PPP CODE

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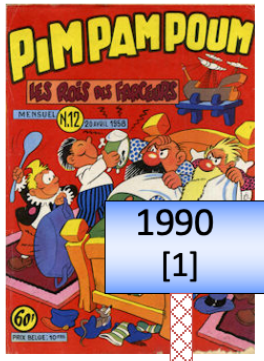

Interference terms

Ion dynamics (FFM model)

Electron broadening

New formulation FFM

New version

1990 [1] — FFM and MD simulation [2] — 2000 — 2010 [3] — 2011 [4] — 2012 — ppp … 2022 [5]

Radiative redistribution function

Code TOTAL LLNL

Code PPP-B Magnetic field

Code PPP-B Intermediate case

[1] A. Calisti, F. Khelfaoui, R. Stamm, B. Talin and R.W. Lee, Phys. Rev. A 42, 5433 (1990)

[2] B. Talin, A. Calisti, L. Godbert, R. Stamm, R.W. Lee and L. Klein, Phys. Rev. A 51, 1918 (1995)

[3] A. Calisti, C. Mossé, S. Ferri, B. Talin, F. Rosmej, L. A. Bureyeva, and V. S. Lisitsa, Phys. Rev. E 81, 016406 (2010)

[4] S. Ferri, A. Calisti, C. Mossé, L. Mouret, B. Talin, M.A. Gigosos, M.A. Gonzalez and V.S. Lisitsa, Phys. Rev. E84, 026407 (2011)

[5] S. Ferri, O. Peyrusse, A. Calisti, Matter Radiat. Extremes 7, 015901 (2022)

Many contributors !

development

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thanks

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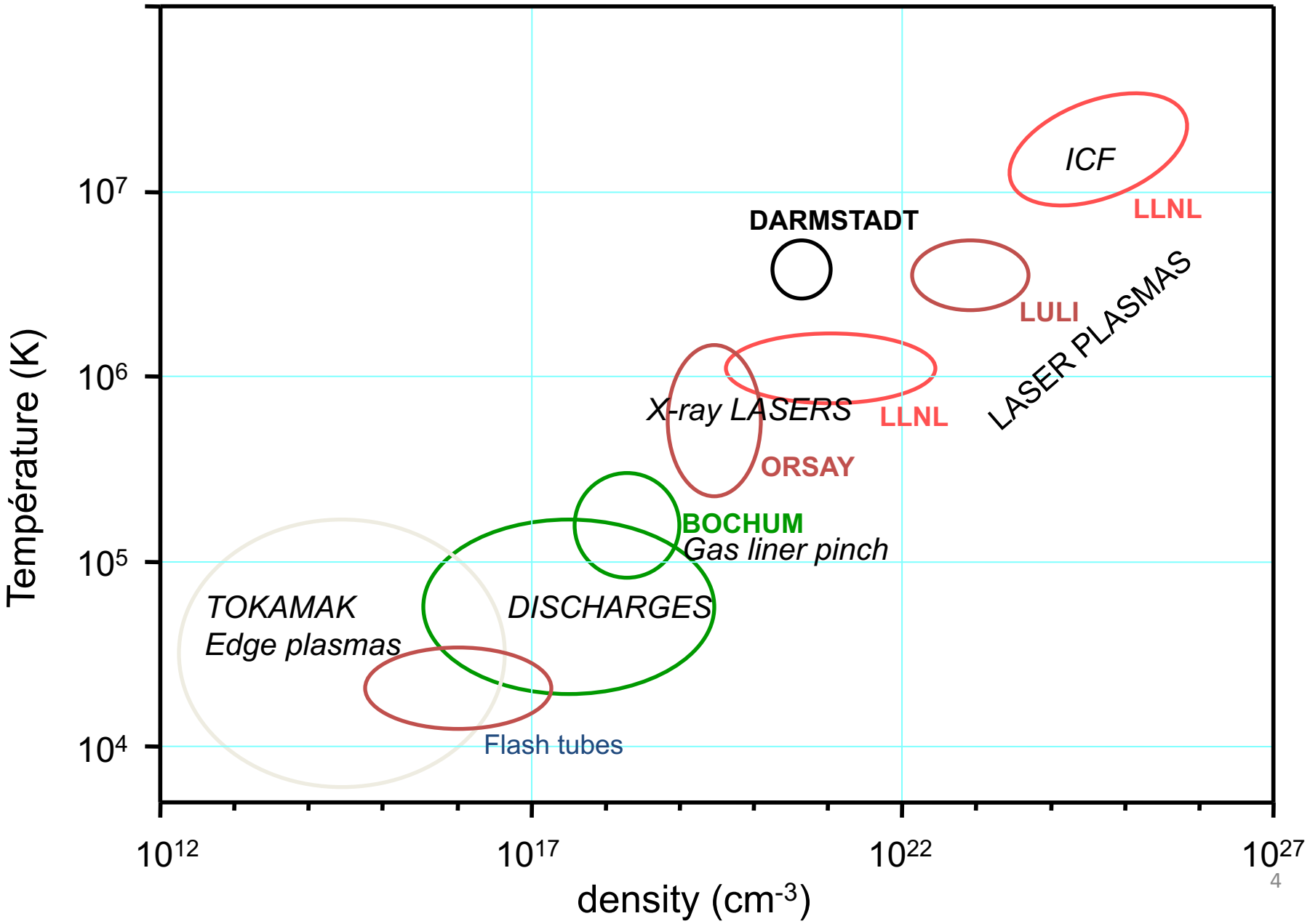
C.Iglesias

The plasma spectroscopy constitutes the main diagnostic tool for a wide range of plasma conditions.



