2   10   0.56267E-03  63.4501      195.428
1  2p3p(3:2)(3:2)3  2p3d(3:2)(5:2)4    8   18   0.11787E-02  64.7600      191.451
1  2p3p(3:2)(3:2)3  2p3d(3:2)(5:2)2    8   19   0.30518E-04  64.8600      191.173
1  2p3p(3:2)(3:2)3  2p3d(3:2)(3:2)3    8   20   0.13733E-03  64.9000      191.058
1  2p3p(3:2)(3:2)3  2p3d(3:2)(5:2)3    8   22   0.16403E-03  70.3800      176.172
$
```

The energy levels for the two case studied are shown on figures 1 and 2. Figures 3 and 4 give the corresponding line profiles. The solid curves are the lines with homogeneous broadening only. The dotted curves are obtained when ionic stark effect is taken into account.

CONCLUSION

We have described a line shape code for multielectron emitters in a plasma environment. The code enables the calculation of stark broadening for complex atomic structures. Our technique demonstrates that stark broadening may affect the profiles of lines

involved in the X-ray laser studies. Further calculations are planned for a comparison with recently obtained experimental line shape of Li-like and Ne-like emitters. These comparisons will serve as a guide for possible improvements of the code. A promising diagnostic tool of hot and dense plasmas should be provided by this fast and interactive code. Others studies planned concern the calculation of line between states of large principal quantum numbers, and the inclusion , by a very fast algorithm, of the effect of ion microfield fluctuations.

APPENDIX I

Brief liouville space review

Liouville space is designed to transform expressions like

$$\left\{ e^{iHt} A e^{-iHt} \right\}_{av} \qquad \text{into} \qquad \left\{ e^{iLt} \right\}_{av} A$$

which disentangles the evolution operator averaged over a stochastic process and any observable A.

The liouville-space $\mathcal{L}$ is defined as the tensorial product of the hamiltonian space $\mathcal{H}$ and is dual $\mathcal{H}^d$. We adopt with the standard notation for vectors in liouville space $|\alpha\beta>>$. The scalar product in $\mathcal{H}$ and $\mathcal{H}^d$ are extended to $\mathcal{L}$:

$$\begin{aligned} &<<\alpha\beta|\gamma\delta>> = <\alpha|\gamma> . (\beta|\delta) \\ &= <\alpha|\gamma> . <\beta|\delta>^* \end{aligned} \qquad 1$$

where bra-ket represent the scalar product in $\mathcal{H}$-space and parenthesis in $\mathcal{H}^d$-space.

It can be seen that

$$Tr\{ A \} = \sum_f <<f\ f|A>> \qquad 2$$

where

$$|A>> = \sum_{\alpha\beta} <\alpha|A|\beta> |\alpha\beta>>$$

according to 1 the "liouville bra" may be defined as

$$<<A| = \sum_{\alpha\beta} <\alpha|A|\beta>^{*} <<\alpha\beta|$$

this gives

$$Tr\{A\,B\} = <<A|B>> \qquad 3$$

Liouville operators are special linear operators P in liouville space such that $P|q>> = |[p,q]>>$ where p and q are linear operator in hamiltonian space. It can be seen that

$$P = p\otimes I^{d} - I\otimes p^{d} \qquad 4$$

For the specific problem of interest it can be seen that

$$Tr(\vec{d}.[\vec{d}(t),\rho_0]) = <<\vec{d}|.[\vec{d}(t),\rho_0]>> \qquad 5$$

which becomes according to 4

$$<<\vec{d}|U(t).\vec{D}|\rho_0>> \qquad 6$$

with the convention $U(t)=e^{-iLt}$.

