

*PHOnon Excitation by Nuclear Inelastic X-ray scattering*

*Software for the evaluation of  
Nuclear Inelastic X-ray Scattering Spectra*

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# About PHOENIX:

- developed 1995 by W. Sturhahn at the APS
  - ☆ incoherent inelastic nuclear resonant scattering
  - ☆ explain first NRIXS experiments (Sturhahn et al. PRL 74, 1995)
  - ☆ FORTRAN code implemented on Sun UNIX
  
- improved 1995-2010 by W. Sturhahn at the APS
  - ☆ resolution function subtraction, 1997
  - ☆ ported to Linux in 2004
  - ☆ sound velocity treatment, 2007
  - ☆ visualization support, version 2.0.0 (2009)
  
- improved 2010- by W. Sturhahn and *NRIXS software*
  - ☆ inverse construction (DOS to spectrum), version 2.1.0 (2012)
  - ☆ API for variable data input formats, version 2.1.0, (2012)

*publications related to PHOENIX:*

*W. Sturhahn, Hyperfine Interact 125 (2000)*

## PHOENIX now supports:

- all Mössbauer isotopes
- addition of raw data sets including normalization
- creation of energy scale from angle/temperature data
- flexible procedure for subtraction of elastic peak
- data normalization
- detailed balance, energy calibration, and moment calculation
- correction routine for limited-range spectra
- partial phonon density-of-states extraction with Fourier-Log method
- consistency checks of moment and PDOS results
- optional deconvolution with resolution function
- flexible extrapolation scheme for Debye sound velocity extraction
- aggregate compressional and shear sound velocities
- reconstruction of spectra from measured or theoretical PDOS
- calculation of various thermodynamic quantities from PDOS

## More on PHOENIX:

- has been used for data evaluation in numerous publications
- distributed under GPL, source code public, evaluations traceable
- can be obtained per e-mail from Wolfgang Sturhahn, no charge
- a major upgrade, PHOENIX-2.0.0, was released in 2009
  
- PHOENIX-2.0.0
  - ☆ has a simple installation procedure for Unix and Mac OS X
  - ☆ offers all previous capabilities of PHOENIX
  - ☆ features run-time graphics
  
- PHOENIX-2.1.0
  - ☆ API for custom data input formats, e.g., SPEC or mda
  - ☆ inverse calculations, i.e., NRIXS spectra from DOS

# PHOX app screen shot:

The screenshot displays the PHOX software interface, which consists of three main windows:

- Terminal (xmgrace):** Shows the execution of the PHOX module. It displays copyright information, version details (2.0.0), and processing results for the file "Fe.dat". Key parameters include:
  - Nuclear transition energy: 14.413 keV
  - Recoil energy of free atom: 1.956 meV
  - Temperature of the material: 297.00 K
  - Constant background: 0.45 cnts/channel
  - Normalization correction: 0.00 %/100meV
 The terminal also shows the fit of the elastic peak, quantities derived directly from the data (e.g., Lamb-Mössbauer factor: 0.7978), and quantities derived after refinement (e.g., Lamb-Mössbauer factor: 0.7980). A warning indicates 1 serious inconsistency was detected.
- Plot Window (Grace):** Contains two plots:
  - peak subtraction:** A plot of counts versus energy (meV) showing the experimental data (green dots) and the fitted peak (red line).
  - partial phonon DOS:** A plot of PDOS (r/eV) versus energy (meV) showing the phonon density of states (blue dots) and the fitted peak (red line).
- Emacs Editor:** Displays the documentation for the PHOX module, including:
  - General information: transition energy (14.4125 keV) and recoil energy (1.956 meV).
  - Input data specific information: sample temperature (297 K), data file name (Fe.dat), and normalization correction (0.45 0).
  - Output data specific information: a table of options and their corresponding file names.