Outline

- Description of the line shape formalism
- The implementation of the PPP code
- How the code runs

Standard spectral line shape theory

The usual starting point for the calculation of a line shape is given by the Fourier transform of the dipole autocorrelation function C(t) :

$$I(\omega) = \frac{1}{\pi} \Re e \int_0^\infty dt\, C(t) e^{i\omega t}$$

in Liouville space notation: $C(t) = \left\langle\left\langle \vec{d}^{\,*} \middle| U(t) \middle| \vec{d}\rho_0 \right\rangle\right\rangle$ with $U(t) = \{U_1(t)\}_{av}$

average over plasma perturber states

U(t) is the evolution operator solution of the stochastic equation :

$$\begin{cases} \dfrac{dU_1(t)}{dt} = -i\left(L_0 + l(t)\right)U_1(t) \\ U_1(0) = 1 \end{cases}$$

$$l(t) = -\vec{d}.\vec{E}_1(t)$$

static ions /impact electrons approximation

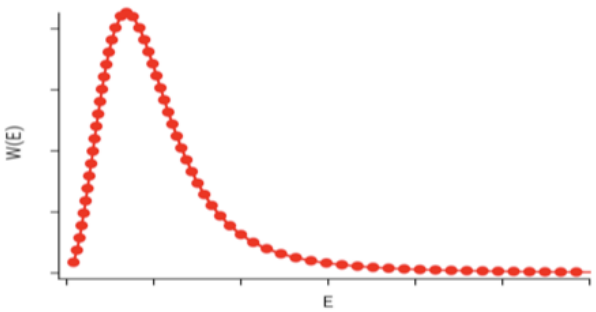
➢The ion microfield is considered as constant during the radiative process

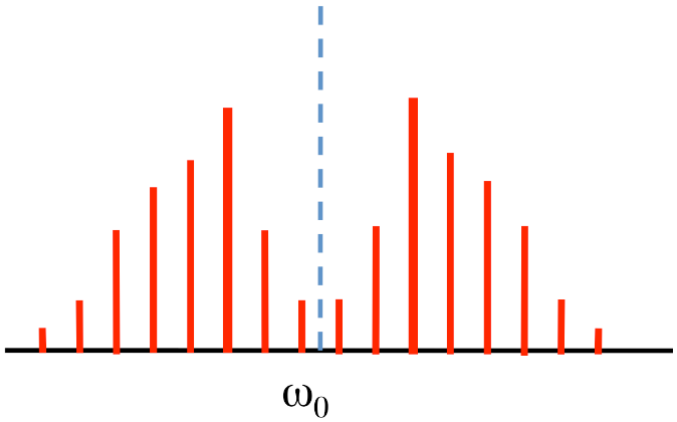
⇒The evolution operator in a constant ion field is given by : $U_E(t) = e^{-i\left(L_0 - \vec{d}.\vec{E} - i\Phi\right)t}$

- *diagonal elements* : atomic frequencies + electronic and natural broadening
- *non-diagonal elements :* Stark interaction terms + interference terms

➢The quasistatic ion approximation leads to an average over a microfield distribution function W(E) :

$$I(\omega) = \sum_E W(E) I_E(\omega)$$





➢We express the evolution operator in a basis in which L is diagonal.

$$I_E(\omega) = \frac{1}{\pi}\Re e\left\langle\left\langle \vec{d}^{\,*} \middle| M_f \int_0^\infty dt e^{i\omega t} e^{-iM_f^{-1}LM_f t} M_f^{-1} \middle| \vec{d}\rho_0 \right\rangle\right\rangle \qquad L = L_0 - \vec{d}.\vec{E} - i\Phi$$

➢We look for the eigenvalues of the operator L : $z_k=\omega_k+i\gamma_k$

➢The Fourier transform in I_E leads to this structure in a constant field E:

$$I_E(\omega) = \frac{-1}{\pi}\Im m\left\langle\left\langle d^* \middle| M_f \begin{pmatrix} \frac{1}{\omega - z_1} & & \\ & \ldots & \\ & & \frac{1}{\omega - z_n} \end{pmatrix} M_f^{-1} \middle| d\rho_0 \right\rangle\right\rangle$$

This expression can be written by a sum of lorentzians:

$$I_E(\omega) = \sum_k \frac{c_k(\omega - \omega_k) + a_k\gamma_k}{(\omega - \omega_k)^2 + \gamma_k^2}$$

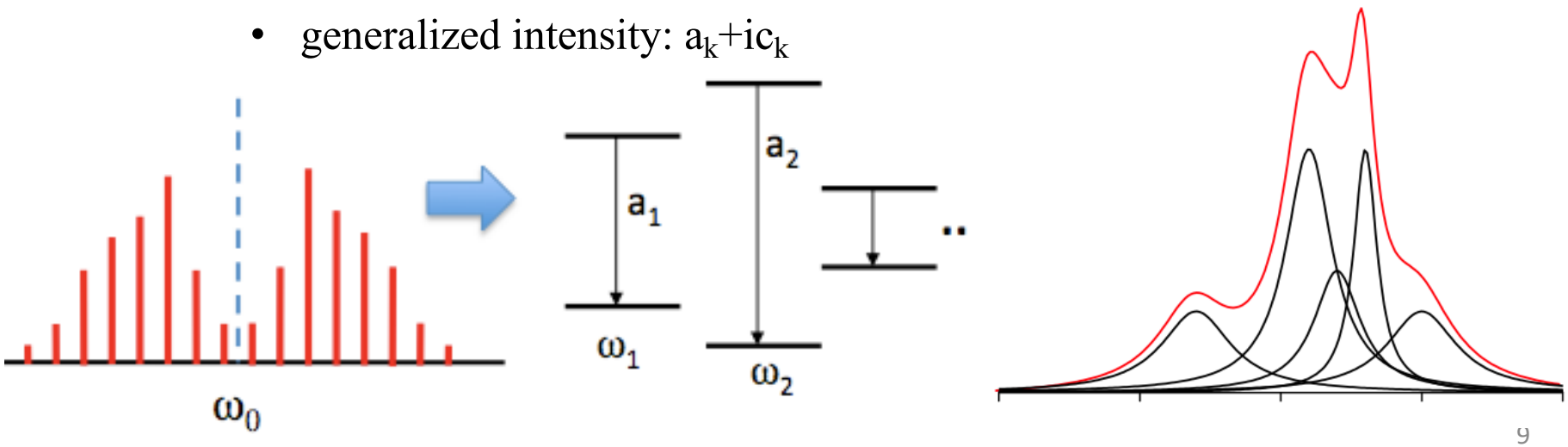
Static profile

Finally, instead of calculating the trace, we need to know the complex coefficients of the Stark components:

$$\omega_{qi} + i\gamma_{qi} = (Z_q)_{ii}$$
$$a_{qi} + ic_{qi} = (\vec{d}^{\,t} M_q)_{ii} \cdot (M_q^{-1} \rho_0 \vec{d}\,)_{ii}.$$

The emitter – plasma interaction can be well represented by a set of two-level systems : the **Stark components** defined by :

