

Density of States Analysis Example

- Given sample and empty-can data, compute phonon DOS
- To use this notebook, first click jupyter menu File->Make a copy
- Click the title of the copied jupyter notebook and change it to a new title
- Start executing cells

Summary of processing steps

- Gather experimental information and experimental raw data
- Reduce raw data to $S(Q,E)$
- Convert $S(Q,E)$ to DOS

Preparation

Create a new working directory and change into it.

Please modify the following path to suit your need!

```
In [1]: import os
workdir = os.path.abspath('./V_Ei120meV')
!mkdir -p {workdir}
%cd {workdir}

/home/linjiao/tmp/multiphonon/examples/V_Ei120meV
```

Get tools ready

```
In [2]: import numpy as np
import histogram.hdf as hh, histogram as H
from matplotlib import pyplot as plt
%matplotlib notebook
# %matplotlib inline

from multiphonon.sqe import plot as plot_sqe
from multiphonon.ui.getdos import Context, NxsWizardStart, QEGridWiza
rdStart, GetDOSWizStart
```

Create a context for getdos

```
In [7]: context=Context()
```

If you want to reuse a previously-saved context, please uncomment the following cell and execute

```
In [ ]: context.from_yaml('./getdos2-V_Ei120meV-context.yaml')
```

Get data

Build download command

```
In [3]: dest = 'ARCS_V_annulus.nxs'
url = "https://www.dropbox.com/s/tbh4jcwiaqs410d/ARCS_V_annulus.nxs?dl=1"
cmd = 'wget %r -O %r' % (url, dest)
print cmd

wget 'https://www.dropbox.com/s/tbh4jcwiaqs410d/ARCS_V_annulus.nxs?dl=1' -O 'ARCS_V_annulus.nxs'
```

Download: this will take a while

```
In [5]: %%time
!{cmd} >log.download 2>err.download
```

```
In [6]: ls

ARCS_V_annulus.nxs  err.download  log.download
```

```
In [9]: context.sample_nxs = './ARCS_V_annulus.nxs'
```

Experimental data and condition

Phonon Density of States (DOS) can be obtained from inelastic neutron scattering (INS) spectrum. This notebook allows for extracting DOS from INS spectrum measured at the ARCS instrument at SNS. To start, we need data files measured for the sample and the empty can, as well as experimental conditions such as incident energy and sample temperature. The following wizard help you go through these steps.

Example datasets:

- `samplenxs = './ARCS_V_annulus.nxs'`
- `mtnxs = Skip`
- `Ei=120`
- `T=300`

```
In [11]: NxsWizardStart(context).show()
```

Done.

Save configuration so you can reuse it

```
In [12]: context.to_yaml('./getdos2-V_Ei120meV-context.yaml')
```

Obtain S(Q,E)

S(Q,E) spectra for both the sample and the empty can is the starting point for getdos processing.

Run the following wizard to define the E and Q axes so that S(Q,E) spectra can be obtained the INS raw data.

- E axis
 - Emin: -115
 - Emax: 115
 - dE: 1
- Q axis
 - Qmin: 0
 - Qmax: 17
 - dQ: 0.1

```
In [16]: QEGridWizardStart(context).show()
```

```
Converting sample data to powder I(Q,E)...
Results: sample IQE, MT IQE, Qaxis, Eaxis
('/home/linjiao/tmp/multiphonon/examples/V_Ei120meV/work/iqe.h5', Non
e, (0.0, 17.05, 0.1), (-115.0, 115.5, 1.0))
Done.
```