## PHOENIX modules:

### ➤ padd

- ☆ interface between data acquisition and user evaluation
- ☆ creates energy scale, adds scans, normalizes data
- ☆ features customizable API for arbitrary data formats

### ➤ phox

- ☆ extracts phonon DOS from NRIXS spectrum
- ☆ calculates moments of NRIXS spectrum
- ☆ performs consistency checks

### ➤ psvl

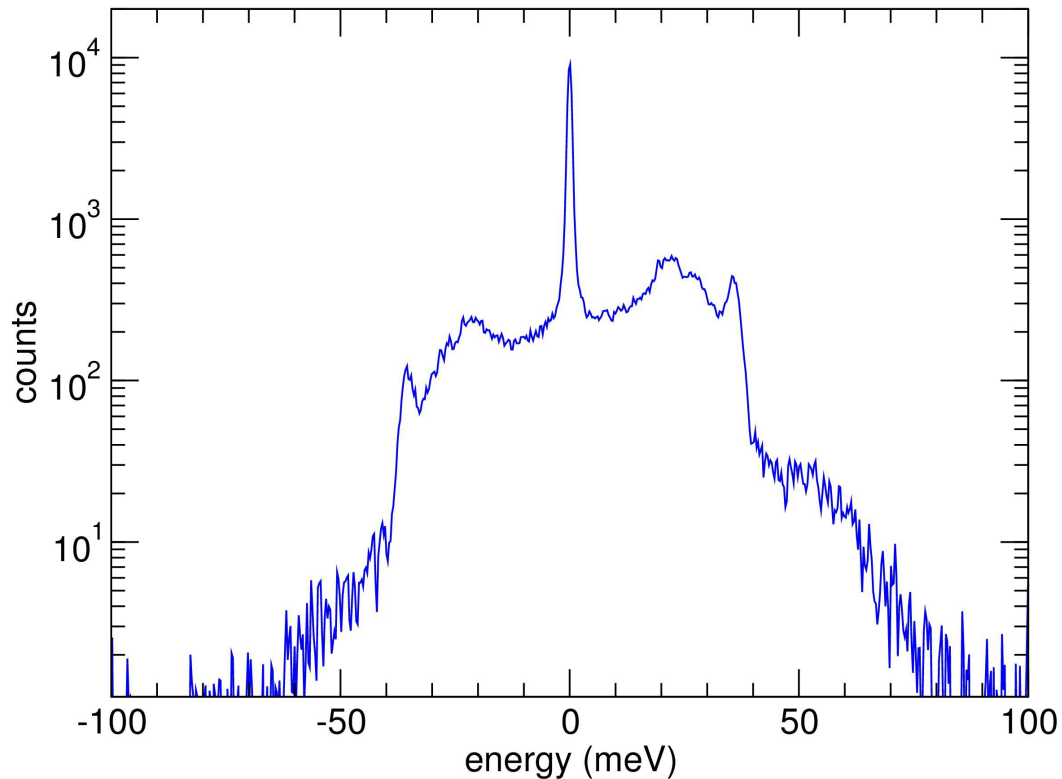
- ☆ extracts aggregate sound velocities from partial phonon DOS

### ➤ psth

- ☆ creates NRIXS spectrum from phonon DOS
- ☆ calculates temperature dependent contractions of phonon DOS

