

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 at <http://www.nrixs.com> – no charge
- a major upgrade, PHOENIX-2.0.0, was released in 2009
 - ☆ simple installation procedure for Unix and Mac OS X
 - ☆ all previous capabilities of PHOENIX
 - ☆ 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 application interface, which consists of three main windows:

- Terminal Window (Left):** 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-Moessbauer factor: 0.7978), and a warning about a serious inconsistency detected.
- Plot Window (Middle):** Contains two graphs:
 - peak subtraction:** A plot of counts versus energy (meV) showing a peak at approximately 20 meV.
 - partial phonon DOS:** A plot of PDOS (r/eV) versus energy (meV) showing a sharp peak at approximately 20 meV.
- Emacs Editor Window (Right):** Displays the documentation for the PHOX application, 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

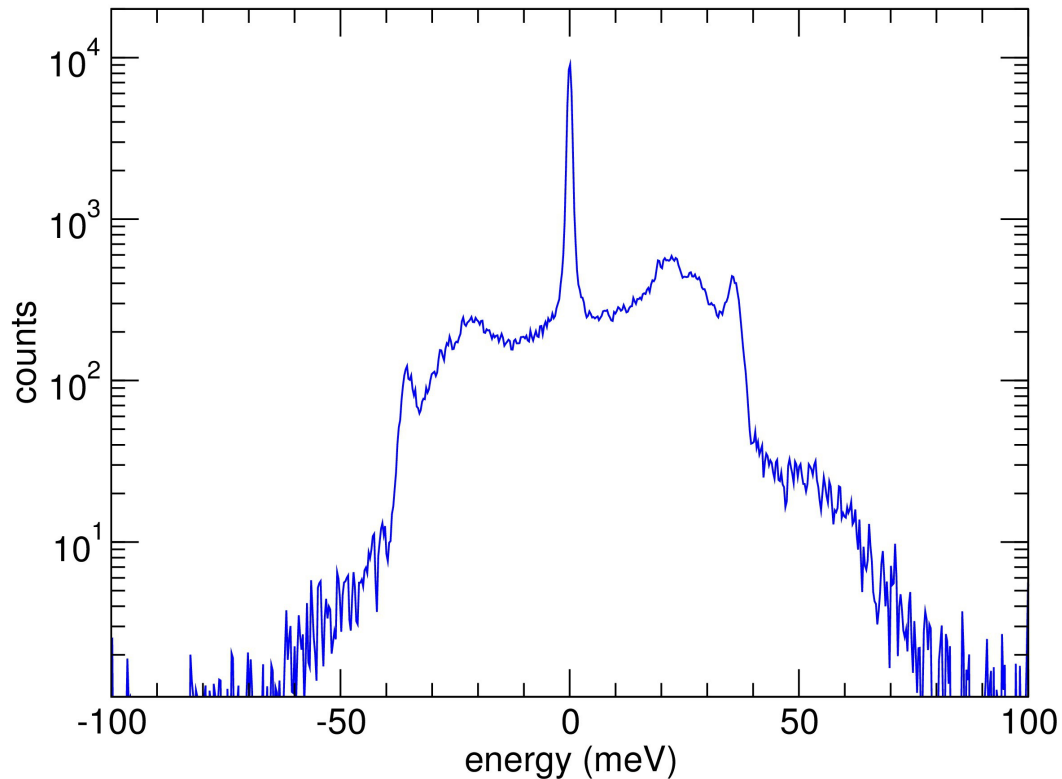
- ☆ extracts aggregate sound velocities from partial phonon DOS

