VIII School of Neutron Scattering "Francesco Paolo Ricci"

Structures and Dynamics of Magnetic Systems

Intermultiplet transitions in Pr: Monte Carlo simulations of High Energy Inelastic Neutron Scattering experiments

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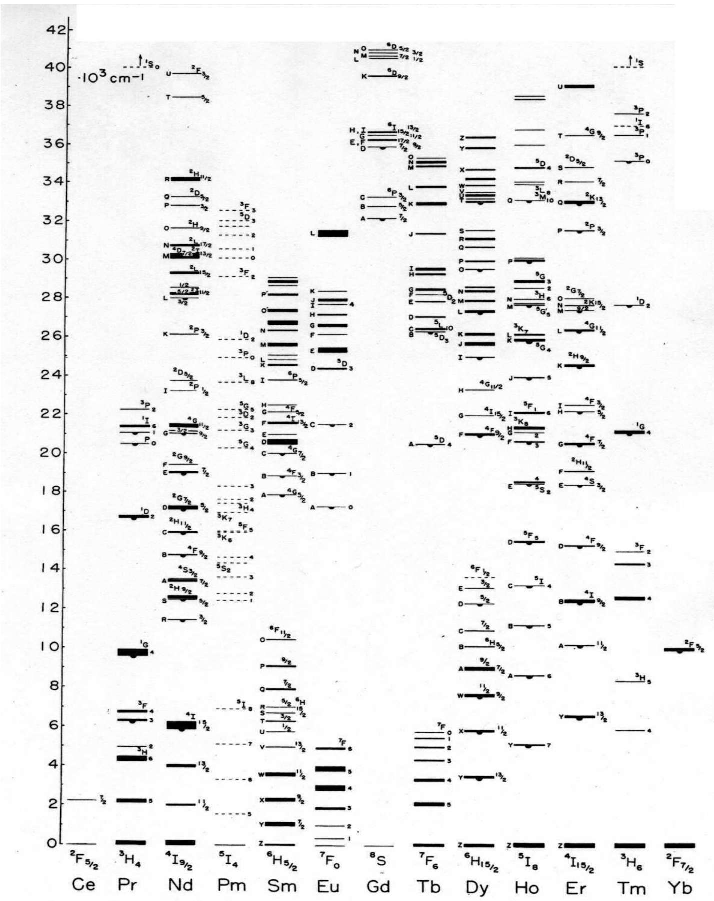
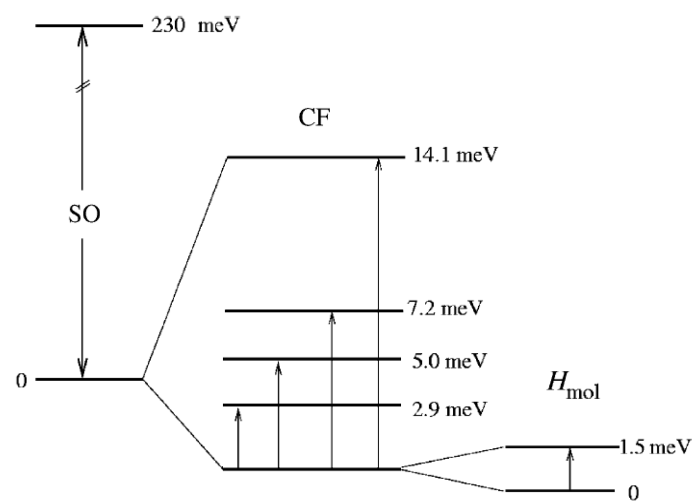
Intermultiplet transitions of rare-earths metals and compounds extend in the eV range. High energy Inelastic Neutron Scattering measurements allow to complement and extend optical measurements into the eV range, including their wavevector dependence. A tutorial on Monte Carlo simulation codes allowing to predict the performances of eV spectrometers for intermultiplet transition experiments is presented.

Typical splitting of levels in a rare-earth system due to the 4*f* electrons lie in the hundreds of meV to eV range.





Typical splitting of levels in a rare earth system due to spin–orbit (SO), crystal-field (CF), and exchange interaction (H_{mol}). Scheme reproducing approximately the situation of Nd^{3+} ions in $NdCu_2$.

Kinematic range:

$$\frac{\hbar^2 Q^2}{2m} = E_0 + E_1 - 2\sqrt{E_0\ E_1}\cos\theta \qquad (1)$$

where m is the neutron mass.