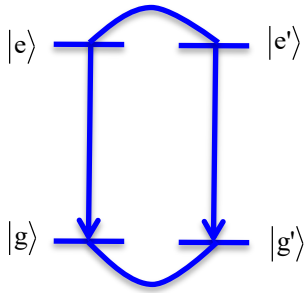
- generalized frequency : $\omega_k + i\gamma_k$
- generalized intensity: $a_k + ic_k$



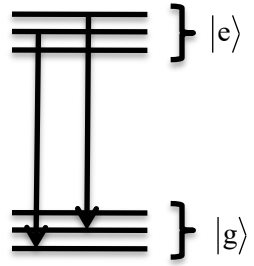
Electron impact approximation

The electronic collision operator represents the effect of the electronic microfield component on the emitter through binary collisions

$$\Phi_{gg',ee'} = \sum_{g''} \delta_{ee'} \vec{d}_{gg''}.\vec{d}_{g''g'} G\left(\Delta\omega_{g''e}\right) + \sum_{e''} \delta_{gg'} \vec{d}_{e'e''}.\vec{d}_{e''e} G\left(-\Delta\omega_{ge''}\right) - \vec{d}_{gg'}.\vec{d}_{e'e}\left[G\left(\Delta\omega_{ge'}\right)+G\left(-\Delta\omega_{g'e}\right)\right]$$



interference terms



with $\Delta\omega_{ge} = \omega - \omega_{ge}$

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

Strong collisions

$$y = \left[\frac{h n^2}{2z}\right]^2 \frac{\omega_p^2 + \omega_{gg''}^2}{E_H kT}$$

* H.R. Griem et al., Phys. Rev. A19, 2421 (1979)

Static profile

The static profile is described by a sum of generalized Lorentzian spectral components: the Stark spectral components or stark dressed components (transitions) –SDT -.

Working in the space of the SDT, we can rewrite the linear response line-shape function in terms of dressed two-level radiators by defining a generalized dipole moment matrix element D_k for the SDT.

$$D_k = r\sqrt{1 + i\frac{c_k}{a_k}} \qquad \text{with} \qquad r = \sqrt{\sum a_k}$$

We also define the probability vector operator p with element p_k describing the instantaneous probability of occurrence of the kth SDT.

$$p_k = \frac{a_k}{r^2}.$$

The spectral line shape in the quasi static approximation is then given by in the basis of the SDT:

$$I(\omega) = \frac{1}{\pi}\Re\sum_{k,j} i \ll D_k|(\omega\mathbf{1} - L_0)^{-1}|D_j \gg p_j,$$

The Frequency Fluctuation Model

To account for microfield fluctuations**, it's postulated that** the Stark components are mixed by using a Markov process with a fluctuation rate

$$\nu = \frac{v_{th}}{r_o}$$

The chosen Markov process is completely determined by, the instantaneous SDT probability operator p and a transition rate operator W such as:

$$\mathbf{W}_{kj} = -\Gamma_j \delta_{kj} + W_{kj}.$$

We get:

$$I(\omega) = \frac{1}{\pi} \Re \sum_{k,j} i \ll D_k | (\omega \mathbf{1} - L_0 - i\Gamma + iW)^{-1} | D_j \gg p_j.$$

Γ is the diagonal matrix of inverse state lifetimes with $\Gamma_{kj} = \nu\delta_{kj}$ and W is the matrix of transition rates between different states such as $W_{kj} = \nu p_k$.

The Frequency Fluctuation Model

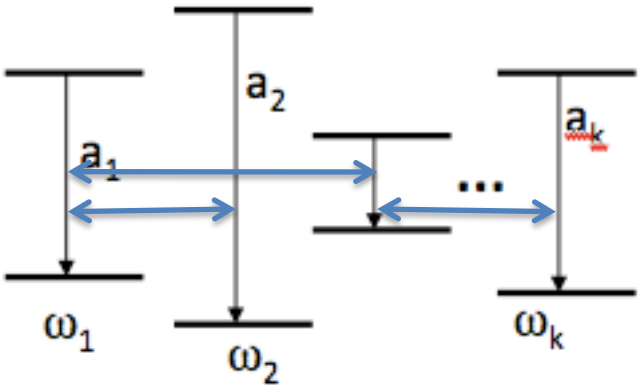
After some algebra (detailed in the PPP user's manual), we get:

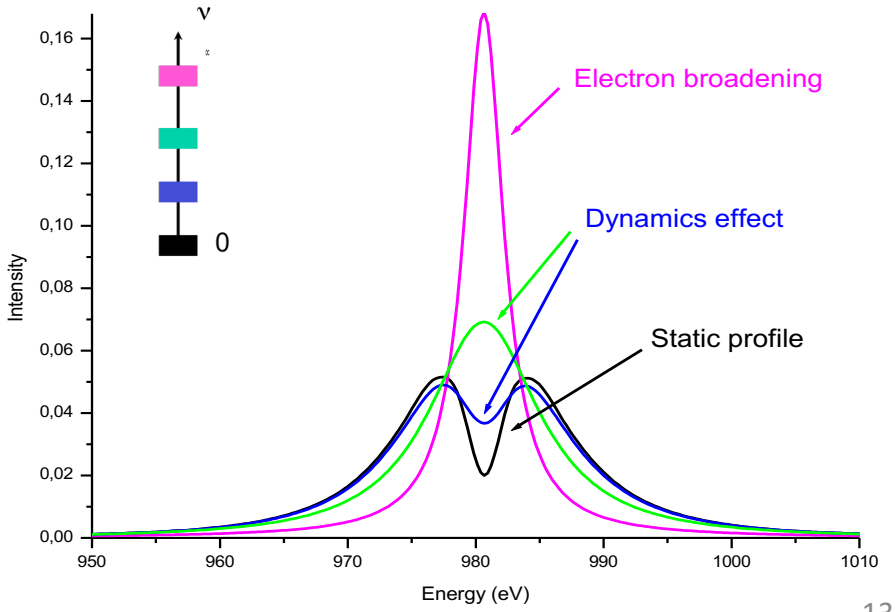
$$I(\omega) = \frac{r^2}{\pi} Re \frac{\sum_k \frac{a_k / r^2}{i(\omega - \omega_k) + \nu}}{1 - \nu \sum_k \frac{a_k / r^2}{i(\omega - \omega_k) + \nu}}$$

or

$$I(\omega) = \frac{r^2}{\pi} Re \frac{\int \frac{W(\omega')d\omega'}{\nu + i(\omega - \omega')}}{1 - \nu \int \frac{W(\omega')d\omega'}{\nu + i(\omega - \omega')}}.$$

With W(ω) being the normalized static line shape.