APPENDIX II

Electronic collision operator

This quantity represents the effect of the electronic component on the radiator. It is usually calculated in the framework of a binary collision impact theory. Using the dipole approximation, a standard expression for this collision operator is generally factorized in two terms:

$\Phi_e = \vec{d}\,.\,\vec{d}\;K(\omega)$

In our code the $\vec{d}\,.\,\vec{d}$ term has been calculated exactly for the selected set of substates. The function $K(\omega)$ depends on the density and temperature of the plasma and is calculated to the second order in the radiator-electron interaction. A thermal average included in $K(\omega)$ may be

performed by using a quantum-mechanical relaxation theory or a classical path assumption for the perturbing electrons. These first calculations have been done with an expression based on a modified semi-classical model, in which a strong-collision term is added to the semi-classical term. As ω tends to zero (center of the line), we satisfy the impact limit conditions, for which $K(\omega)$ tends to a constant value given by:

$$K(\omega=0) = -\frac{4\pi}{3}\left(\frac{2m}{\pi kT}\right)^{1/2} N_e \left(\frac{h}{me}\right)^2 \left(C + \int_y^{\infty} e^{-x}\frac{dx}{x}\right)$$

where y is given by the ratio $y=(\rho_{min}/\rho_{max})^2$, ρ_{min} and ρ_{max} being respectively the minimum and maximum values of the impact parameter range. The maximum value ρ_{max} is taken to be the smallest of the Debye radius or a cutoff $v/\Delta\omega_{ii'}$, where v is the mean thermal velocity and $\Delta\omega_{ii'}$ is the frequency difference between the two nearest interacting levels. The minimum value ρ_{min} is a strong collision radius which is the largest of the emitters Bohr radius or the so called Weisskopf radius ρ_w . The latter quantity is defined by the relation $V\tau/h \approx 1$, where V is the emitter-perturber interaction at distance ρ.

For values of ω of the order or larger than v/ρ_w , $K(\omega)$ enters the binary strong collision regime, where the motion of the perturber can be neglected. $K(\omega)$ should then be proportional to $\omega^{-1/2}$, ensuring that the wing of the line profile has the usual static asymptotic $\omega^{5/2}$ dependance. For this domain of large frequencies, our calculation switches in a continuous way from the constant impact value of $K(\omega=0)$, to a static $\omega^{1/2}$ behaviour.

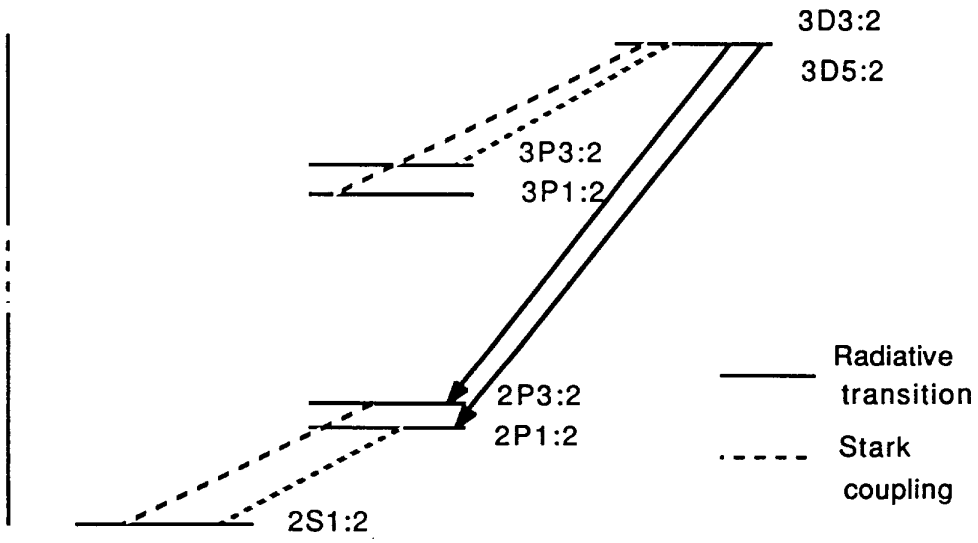

Fig.1. Energy diagram for the Lithium-like Oxygen case.