## example 1.1:

- add data of several NRIXS scans on bcc-Fe, ASCII input format



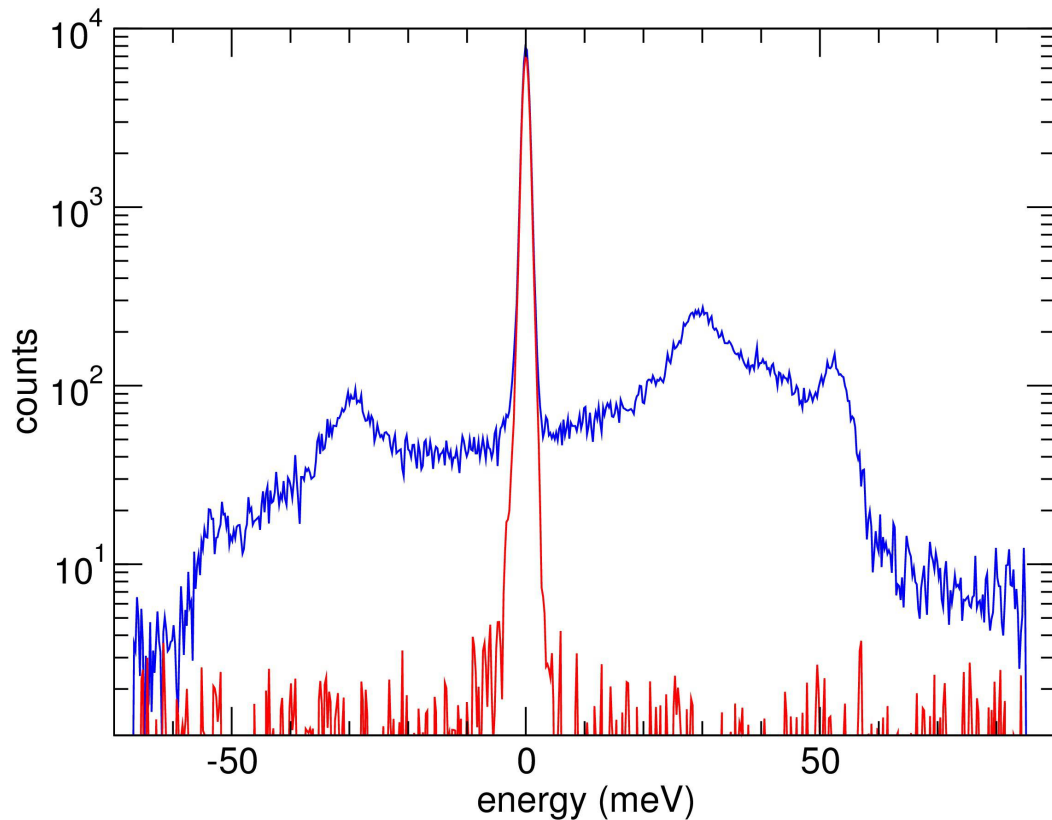
- ☆ construct the input file `in_padd`
- ☆ inspect output files  
`*.shf`, `*.mon`, `*.ptp`

Command:

`padd`

## example 1.2:

- add data of several NRIXS scans on hcp-Fe, ASCII input format, simultaneous creation of resolution function