The code description

The code PPP is divided into three independent parts that prepare, process and build the spectra:

- **pim**: Sets the necessary links with the external data bases and the output files and the plasma parameters. It also selects the relevant quantum systems.
- **pam**: Processes the hard algebra stage
- **poum**: Carries out the final calculation of lineshapes according to particular options and formats. Account for ionic dynamics effects.

*The first phase **pim** is a dialog with the code which helps the user to extract a well-shaped data subset from the atomic database according to both the constraints of computer time-saving and appropriate selection of the relevant couplings for Stark effect calculations.*

*The algebra involved in the second phase **pam** is basically a sequence of quantum mechanical calculations of the same trace necessary to account for the average on the microfield distribution. The numerical difficulty here lies in the diagonalization of complex matrices.*

*The third phase **poum** includes the FFM procedure and sums of elementary Lorentzian profiles defined with the above parameters and, if necessary, convolutions.*

The code description

The PIM phase:

-Phase 1 :

- defines the plasma characteristics : N_e, T_e, T_i and mass, charge of emitters and perturbers

-extracts the data (energy levels and reduced dipole matrix elements) from the atomic database (MCDF, COWAN, HULLAC, FAC…)

-can use populations from dedicated codes or assign LTE populations by default

-can calculate the field distribution or input any distribution

The microfield distribution can be calculated in the code with APEX for ions

In the case of neutrals, with Hooper's distribution.

Example :Lineshape of Lyman α with fine structure for hydrogen like argon with protons

If "PPP" is run for the first time, a default set of variables is typed into the screen and the default file "in_new.txt" is created in the user's directory. Subsequent executions reopen the modified file "in_new.txt" and ask to choose whether to execute "pim","pam",or "pum".

default set of variables

```
1  Ar17.dat      ****          (base,pfi) atom data base/ pop file
2  3300.00    3340.00          (da, db) frequency interval bounds - eV
3  40.000       1.000          (em, pm) emitter/ perturber mass
4  17.000       1.000          (ze,zp) net emit. charge/ pert. charge
5  0.10000E+08 0.10000E+08     (tmpe, tmpi) electron temp/ ion temp. - K
6  0.10000E+25 0.10000E-01     (dens,per) elec dens/ emit/pert concent
7  2.              10.         (lay,set) layer b/ stark trans cutoff
8  2                           (nu) block rad trans nb
9  outd           outs         (out, sdof) Stark data, output file
10 n                           (ric) interference terms (y/n)
11 50            25.           (nmc, ecut) fld number/ max field value
12 new data? or help
```

To modify this file and enter a new data one can simply write `variablename=new data` *without space character (note that* `in_new.txt` *can also be edited).*

Example :Lineshape of Lyman α with fine structure for hydrogen like argon with protons

default set of variables

```
1  Ar17.dat      ****          (base,pfi) atom data base/ pop file
2  3300.00    3340.00          (da, db) frequency interval bounds - eV
3  40.000       1.000          (em, pm) emitter/ perturber mass
4  17.000       1.000          (ze,zp) net emit. charge/ pert. charge
5  0.10000E+08 0.10000E+08     (tmpe, tmpi) electron temp/ ion temp. - K
6  0.10000E+25 0.10000E-01     (dens,per) elec dens/ emit/pert concent
7  2.              10.         (lay,set) layer b/ stark trans cutoff
8  2                           (nu) block rad trans nb
9  outd           outs         (out, sdof) Stark data, output file
10 n                           (ric) interference terms (y/n)
11 50            25.           (nmc, ecut) fld number/ max field value
12 new data? or help
```

base: Atomic database filename. Provided by known atomic physic codes and written with a format that can be read by the PPP code.

pfi: Optional level population filename.

nu: Sets the number of radiative transitions which can be processed at a time.

out: Output filename for the Stark component data, to be post-processed by pum

sdof: Output filename for the profiles.

ric: By default, ric=n. Without or with interference terms.

nmc: Gives the number of significant points for the micro field distribution.

ecut: Maximum field values of the microfield distribution by default, ecut=25.

Example :Lineshape of Lyman α with fine structure for hydrogen like argon with protons

The automatic selection of a quantum system for a given problem is a nontrivial optimization process. Many constraints must be considered at a time.

- the bigger the system is, the better the Stark effect is accounted for.
- the smaller the system is, the faster the calculations are.
- big systems could deal with numerical traps.

The selection algorithms work finding the successive neighbors of a radiative transition. The first neighbors are selected using the mean Stark shift but the following ones are characterized by the blending ratios due to Stark couplings.

The mean electric field enters into the calculation of the mean Stark shift that thus depends on the electronic density. Therefore, the selected quantum systems can vary with the plasma conditions.

`lay`: number of successive neighbor shells to be considered.
`xset`: minimum relative strength of a state taken into account. If q is the larger Stark shift induced by the first neighbors, one must have :

$$u(a,b) = \frac{q}{xset}.$$

`u` being the estimated coupling strength of a state `b` on a state `a`.

Example :Lineshape of Lyman α with fine structure for hydrogen like argon with protons

The atomic database must be in the user's directory when the PPP code is executed. If this is not the case, the following message appears on the screen.

```
check if atomic database is in your folder
```

The default `in_new.txt` file is created in the user directory:

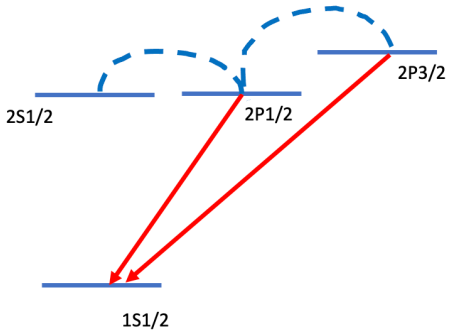
in_new.txt

```
Ar17.dat      ****        (base,pfi) atom data base/ pop file
3300.00    3340.00        (da, db) frequency interval bounds - eV
40.000      1.000         (em, pm) emitter/ perturber mass
17.000      1.000         (ze,zp) net emit. charge/ pert. charge
0.10000E+08 0.10000E+08   (tmpe, tmpi) electron temp/ ion temp. - K
0.10000E+25 0.10000E-01   (dens,per) elec dens/ emit/pert concent
2.             10.        (lay,set) layer b/ stark trans cutoff
2                         (nu) block rad trans nb
outd           outs       (out, sdof) Stark data, output file
n                         (ric) interference terms (y/n)
50           25.          (nmc, ecut) fld number/ max field value
 e            300         (units,npt)(e/a)eV or A/curve point numb.
3300.00    3340.00        (ai,af) default frequency range
n              f          (dop,cv)doppler (y/n)-convol(f)fft(v)voigt
 0.00000   0.00000        (wg,wl) Gauss FWHM/ Lorentz HWHM eV
  n                       (nyn) profile normalization  y/n
  0.00000                 (shft) shift in output units
```