Kinematical restrictions to high energy - low wavevector transfers.

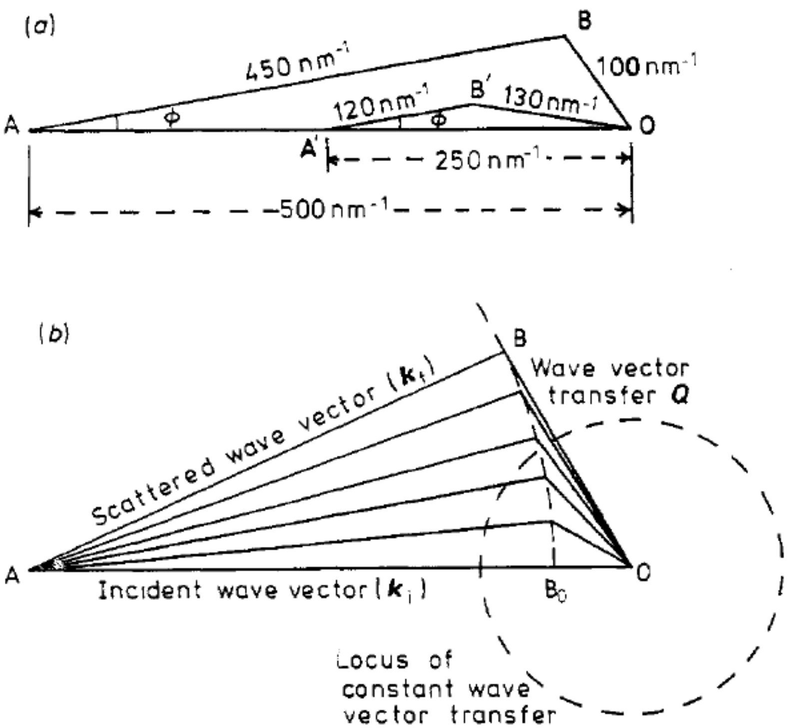


Figure 1 Vector scattering diagrams.

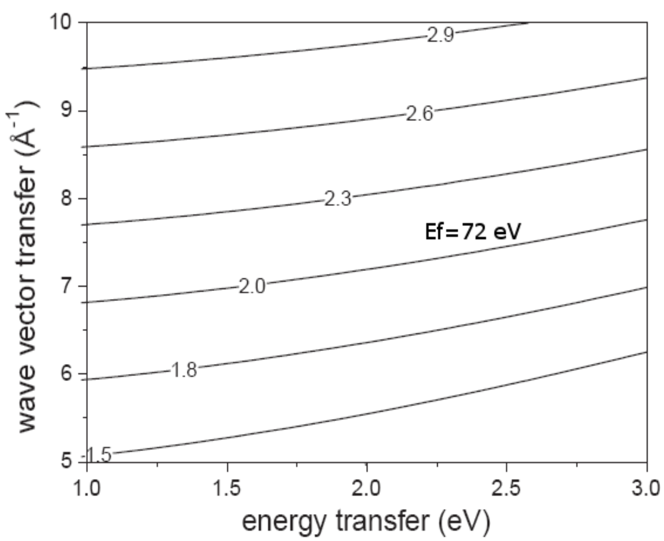
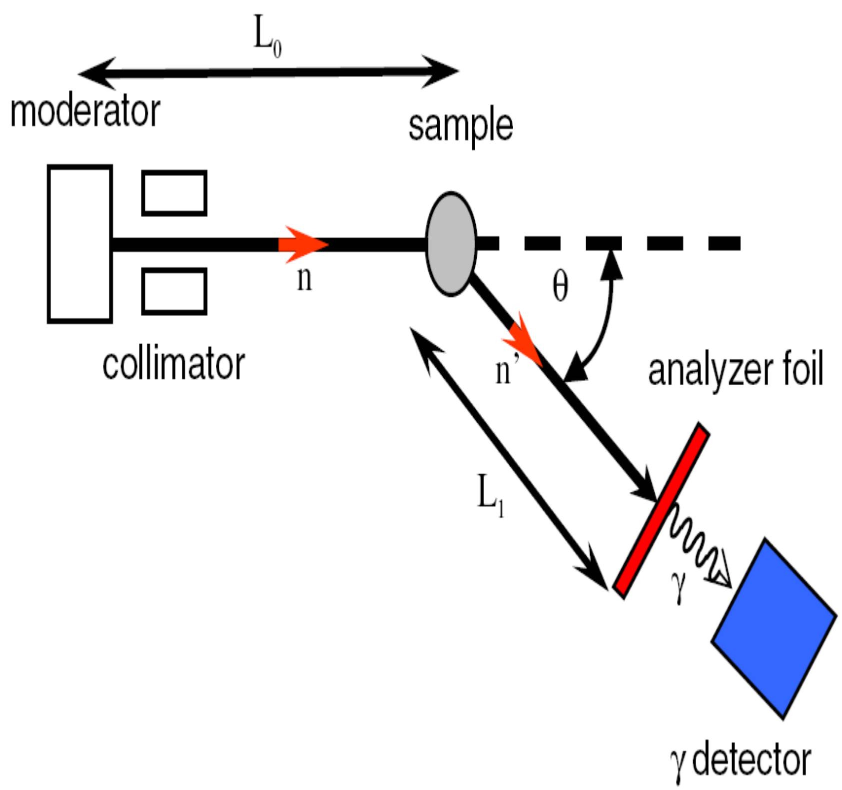