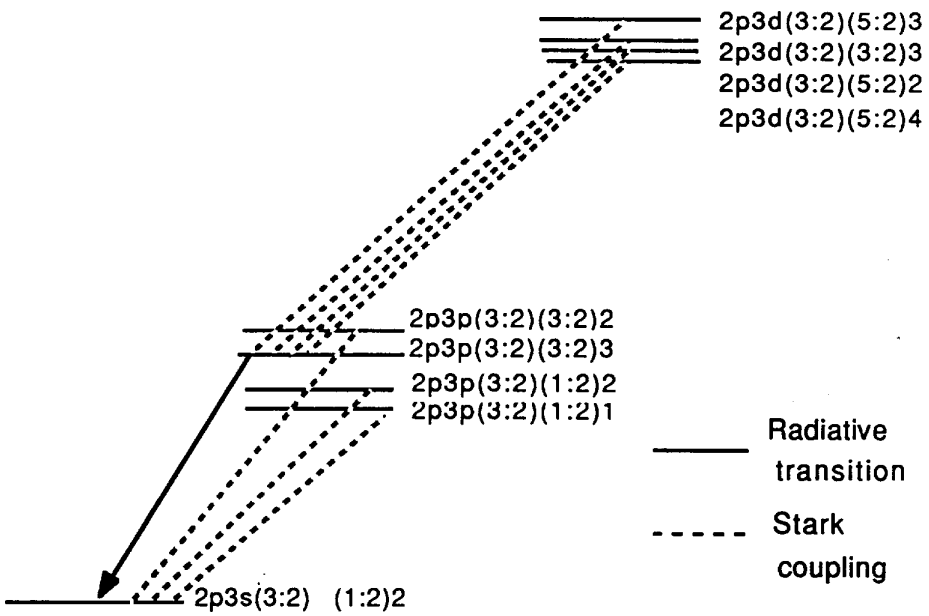

Fig.2 Energy diagram for the Neon-like Selenium case.

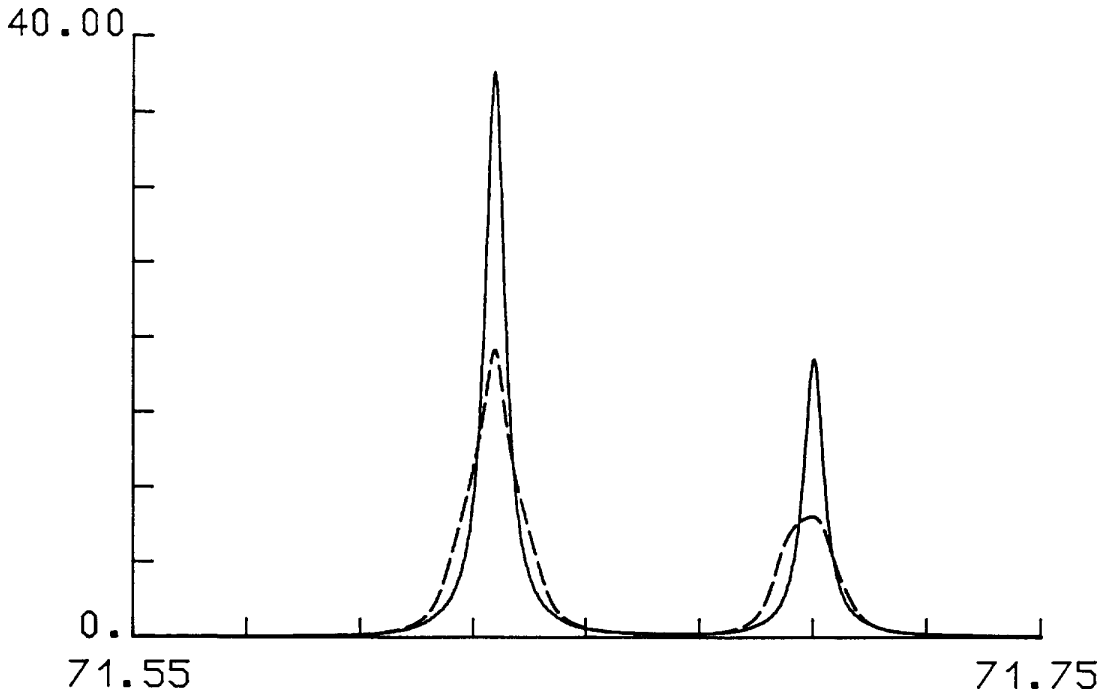