- ☆ construct the input file in\_padd
- ☆ inspect output directories/files

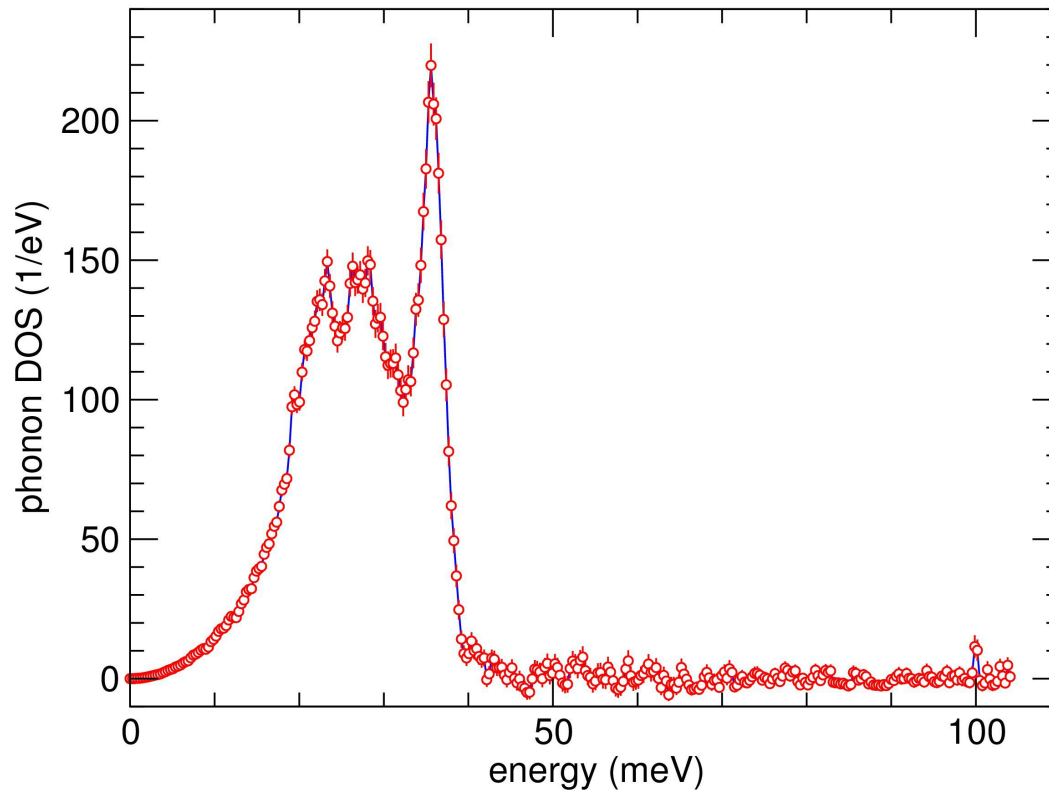
Command:

```
mpadd NRIXS:11 NFS:9
```



## example 2.1:

- extract phonon DOS from bcc-Fe spectrum created in exp. 1.1



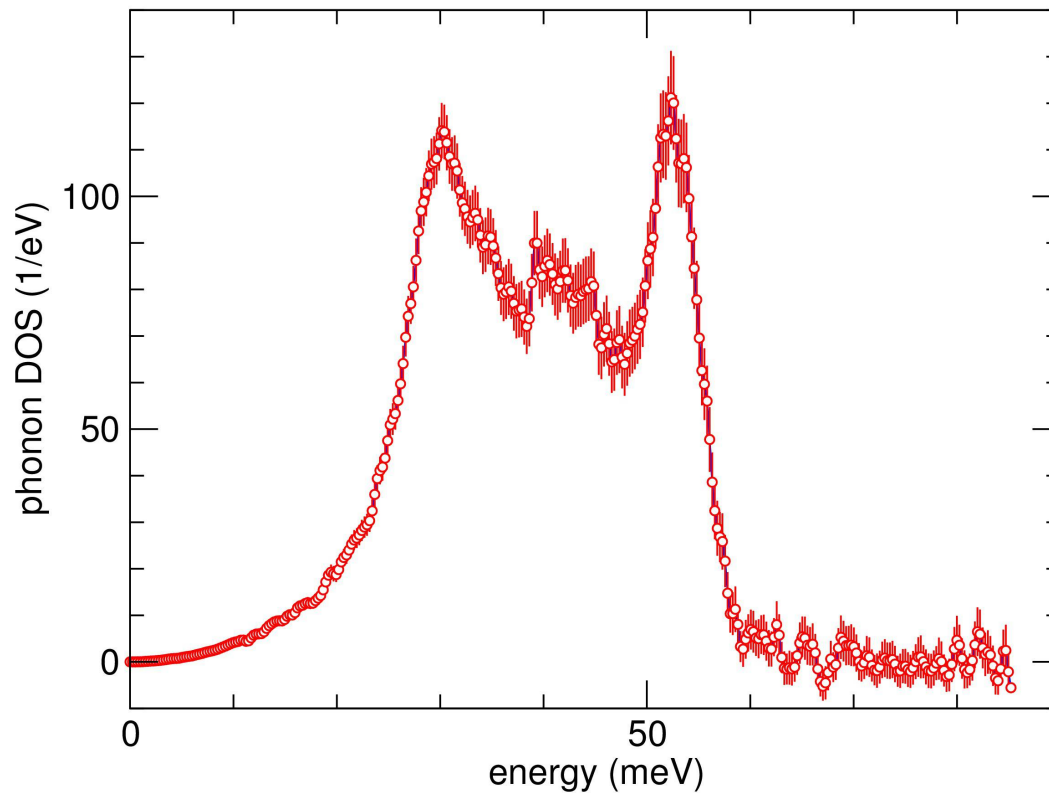
- ☆ construct the input file `in_phox`
- ☆ inspect output files