➤ 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



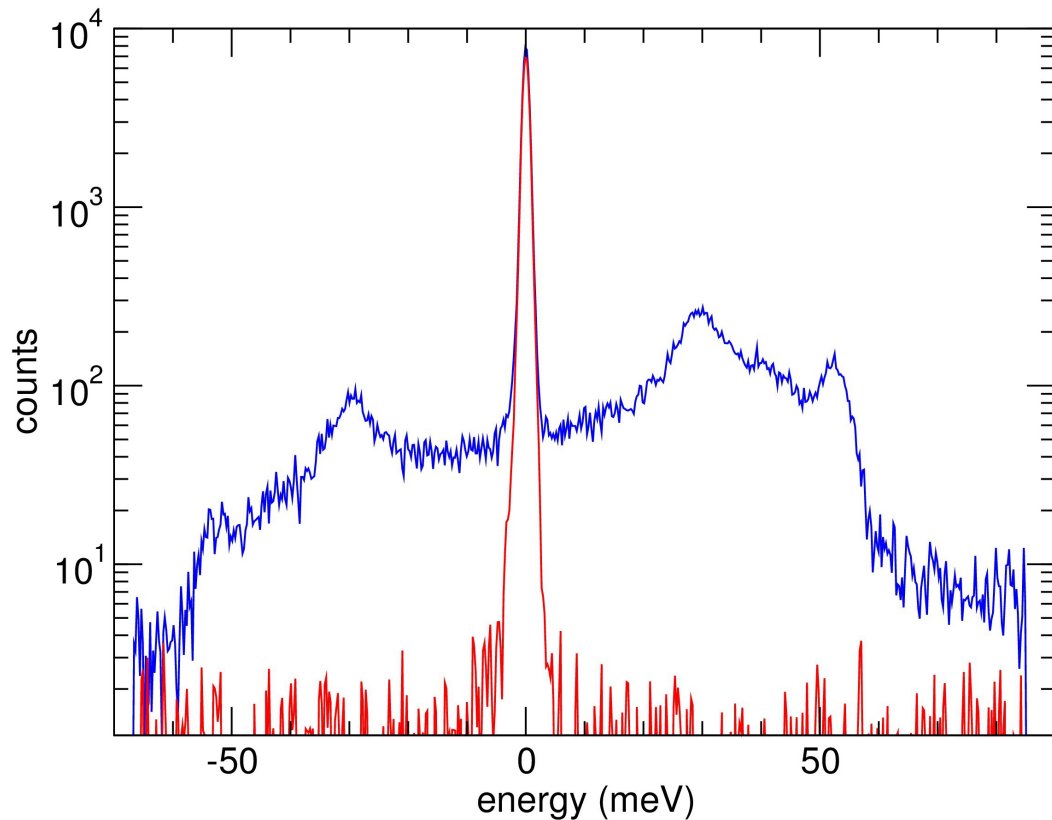
- ☆ construct the input file `in_padd`
- ☆ inspect output files
`*.shf`, `*.mon`, `*.ptp`

Command:

`padd`

example 1.2:

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



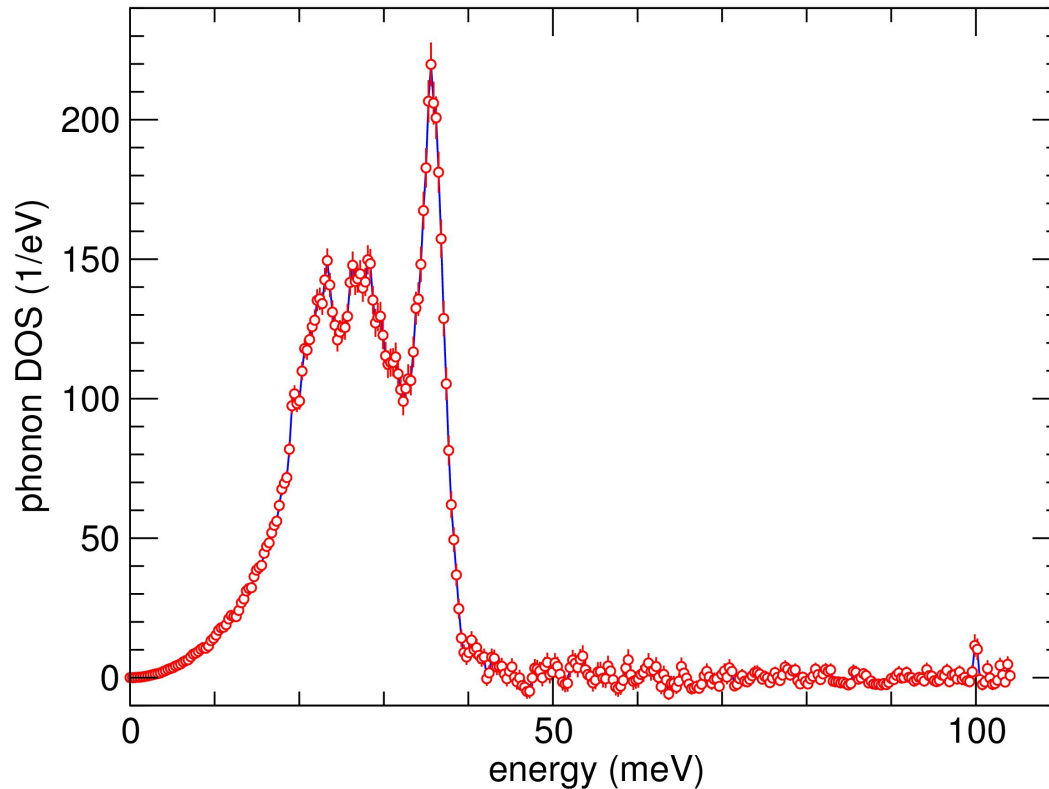
- ☆ construct the input file `in_padd`
- ☆ inspect output directories/files

Command:

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


example 2.1:

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



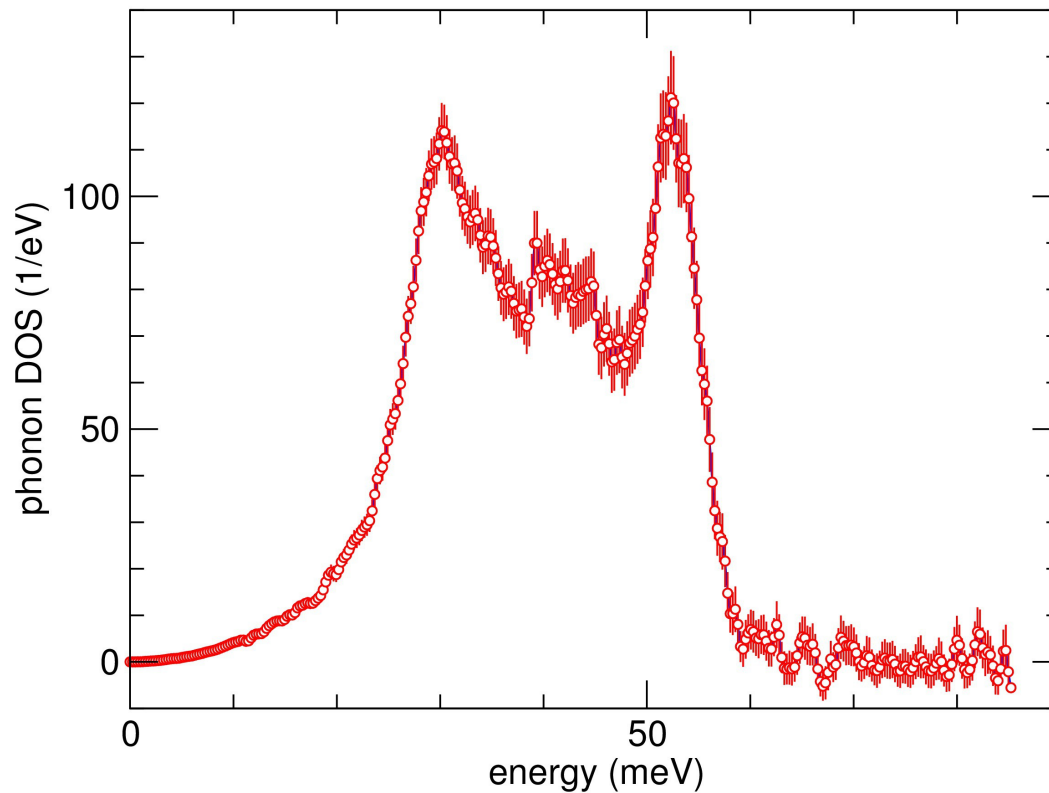
- ☆ construct the input file `in_phox`
- ☆ inspect output files