Example :Lineshape of Lyman α with fine structure for hydrogen like argon with protons

After the choice of the data:

```
 Ar17.dat          ****              (base,pfi) atom data base/ pop file
  3300.00           3340.00          (da,db) frequency interval bounds - eV
   40.000            1.0000          (em,pm) emitter/ perturber mass
   17.000            1.0000          (ze,zp) net emit. charge/ pert. charge
  0.10000E+08       0.10000E+08      (tmpe,tmpi) electron temp/ ion temp. - K
  0.10000E+25       0.10000E-01      (dens,per) elec dens/ emit/pert concent
   2                 10.             (lay,xset) layer nb/ stark trans cutoff
    2                                (nu) block rad trans nb
 outd              outs              (out,sdof) Stark data,output file
 n                                   (ric) interference terms  (y/n)
  50               25.               (nmc,ecut) fld number/ max field value
is this Ok? y(def)/n

zmoy   1.15999997
Gamma =   2.56348401E-02   el*el/(r0*bolt*tmpi)   !q*q/r0*K*Ti

!!!!!!!!!!!!!  population -->  Boltzmann!!!!!!!!!

 discard radiative transitions? y(es) (def. no)

 radiative transition number (krad)          2

    ss1s00 -->    pp2p00
    ss1s00 -->    pp2p01

nb transitions radiatives / bloc          2
 number of blocs (miscel)          1
```



Example :Lineshape of Lyman α with fine structure for hydrogen like argon with protons

For the next step the user may optionally direct the code to process a microfield distribution function, answering the question with ”y” or an appropriate filename. :

```
  m-field calculation y(es) (no def.)
  or filename (other distribution)
y

  view miscel ? y/(n def --> pam)
```

At this stage two files are created in the user directory: `field` and `samfld.dat`. `Field` corresponds to the raw calculation made by Apex (or other method). These data are then processed in order to interpolate the required number `nmc` of significant probabilities on points, regularly displayed on the distribution function. The result is stored in the file `samfld.dat` which will used by `pam`.

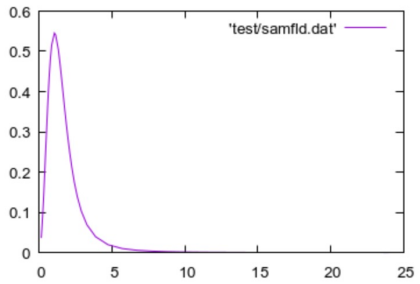
```
  view miscel ? y/(n def --> pam)
y
```

If you answer `y` to this question, you can see:

```
annette.calisti@univ-amu.fr@jupyter:~/test$ ls
Ar17.dat  bars  field  in_new.txt  miscel.  samfld.dat
annette.calisti@univ-amu.fr@jupyter:~/test$
```

Gnuplot Kernel

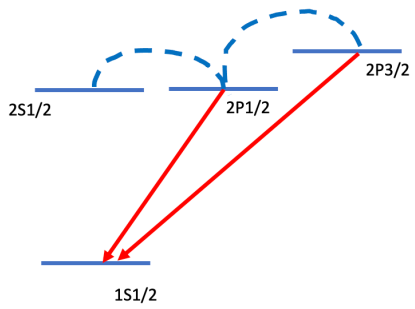
```
[1]: plot 'test/samfld.dat' w l
```



Example :Lineshape of Lyman α with fine structure for hydrogen like argon with protons

pim writes the second file needed for the following phase **pam** whose name is `miscel.`

```
annette.calisti@univ-amu.fr@jupyter:~/test$ more miscel.
  Ar17.dat           ****               (base,pfi) atom data base/ pop file
   3300.00            3340.00           (da,db) frequency interval bounds - eV
    40.000             1.0000           (em,pm) emitter/ perturber mass
    17.000             1.0000           (ze,zp) net emit. charge/ pert. charge
   0.10000E+08        0.10000E+08       (tmpe,tmpi) electron temp/ ion temp. - K
   0.10000E+25        0.10000E-01       (dens,per) elec dens/ emit/pert concent
    2                  10.              (lay,xset) layer nb/ stark trans cutoff
     2                                  (nu) block rad trans nb
  outd               outs               (out,sdof)Stark data, output file
  n                                     (ric) interference terms  (y/n)
   50                25.               (nmc,ecut) fld number/ max field value
  e                     300             (units,npt)(e/a)eV or A/curve point numb.
   3300.00            3340.00           (ai,af) default frequency range
  n                  f                  (dop,cv)doppler (y/n)-convol(f)fft(v)voigt
   0.00000            0.00000           (wg,wl) Gauss FWHM/ Lorentz HWHM eV
  n                                     (nyn) profile normalization  y/n
   0.00000                              (shft) shift in output units
    2.937                                (t) fluctuation rate
      2                                 (krad) radiative transition number
    1    4      4                       (levg,lev,ltrs) ground level,total level & trans. number
  lab. /name /energy /spont. /popu. /2j+1 / /n
   1       ss1s00        0.000000   0.00000E+00   0.10000E+01    2    1
   2       pp2p01     3318.220703   0.42603E-01   0.21268E-01    2    2
   3       ss2s00     3318.388428   0.90349E-13   0.21264E-01    2    2
   4       pp2p00     3323.036377   0.43184E-01   0.42299E-01    4    2
  i-lab. /j-lab. /redu. /  /dlambda /xstrs
   1    2   -0.57735E-01    0.37366E+01    0.39595E-03    2
   2    3   -0.23400E+00    0.73932E+05    0.45626E+01    1
   1    4   -0.82023E-01    0.37311E+01    0.79800E-03    2
   3    4   -0.33237E+00    0.26675E+04    0.46720E+01    1
annette.calisti@univ-amu.fr@jupyter:~/test$
```



Example :Lineshape of Lyman α with fine structure for hydrogen like argon with protons

pim writes the second file needed for the following phase **pam** whose name is `miscel.`

In addition to the header that corresponds to the file `in_new.txt` modified by **pim**, the code writes an estimate of the fluctuation rate for the Markovian fluctuation model and four integers corresponding respectively to:

`t`: the frequency fluctuation rate to be used in the FFM procedure
`krad`: number of radiative transitions actually considered
`levg`: number of ground levels
`lev`: total number of levels
`ltrs`: total number of transitions

The remaining part of the file embodies the atomic data for the problem, the level data package and the transition data package.
In the level data package, the only relevant data used by the main processing are:

```
lab. /energy /popu. /2j+1 / /n
```

In the transition data one, only the first three columns and the last one are used.