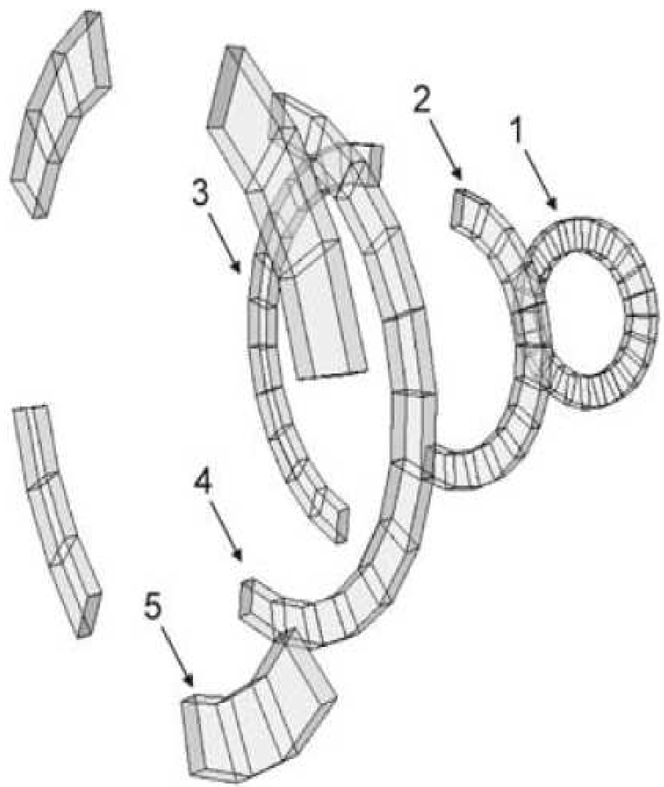
Fig. 3. Contour plot of equal scattering angle as a function of wave vector transfer and energy transfer for a fixed final neutron energy of 72 eV (lantanum resonance).

Inverse geometry (E_1 fixed) unlimited in energy loss.

This means final energy in the $\geq$ 10 eV: i.e. detection and energy selection technologies for eV neutrons. VESUVIO spectrometer.
1) Resonant detector configuration