Fig. 3 Oxygen Lithium-like case. x-scale in eV

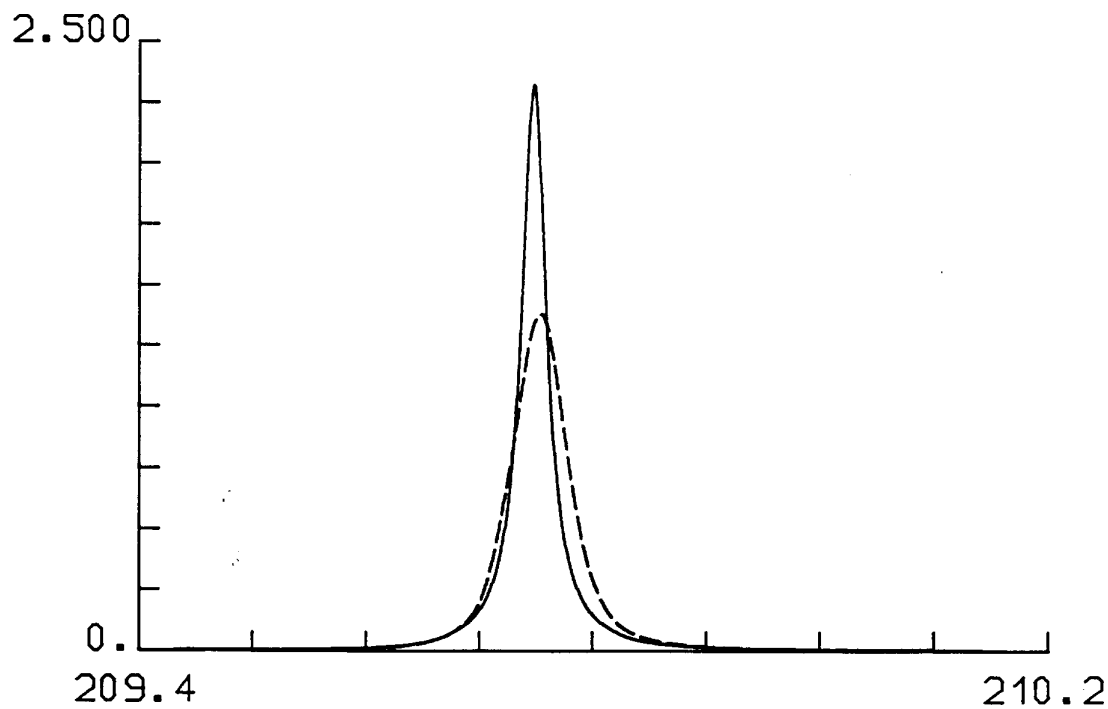

Fig. 4 Selenium Neon-like case. x-scale in Angström

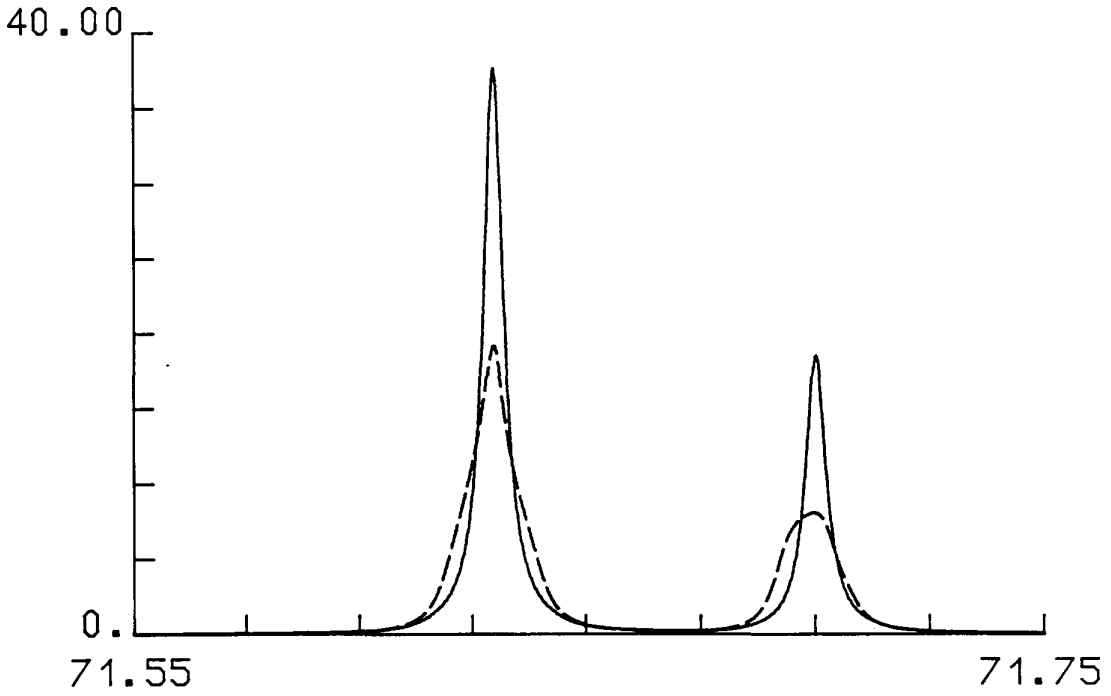