Command:

`phox`

## example 2.2:

- extract phonon DOS from hcp-Fe spectrum created in exp. 1.2 using data and resolution function



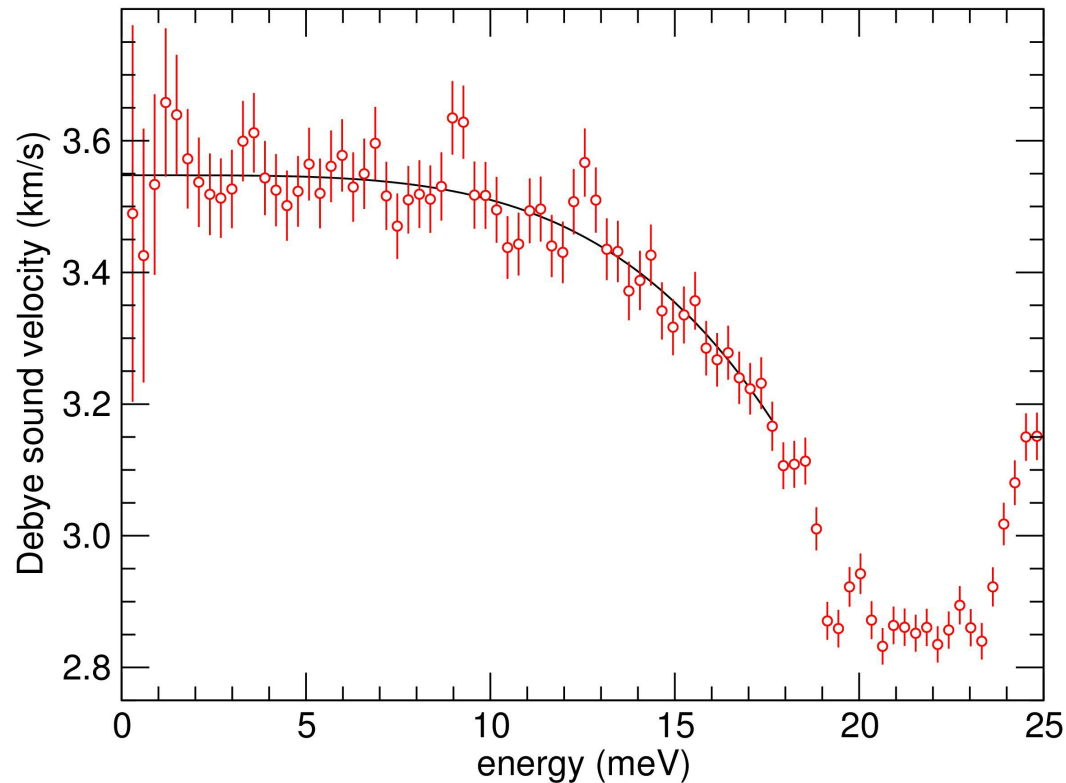
- ☆ construct the input file `in_phox`
- ☆ inspect output files

Command:

`phox`

## example 3.1:

- extract sound velocities from phonon DOS created in exp. 2.1



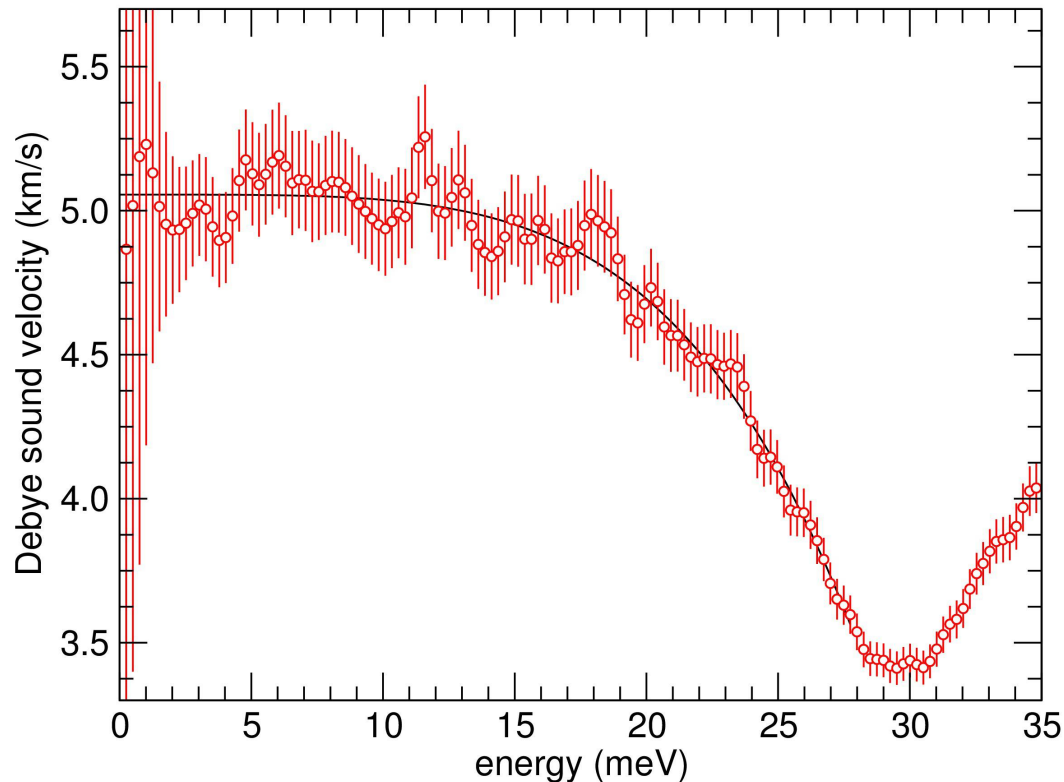
- ☆ construct the input file `in_psv1`
- ☆ inspect output files

Command:

`psv1`

## example 3.2:

- extract sound velocities from phonon DOS created in exp. 2.2



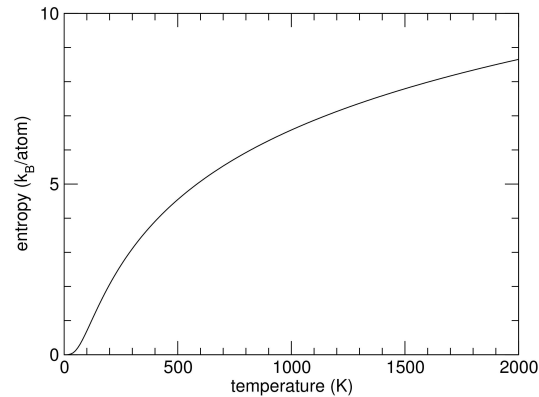
- ☆ construct the input file `in_psv1`
- ☆ inspect output files

Command:

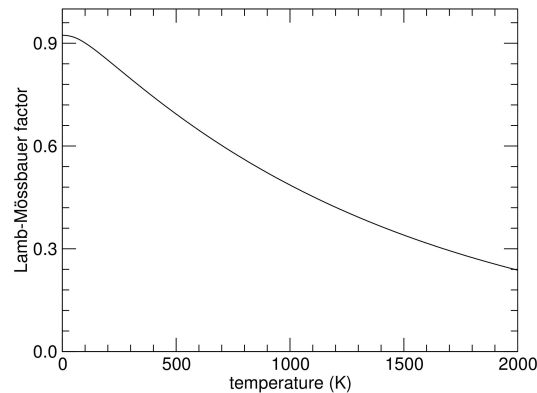
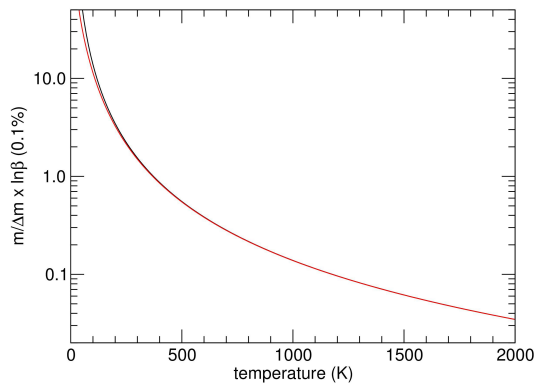
`psv1`