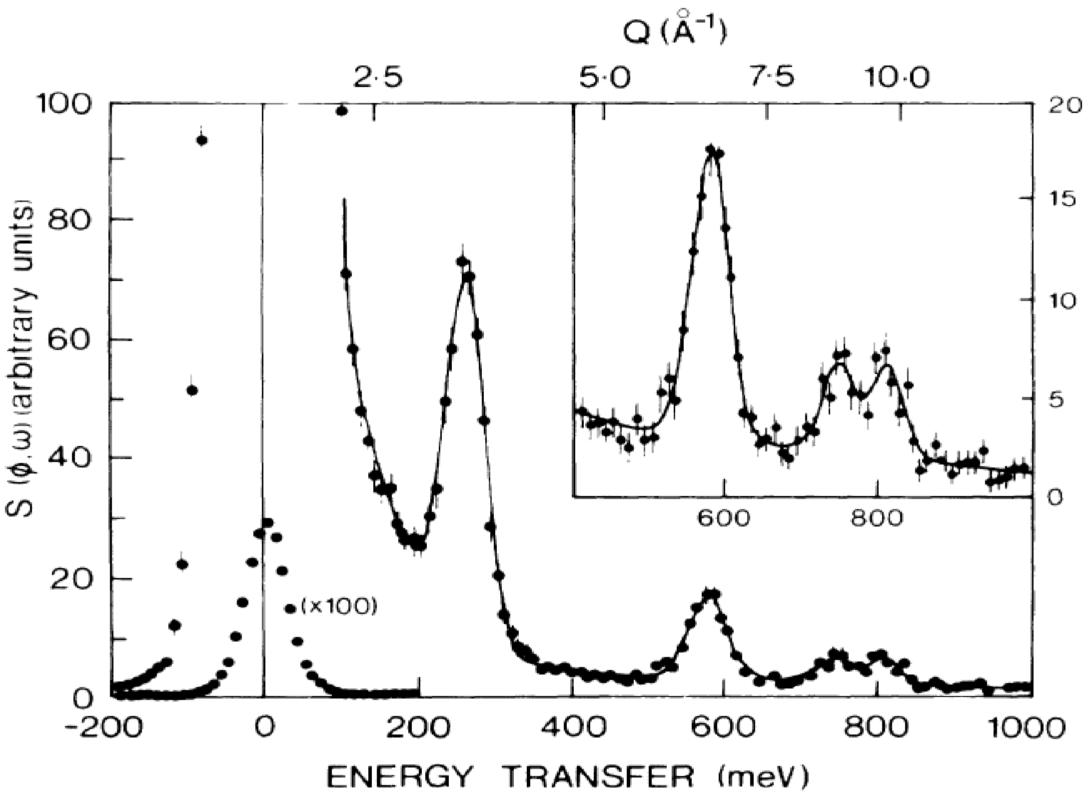


VESUVIO spectrometer.
2) Very Low Angle Detector bank



Scattering angles in the range $1^\circ \leq \phi \leq 4^\circ$

Background: Intermultiplet transitions observed in metallic Pr in the range: $0 \leq \hbar\omega \leq 1600$ meV;$1 \leq Q \leq 15$ $\dot{A}^{-1}$; (A.D. Taylor et al., PRL, 61, 1309 (1988)). Transition $^3H_4 \rightarrow ^1G_4$ @1170 meV was not observed.



Proposed experiment using the VLAD detector on VESUVIO.

Assessment of experiment through a Monte Carlo simulation of the scattering spectra. USE of DINSMS code (J. Mayers et al. NIM-A 481, 454 (2002).

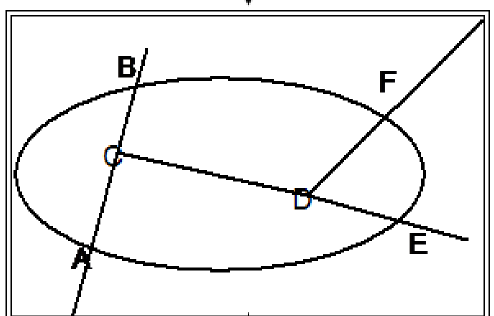
VESUVIO spectrometer

Source: Time-energy distribution

Assign initial weight
1 neutron=weight 1

collimation

$$\frac{\partial^2 \sigma}{\partial \Omega \partial E_1} = \frac{\sigma}{4\pi} \frac{k_1}{k_0} S\,(q,\omega)$$



Attenuation:
Scattering,
absorption
transmission

•Increment TOF and weight

Analyzer- E1

Detector

Final weight in time bin

Tutorial task: simulate scattering spectra from Pr using VLAD detector bank on VESUVIO. Estimate Q,$\hbar\omega$ range accessed on each fixed-angle element.