The code description

The PAM phase:

- **Phase 2** : Stark effect calculation – expensive in computation time which is increased when interference terms are taken into account (much more extra-diagonal terms)

```
annette.calisti@univ-amu.fr@jupyter:~/test$ ../PPP
 hit pim, pam, poum (pum) or help ?
pam
  outd              outs              (out,sdof) Stark data, output file
  n                                   (ric) interference terms  (y/n)
  new data? or help

  outd              outs              (out,sdof) Stark data, output file
  n                                   (ric) interference terms  (y/n)
 is this Ok? y(def)/n

 zmoy   1.15999997
 Gamma =   2.56348401E-02   el*el/(r0*bolt*tmpi)   !q*q/r0*K*Ti

 nb transitions           4
 ******************************
 nb total de composantes Stark:         686

 nb transitions           4


 view outd        ? y/(n def) ; poum (pum)
y
annette.calisti@univ-amu.fr@jupyter:~/test$
```

The code description

The PAM phase:

At the end of the whole process, the complex coefficients are written down into the file `outd`, which will be read and processed by **poum**.

```
annette.calisti@univ-amu.fr@jupyter:~/test$ ls
Ar17.dat  bars  field  in_new.txt  miscel.  outd  samfld.dat
annette.calisti@univ-amu.fr@jupyter:~/test$ more outd
  3318.132324    0.1658920E-07    0.5967404E-08    0.477309          1
  3318.440186   -0.2275299E-08   -0.5980124E-08    0.717935          1
  3323.072754    0.1079466E-09    0.1272004E-10    0.321601          1
  3318.132324    0.3005939E-07    0.1421771E-07    0.477309          1
  3318.440186   -0.1108918E-08   -0.1420527E-07    0.717935          1
  3323.072754   -0.1067625E-09   -0.1243582E-10    0.321601          1
  3323.036377    0.2170945E-07     0.000000        0.317204          2
  3323.036377    0.2170945E-07     0.000000        0.317204          2
  3318.132324    0.1024035E-08   -0.8536568E-09    0.477309          2
  3318.440186   -0.9122296E-09    0.8942475E-09    0.717935          2
  3323.072754    0.2883412E-07   -0.4059071E-10    0.321601          2
  ...
```

The code description

The POUM phase:

- **Phase 3** : Data post processing
Applying FFM
Dressing of the Stark components with lorentzians
Convolution with Doppler or apparatus function is possible

```
annette.calisti@univ-amu.fr@jupyter:~/test$ ../PPP
 hit pim, pam, poum (pum) or help ?
poum
  outd                outs                (out,sdof) Stark comp. data, output file
  e                      300              (units,npt)(e/a)eV or A/curve point numb.
   3300.00             3340.00             (ai,af) default frequency range
  n                   f                   (dop,cv)doppler(y/n)-convl(f)fft(v)voigt
   0.00000             0.00000             (wg,wl) Gauss FWHM/ Lorentz HWHM eV
  n                                       (nyn) profile normalization  (y/n)
   0.00000                                (shft) shift in output units
  new data? or help
```

At the end of execution, poum writes the files `s_sdof` and `d_sdof` with the two columns intensity versus energy (or wavelength) with `npt` values of energy (or wavelength).

The code description

The POUM phase:

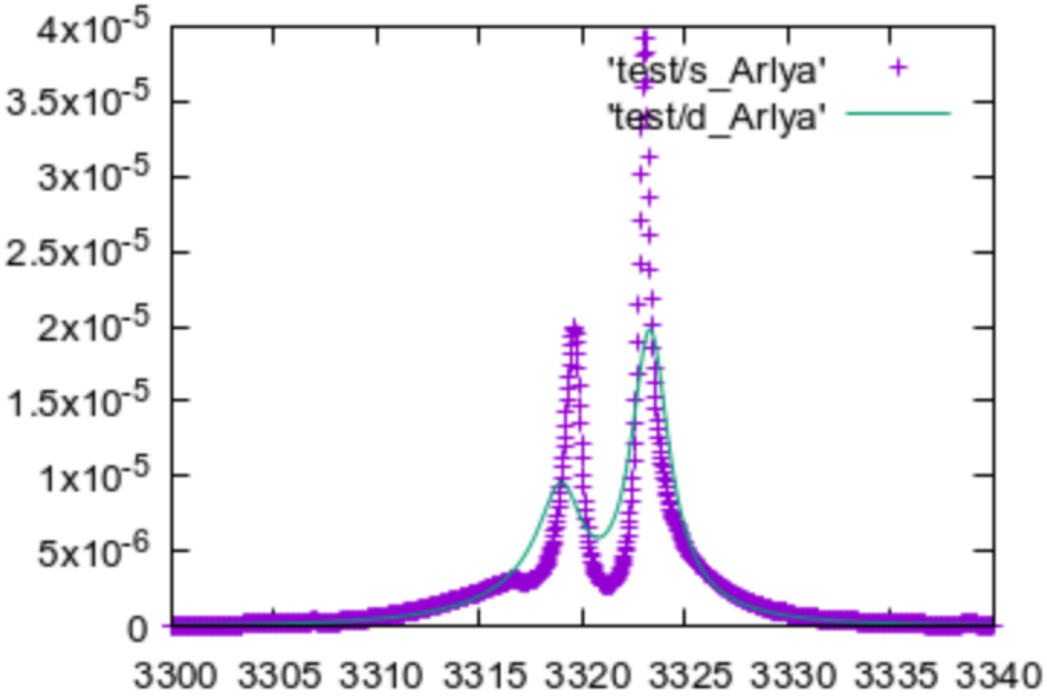
```
annette.calisti@univ-amu.fr@jupyter:~/test$ ../PPP
 hit pim, pam, poum (pum) or help ?
poum
  outd               outs              (out,sdof) Stark comp. data, output file
  e                     300            (units,npt)(e/a)eV or A/curve point numb.
   3300.00            3340.00          (ai,af) default frequency range
  n                  f                 (dop,cv)doppler(y/n)-convl(f)fft(v)voigt
   0.00000            0.00000          (wg,wl) Gauss FWHM/ Lorentz HWHM eV
  n                                    (nyn) profile normalization  (y/n)
   0.00000                             (shft) shift in output units
  new data? or help
npt=1000
  new data? or help
sdof=Arlya
  new data? or help

  outd               Arlya             (out,sdof) Stark comp. data, output file
  e                    1000            (units,npt)(e/a)eV or A/curve point numb.
   3300.00            3340.00          (ai,af) default frequency range
  n                  f                 (dop,cv)doppler(y/n)-convl(f)fft(v)voigt
   0.00000            0.00000          (wg,wl) Gauss FWHM/ Lorentz HWHM eV
  n                                    (nyn) profile normalization  (y/n)
   0.00000                             (shft) shift in output units
 is this Ok? y(def)/n

 zmoy   1.15999997
 Gamma =   2.56348401E-02   el*el/(r0*bolt*tmpi)   !q*q/r0*K*Ti
 Stark transitions number         686
  total intensity=   1.06642481E-04
  total intensity=   1.06642481E-04
 taux melange   2.93729734
           1   Stark comp. :         294
           2   Stark comp. :         392
 norme:  0.983122051

 CPU time =   -4.06799978E-03 seconds
  total intensity=   1.06642481E-04
annette.calisti@univ-amu.fr@jupyter:~/test$
```