## example 4.1:

- calculate temperature dependent functions  
from phonon DOS created in exp. 2.1



- ★ construct the input file `in_psth`
- ★ inspect output files

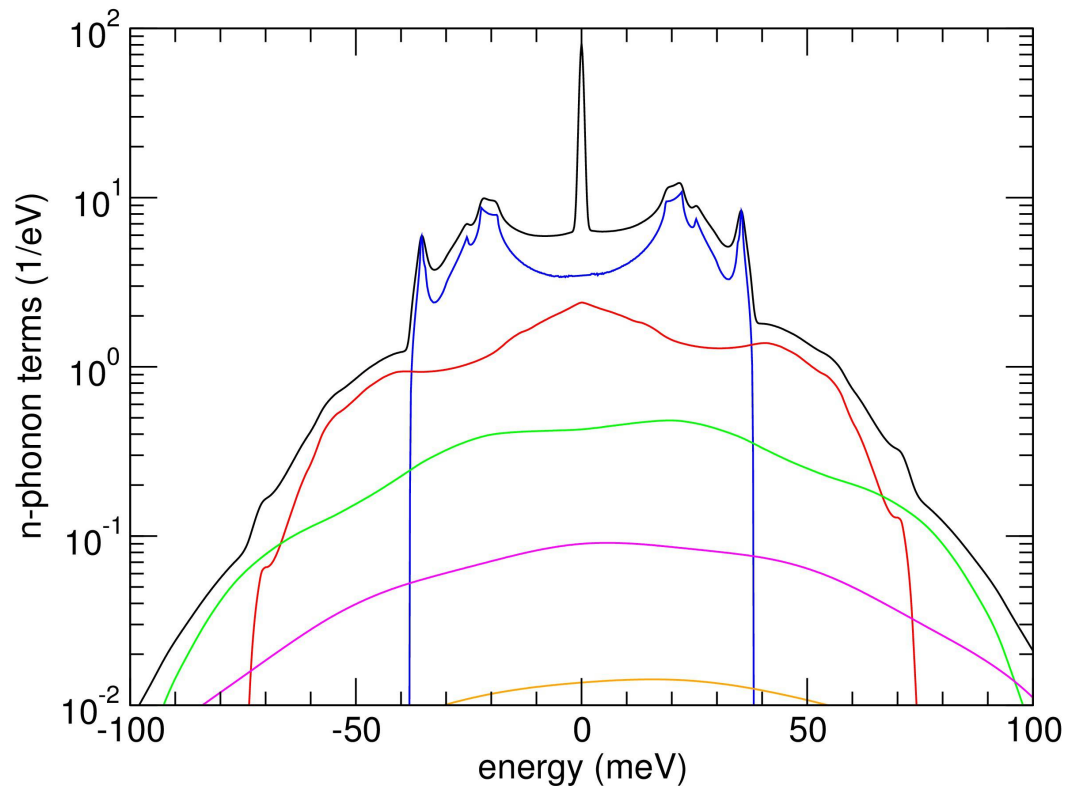


Command:

`psth`

## example 4.2:

- calculate normalized NRIXS spectrum from a theoretical phonon DOS



- ★ construct the input file `in_psth`
- ★ inspect output files

Command:

`psth`