1 1 Fortran source code file - 1 executable

2 1 command file

3 1 instrument parameter file

4 output: ascii files of time of flight - intensity spectra

Notes on source code: 1) energy analyser: ^{238}U resonant filter

Senza nome - Blocco note

File Modifica Formato Visualizza ?

```
FUNCTION TO GENERATE FINAL ENERGY VALUES FOR URANIUM FOIL ANALYSER AT 293K
 WITH NUMBER DENSITY OF 1.456E20 ATOMS/SQ CM.
 modificata 3/6/2003
    FUNCTION U1GEN(XV)
    PARAMETER(N=2665)
    REAL E(N),X(N)
    DATA (E(I),I=1,N)
   $/1027.6,1127.6,1261.0,1378.3,1504.3,1630.3,1749.0,1867.6,
   $2049.4,2231.2,2428.8,2581.5,2734.1,2886.8,2963.2,3155.5,
   $3299.7,3443.9,3588.2,3684.3,3789.4,3903.3,3988.7,4074.2,
   $4131.1,4188.1,4231.7,4257.9,4275.4,4284.1,4292.9,4299.4,
   $4306.0,4312.5,4316.9,4321.2,4325.6,4329.8,4333.8,4337.8,
   $4343.8,4349.9,4367.2,4372.8,4377.7,4382.3,4386.8,4391.5,
   $4393.0,4397.6,4402.2,4406.8,4411.4,4416.9,4426.1,4435.2,
   $4442.0,4446.6,4451.1,4455.6,4460.2,4464.4,4470.3,4476.1,
   $4482.0,4489.8,4497.2,4507.6,4514.5,4535.3,4563.0,4604.5,
   $4659.9,4715.2,4770.1,4825.1,4880.0,4934.9,4989.8,5044.7,
   $5099.6,5154.5,5197.4,5240.3,5283.2,5326.1,5369.0,5411.9,
   $5454.8,5497.6,5531.1,5564.5,5597.9,5631.4,5664.8,5698.2,
   $5731.6,5765.1,5793.5,5822.0,5850.5,5879.0,5907.4,5928.8,
   $5950.1,5971.5,5992.8,6014.0,6035.1,6056.2,6077.4,6098.5,
   $6114.3,6130.2,6146.0,6161.9,6177.8,6193.7,6209.6,6225.5,
   $6237.5,6249.4,6261.4,6273.3,6285.2,6295.1,6306.9,6318.7,
   $6330.5,6342.3,6351.1,6359.9,6368.8,6377.6,6383.5,6392.5,
   $6401.6,6410.6,6417.4,6424.2,6430.9,6437.7,6444.5,6451.3,
   $6458.1,6465.1,6469.8,6474.5,6479.2,6483.9,6488.6,6493.2,
   $6498.1,6502.9,6506.1,6509.7,6513.3,6516.2,6519.2,6522.0,
   $6524.7,6527.4,6530.1,6532.8,6535.4,6538.4,6541.4,6543.4,
   $6545.8,6548.2,6550.6,6553.0,6555.1,6557.3,6559.4,6561.6,
   $6563.7,6565.8,6567.9,6570.0,6572.1,6574.6,6576.4,6578.2,
   $6580.0,6581.8,6583.6,6585.4,6588.0,6590.4,6592.8,6595.2,
   $6597.6,6600.0,6602.8,6605.6,6608.4,6611.2,6614.9,6618.7,
   $6623.5,6630.3,6640.7,6644.7,6648.7,6652.5,6656.1,6659.5,
   $6663.3,6666.5,6669.7,6672.9,6674.0,6676.9,6680.8,6684.0,
```

Notes on source code: 2) γ detectors for tagging in time the radiative resonant absorption in ^{238}U filter. 3) Partial differential cross section: nuclear+magnetic scattering.