The code description

The POUM phase:

```
annette.calisti@univ-amu.fr@jupyter:~/test$ ls
Ar17.dat  bars  d_Arlya  field  in_new.txt  miscel.  outd  samfld.dat  s_Arlya
annette.calisti@univ-amu.fr@jupyter:~/test$
```

```
[3]: plot 'test/s_Arlya' w p, 'test/d_Arlya' w l
```



Examples of application

By increasing density:

```
annette.calisti@univ-amu.fr@jupyter:~/test$ ../PPP
 hit pim, pam, poum (pum) or help ?
pim

 new calculation ? y(def)/n


 Search of Atomic Database ? y/n(def)

  Ar17.dat           ****              (base,pfi) atom data base/ pop file
   3300.00            3340.00          (da,db) frequency interval bounds - eV
    40.000             1.0000          (em,pm) emitter/ perturber mass
    17.000             1.0000          (ze,zp) net emit. charge/ pert. charge
   0.10000E+08        0.10000E+08      (tmpe,tmpi) electron temp/ ion temp. - K
   0.10000E+25        0.10000E-01      (dens,per) elec dens/ emit/pert concent
    2                  10.             (lay,xset) layer nb/ stark trans cutoff
     2                                 (nu) block rad trans nb
  outd               Arlya             (out,sdof) Stark data,output file
  n                                    (ric) interference terms  (y/n)
   50                25.               (nmc,ecut) fld number/ max field value
  new data? or help
dens=2.e24
  new data? or help
```

Run again PIM

for a new calculation

Change the density

And also calculate the field distribution function with the new density:

```
  m-field calculation y(es) (no def.)
  or filename (other distribution)
y
```

Examples of application

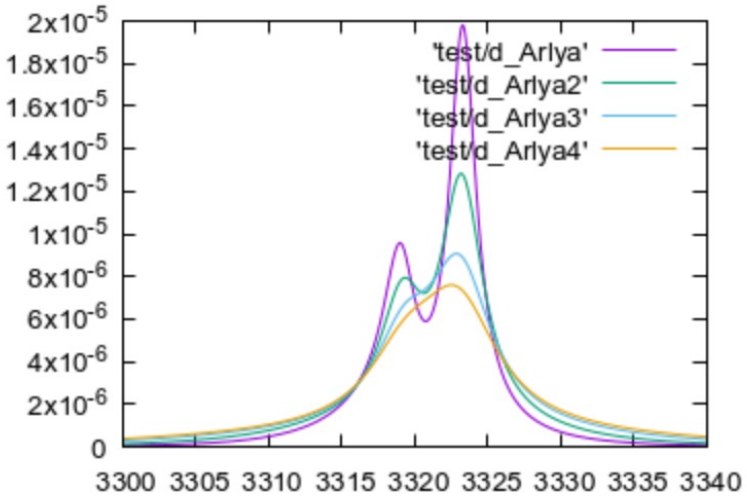
By increasing density:

```
 view outd          ? y/(n def) ; poum (pum)

  outd                Arlya              (out,sdof) Stark comp. data, output file
  e                     1000             (units,npt)(e/a)eV or A/curve point numb.
   3300.00             3340.00           (ai,af) default frequency range
  n                   f                  (dop,cv)doppler(y/n)-convl(f)fft(v)voigt
   0.00000             0.00000           (wg,wl) Gauss FWHM/ Lorentz HWHM eV
  n                                      (nyn) profile normalization  (y/n)
   0.00000                               (shft) shift in output units
  new data? or help
sdof=Arlya2
  new data? or help
```

Change the name of the output file

Do it for n_e between 1.10^{24} and 1.10^{25} and plot the results on the same graph.

```
[5]: plot 'test/d_Arlya' w l, 'test/d_Arlya2' w l, 'test/d_Arlya3' w l, 'test/d_Arlya4' w l
```



note: the profile becomes wider and wider, and the selected energy range becomes too narrow. You need to set it wider to see the whole profile.