Fig. 3 Oxygen Lithium-like case. x-scale in eV

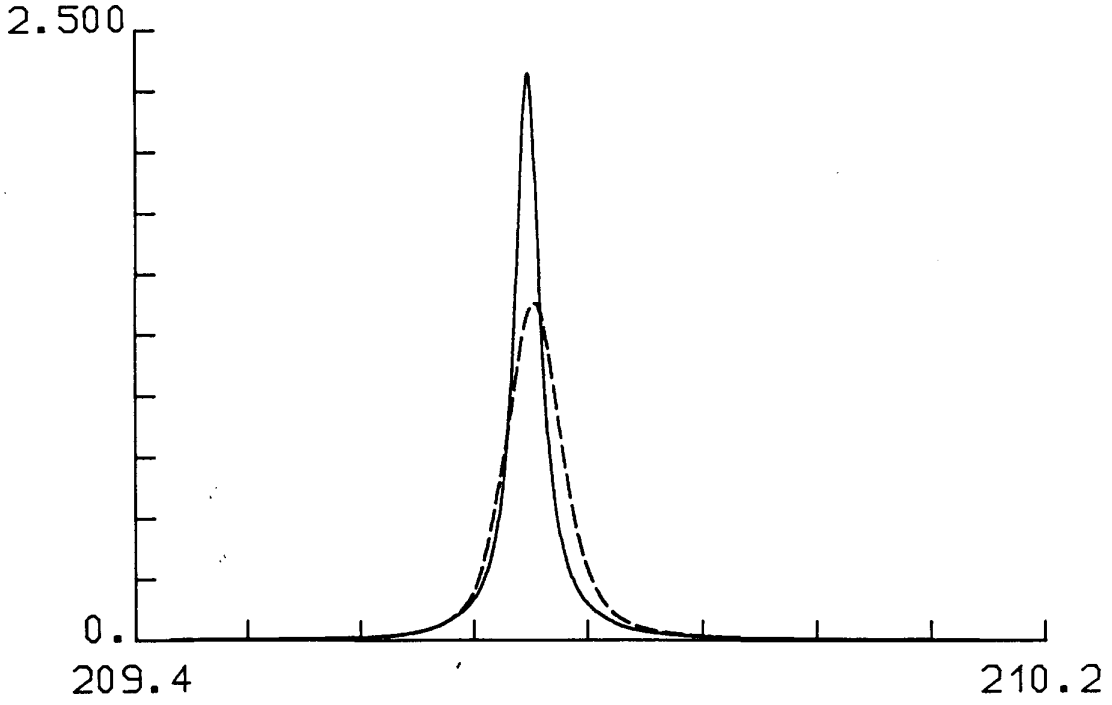

Fig. 4 Selenium Neon-like case. x-scale in Angström