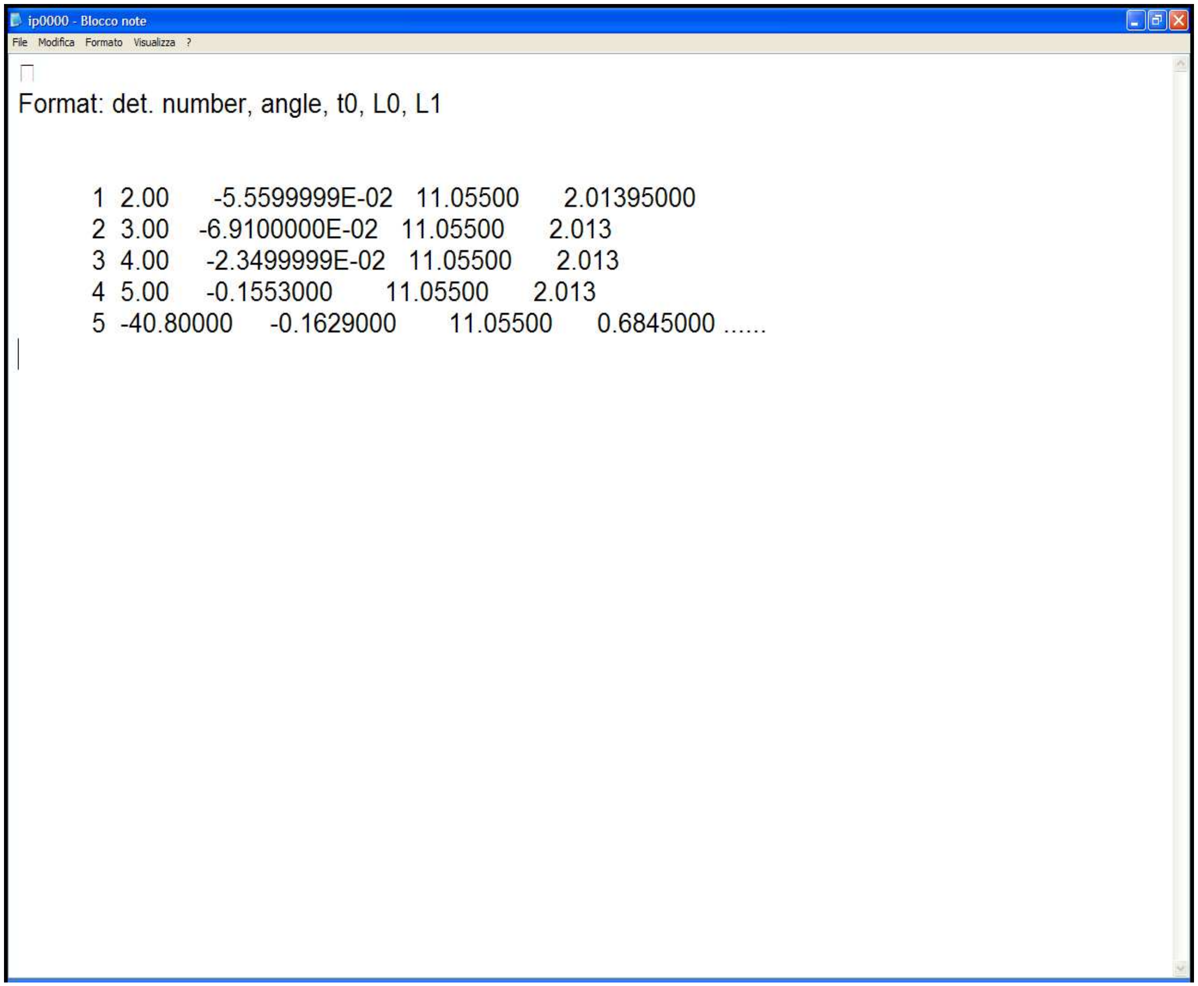
$$\frac{d^2\sigma}{d\Omega dE_1} = \frac{k_1}{k_0}\sigma_n S_n(\mathbf{Q},\omega) + \frac{k_1}{k_0}\, r_0^2\, G(\mathbf{Q};\mu,\nu)\,\delta(\hbar\omega + E_\mu - E_\nu) \quad (2)$$

Senza nome - Blocco note

File Modifica Formato Visualizza ?

```
*mod 26-6-06 added magnetic XS form Praseodimium
      FUNCTION PDCS(E0,E1,TH,NM,M,B,SIG)
      REAL M(NM),SIG(NM),B(NM),K0,K1,J
      REAL j1,j2,j3,jj
      real acca3,acca4,acca6,x2medio,x

*       write(6,*) ' pdcs. e0=',e0,' e1=',e1,' th=',th
      RT2PI=SQRT(2.0*ACOS(-1.0))
      K0=SQRT(E0/2.0717)
      K1=SQRT(E1/2.0717)
      Q=SQRT(K0**2+K1**2-2.0*K0*K1*COS(TH))
      W=E0-E1
      w0M1=417.
   gdip=0.0016+0.0984*exp(-Q/2.009)
   gnodip=-0.00933/(1+exp((Q-3.85)/0.63))+0.00933
   peak1=EXP(-(w-261.)**2/(20.**2))/(20.*RT2PI)
   peak2=EXP(-(w-578.)**2/(20.**2))/(20.*RT2PI)
   peak3=EXP(-(w-747.)**2/(20.**2))/(20.*RT2PI)
   peak4=EXP(-(w-809.)**2/(20.**2))/(20.*RT2PI)
   peak5=EXP(-(w-1170.)**2/(20.**2))/(20.*RT2PI)
   sqwmag=gdip*peak1+gnodip*(peak2+peak3+peak4+peak5)
* n.b. w0M1 e' per M=1 amu
      PDCS=0.0
*   4.18036=hbar^2 in meV*amu*A^2
      ................................................


        SQW=M(I)*J/(4.18036*Q)
        PDCS=PDCS+B(I)**2*(K1/K0)*SQW
   PDCS=PDCS+0.29*sqwmag
```