Examples of application

Illustrating the choice of atomic system::

```
annette.calisti@univ-amu.fr@jupyter:~/test$ more miscel.
  Ar17.dat          ****              (base,pfi) atom data base/ pop file
   3300.00           3340.00          (da,db) frequency interval bounds - eV
    40.000            1.0000          (em,pm) emitter/ perturber mass
    17.000            1.0000          (ze,zp) net emit. charge/ pert. charge
   0.10000E+08       0.10000E+08      (tmpe,tmpi) electron temp/ ion temp. - K
   0.10000E+25       0.10000E-01      (dens,per) elec dens/ emit/pert concent
     2                 1.             (lay,xset) layer nb/ stark trans cutoff
      1                               (nu) block rad trans nb
  outd              ArlyaSplit       (out,sdof)Stark data, output file
  n                                  (ric) interference terms  (y/n)
   50               25.               (nmc,ecut) fld number/ max field value
  e                   1000           (units,npt)(e/a)eV or A/curve point numb.
   3300.00           3340.00          (ai,af) default frequency range
  n                 f                 (dop,cv)doppler (y/n)-convol(f)fft(v)voigt
   0.00000           0.00000          (wg,wl) Gauss FWHM/ Lorentz HWHM eV
  n                                  (nyn) profile normalization  y/n
   0.00000                           (shft) shift in output units
    2.937                            (t) fluctuation rate
      2                              (krad) radiative transition number
    1    3      2                    (levg,lev,ltrs) ground level,total level & trans. number
  lab. /name /energy /spont. /popu. /2j+1 / /n
   1       ss1s00        0.000000   0.00000E+00   0.10000E+01    2    1
   3       ss2s00     3318.388428   0.90349E-13   0.21264E-01    2    2
   4       pp2p00     3323.036377   0.43184E-01   0.42299E-01    4    2
  i-lab. /j-lab. /redu. /  /dlambda /xstrs
   1    4   -0.82023E-01    0.37311E+01    0.79800E-03    2
   3    4   -0.33237E+00    0.26675E+04    0.46720E+01    1
    1    3      2                    (levg,lev,ltrs) ground level,total level & trans. number
  lab. /name /energy /spont. /popu. /2j+1 / /n
   1       ss1s00        0.000000   0.00000E+00   0.10000E+01    2    1
   2       pp2p01     3318.220703   0.42603E-01   0.21268E-01    2    2
   3       ss2s00     3318.388428   0.90349E-13   0.21264E-01    2    2
  i-lab. /j-lab. /redu. /  /dlambda /xstrs
   1    2   -0.57735E-01    0.37366E+01    0.39595E-03    2
   2    3   -0.23400E+00    0.73932E+05    0.45626E+01    1
```

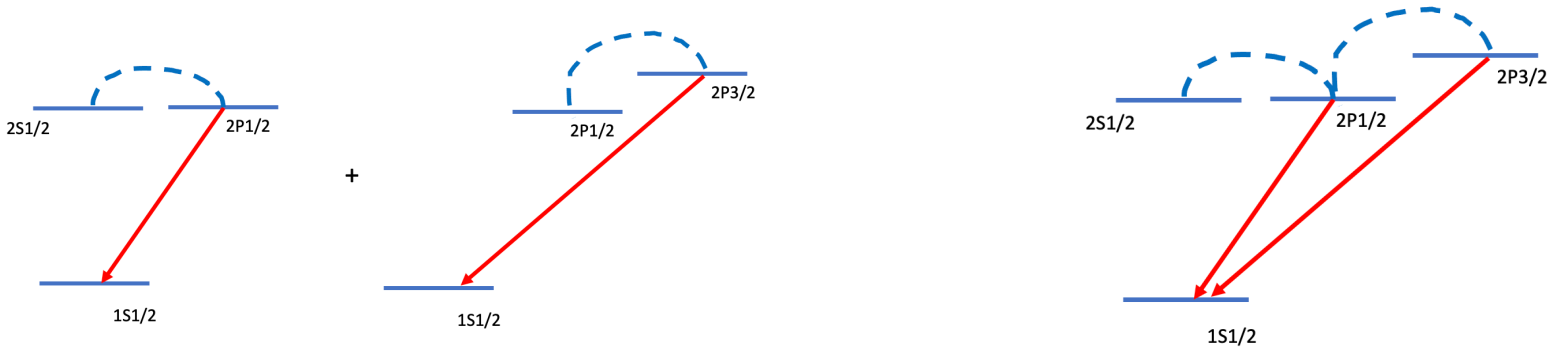
`xset` is chosen too small

`Xset=1.2`

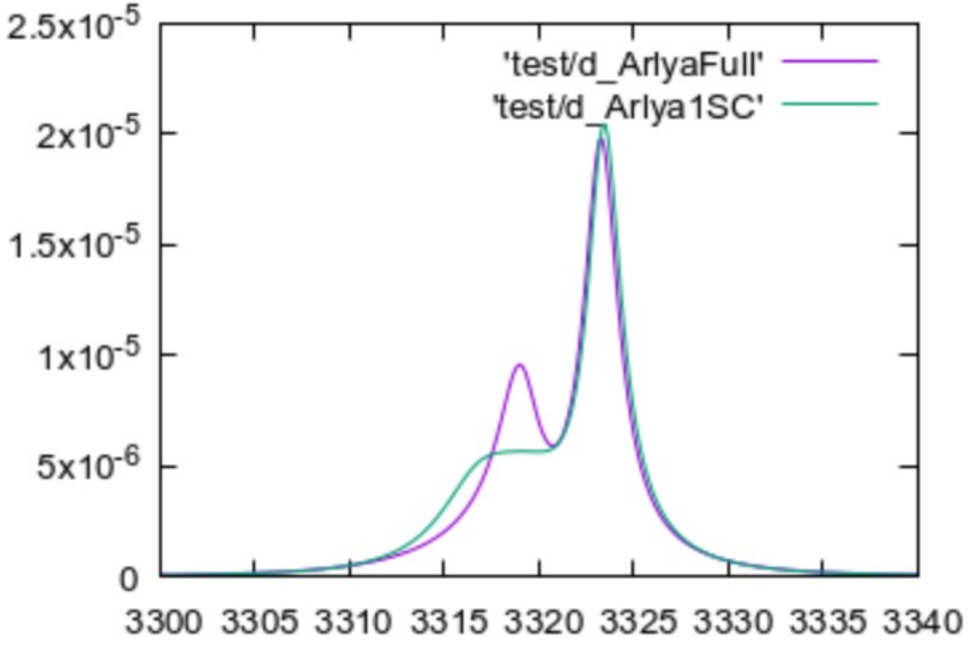
transition-by-transition calculation

Examples of application

Illustrating the choice of atomic system::




```
[13]: plot 'test/d_ArlyaFull' w l, 'test/d_Arlya1SC' w l
```



note: Calculating the profile transition by transition is not a very strong approximation, but Stark couplings must be carefully selected.