Command:

`phox`

example 2.2:

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



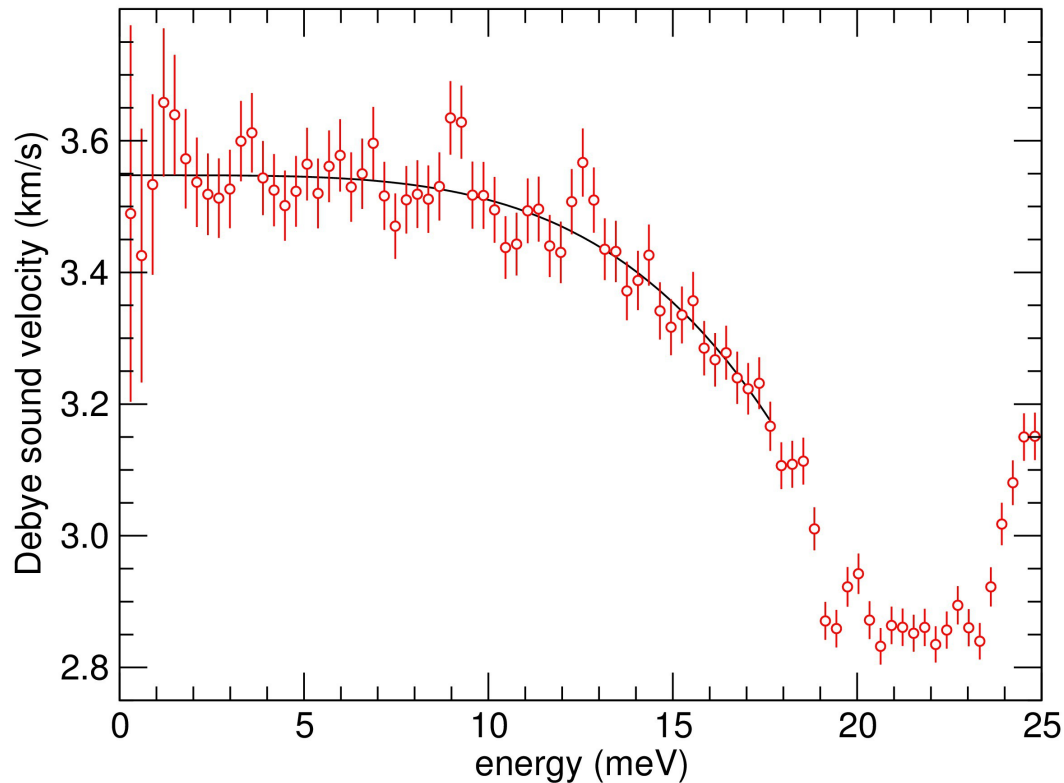
- ☆ construct the input file `in_phox`
- ☆ inspect output files

Command:

`phox`

example 3.1:

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



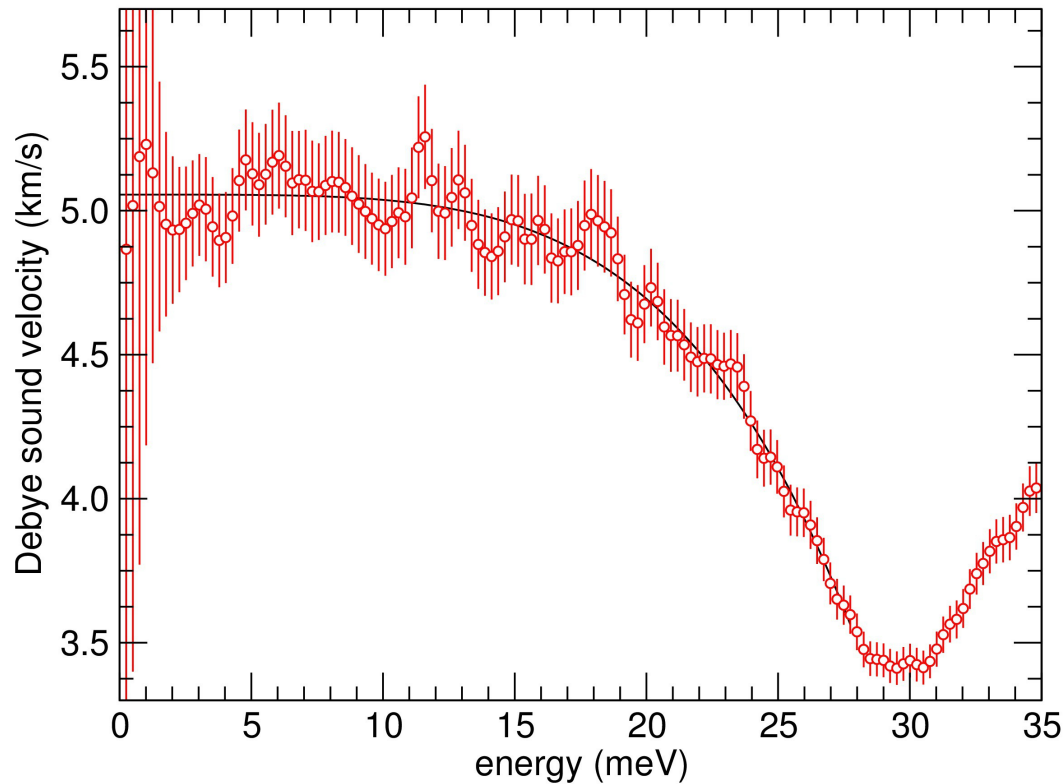
- ☆ construct the input file `in_psv1`
- ☆ inspect output files

Command:

`psv1`

example 3.2:

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

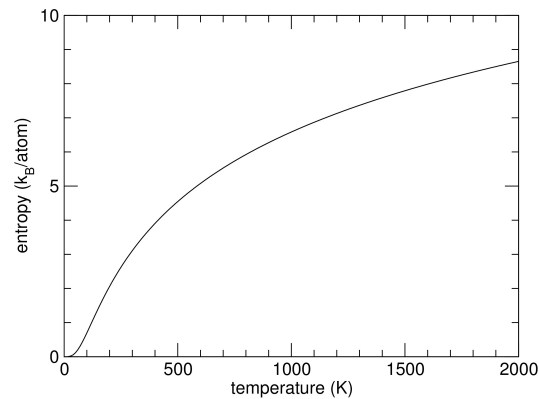


- ☆ construct the input file `in_psv1`
- ☆ inspect output files

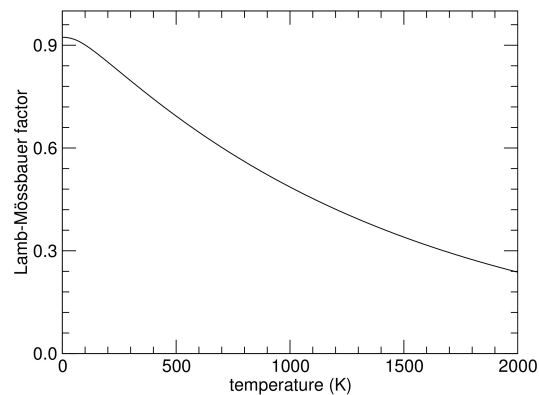
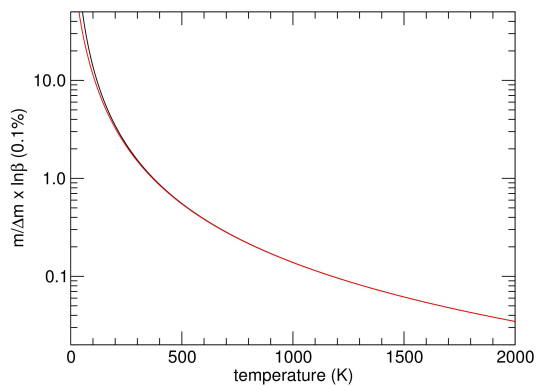
Command:
`psv1`

example 4.1:

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



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

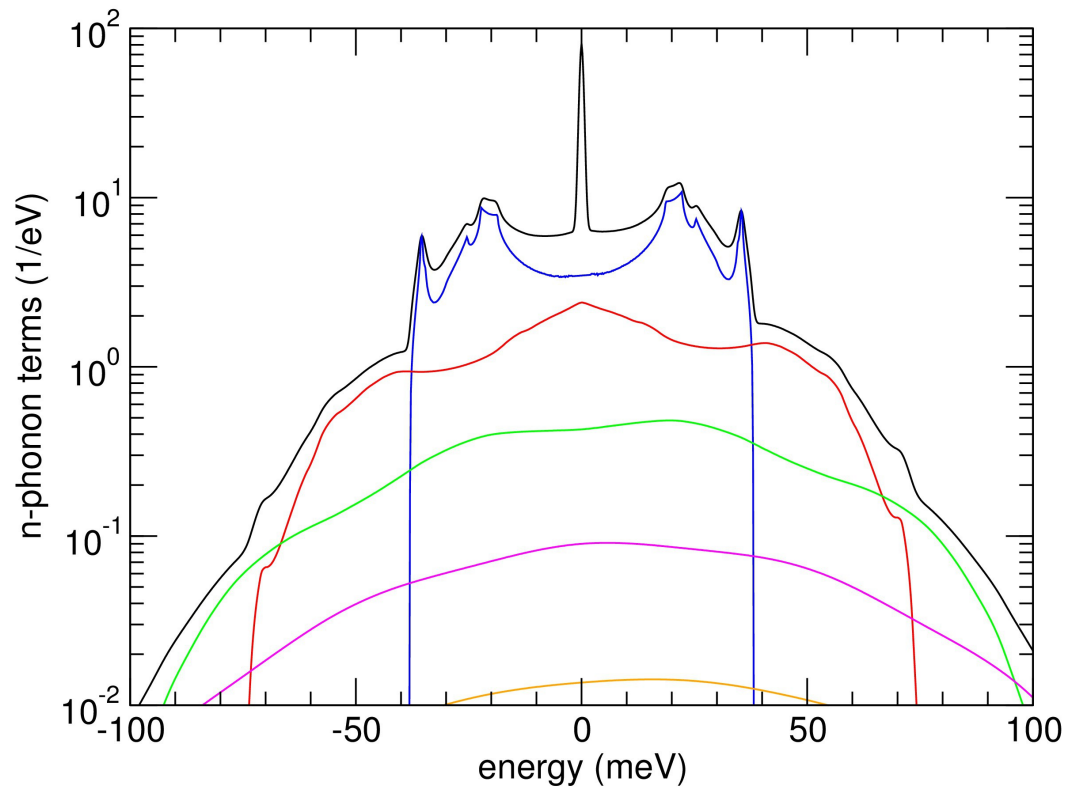


Command:

`psth`

example 4.2:

- calculate normalized NRIXS spectrum from a theoretical phonon DOS



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

Command:

`psth`