Notes on instrument parameter file:



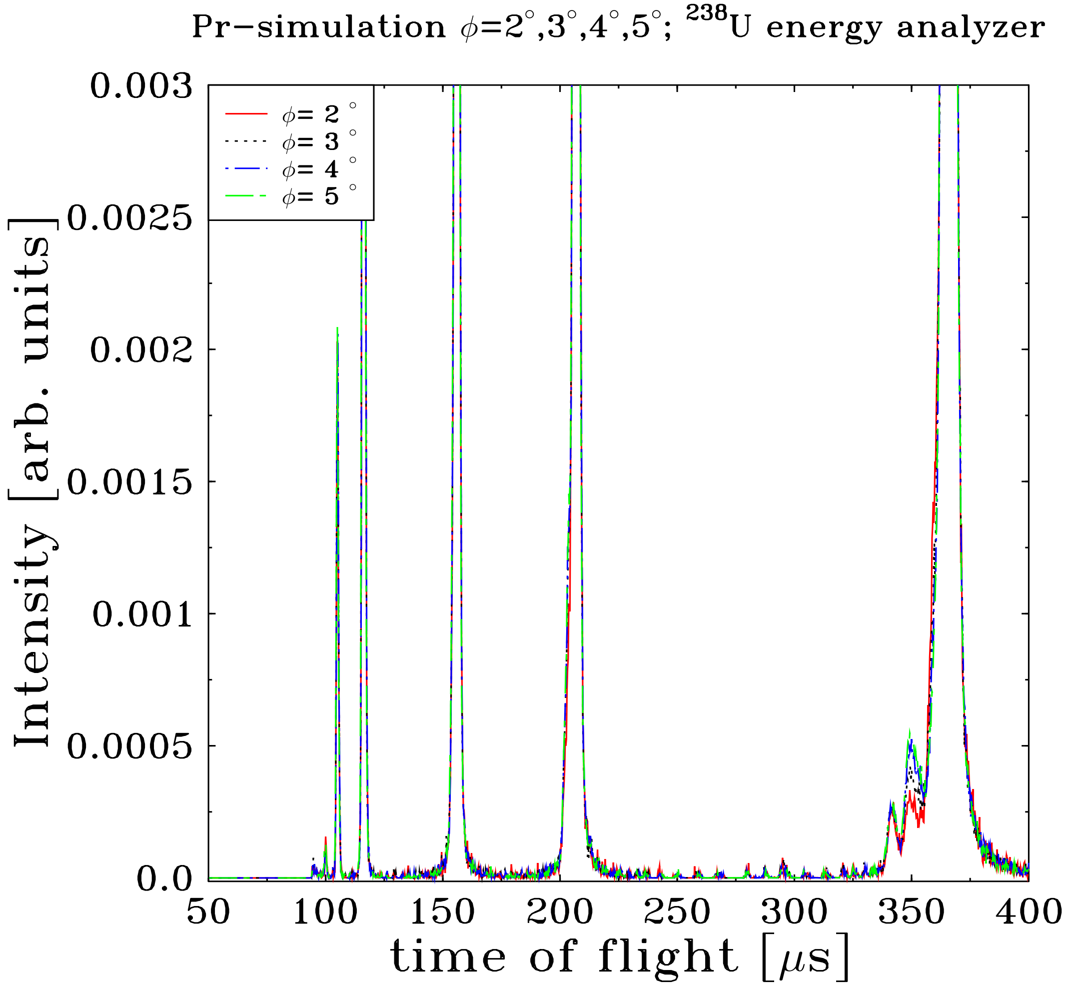

```
Format: det. number, angle, t0, L0, L1


        1  2.00     -5.5599999E-02   11.05500     2.01395000
        2  3.00   -6.9100000E-02   11.05500     2.013
        3  4.00    -2.3499999E-02   11.05500     2.013
        4  5.00    -0.1553000      11.05500     2.013
        5  -40.80000    -0.1629000      11.05500     0.6845000 ......
```

pr.com - Blocco note

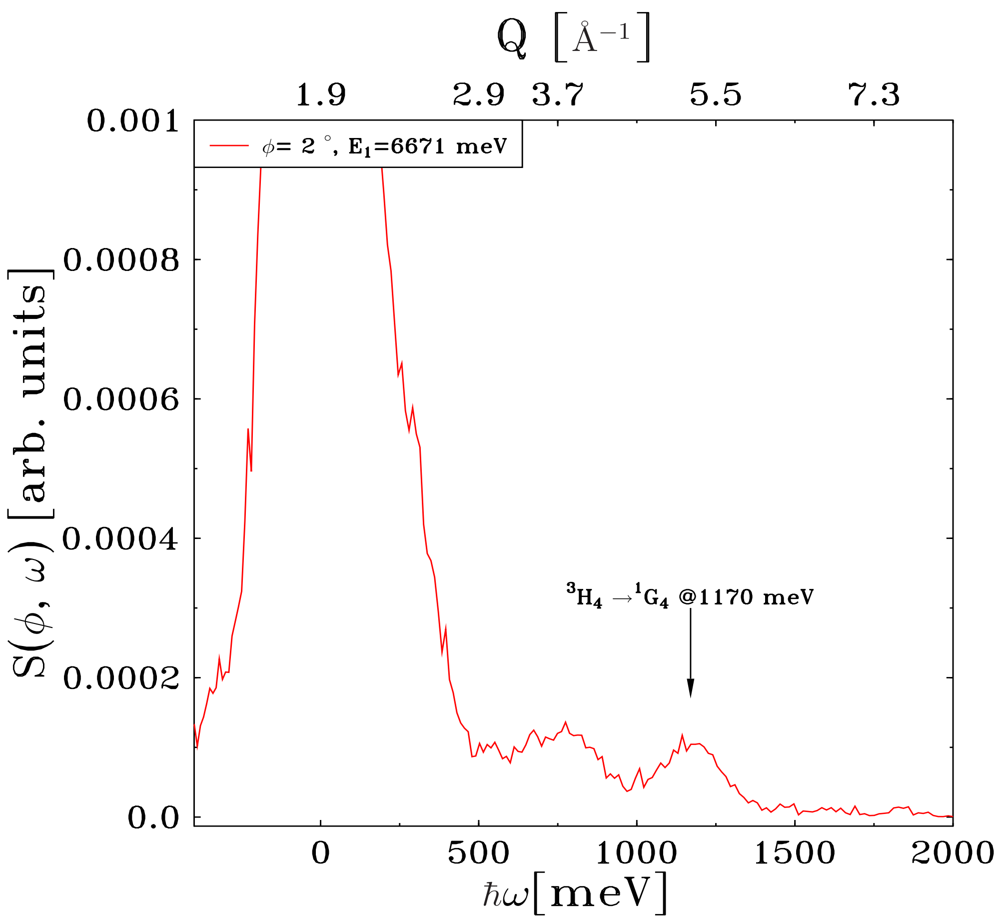
File Modifica Formato Visualizza ?

```
0001             ! No of instrument parameter file.
1 1              ! First and last detectors
66671. 100         ! Final energy and HWHM of res fn (meV)
0.3 2.1          ! Dt0 in microsec, DL0 in cm.
50 400 0.25       ! Minimum and maximum tof+ channel width (micro-sec)
1.5 2.0          ! Radius of umbra and penumbra in c.m.
3.5 3.5 1.0       ! Height, width and depth of detector in cm.
1                ! Sample geometry. 1=slab,2=cylinder'
0                ! Sample angle
10.0 10.0 0.2    ! R and Height of cylinder or thickness, ht,width of slab.
1                           ! Number of different atomic masses.
140. 10. 20. 1.  ! Mass, xsect, s.d. of J(y),no atoms Pb
11.3             ! Density of sample in gm/cubic cm.
6.0e6             ! Number of events
1                ! Maximum order of scattering
tutorial_pr          !name of output file
```

Example of a time of flight spectrum:



Example of an $S(\phi, \omega)$ spectrum:



- Simulate tof spectra
- Transform into $S(\phi, \omega)$
- Adjust simulation parameters
- Estimate Q-dependence