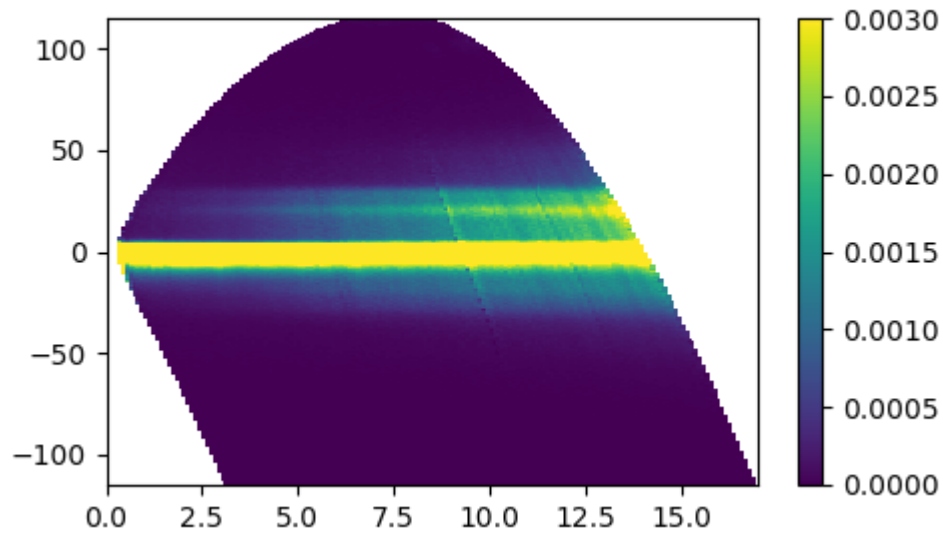
Parameters are saved in the work dir. Uncomment the script below to see.

```
In [ ]: %%script bash
# ls work/
# cat work/raw2iqe-sample.params
```

Plot sample IQE

```
In [17]: iqe = hh.load('work/iqe.h5')
```

```
In [18]: plt.figure(figsize=(6,4))
plot_sqe(iqe)
# plt.xlim(0, 11)
plt.clim(0, 3e-3)
```

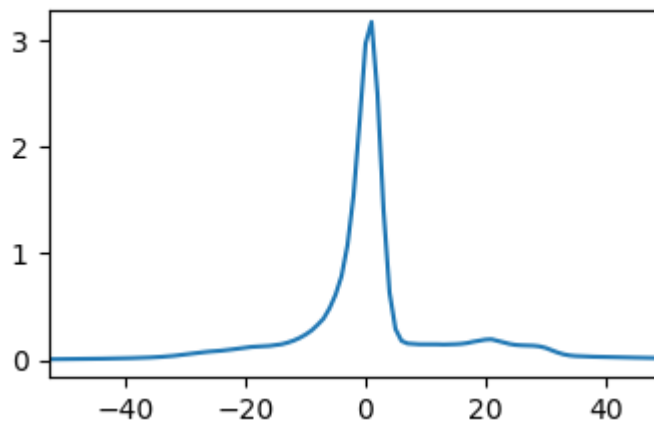


You can improve the Q,E grid parameters if you like, by re-executing the above cell of

```
QEGridWizardStart(context).show()
```

Plot I(E)

```
In [19]: iqe2 = iqe.copy()
I = iqe2.I; I[I!=I] = 0 # remove NaNs
IE = iqe2.sum('Q') # sum over Q
plt.figure(figsize=(6,4))
plt.plot(IE.energy, IE.I)
```



```
Out[19]: [<matplotlib.lines.Line2D at 0x7f240af10490>]
```

The plots above provide clues to selecting parameters for the getdos procedure

Save configuration so you can reuse it

```
In [20]: context.to_yaml('./getdos2-V_Ei120meV-context.yaml')
```

Run GetDOS

DOS will be obtained from SQE by an iterative procedure where multiphonon and multiple scattering corrections are applied to the measured SQE spectrum, assuming incoherent approximation, and the corrected spectrum is then converted to DOS.

- Skip initdos
- Parameters:
 - Emin of elastic peak: -15
 - Emax of elastic peak: 7
 - Average atom mass: 50.94
 - mt_faction: 0.9
 - Max phonon energy: 40
 - C_ms: 0.26
 - const_bg_fraction: 0.004

```
In [83]: context.initdos = ''  
         GetDOSWizStart(context).show()
```

Save context

```
In [84]: context.to_yaml('./getdos2-V_Ei120meV-context.yaml')
```

Print context

```
In [33]: # print context
```

Check output

Results are saved in "work" directory

In [85]: `ls work/`

```

dirddydos/          iqe.h5          raw2iqe-sample.params  rou
nd-2/
final-dos.h5        iqe.nxs          residual_E-posE.h5     rou
nd-3/
getdos-kargs.yaml   plot_dos_iteration.py* round-0/                rou
nd-4/
I_E-exp-posE.h5     plot_residual.py*  round-1/                rou
nd-5/

```

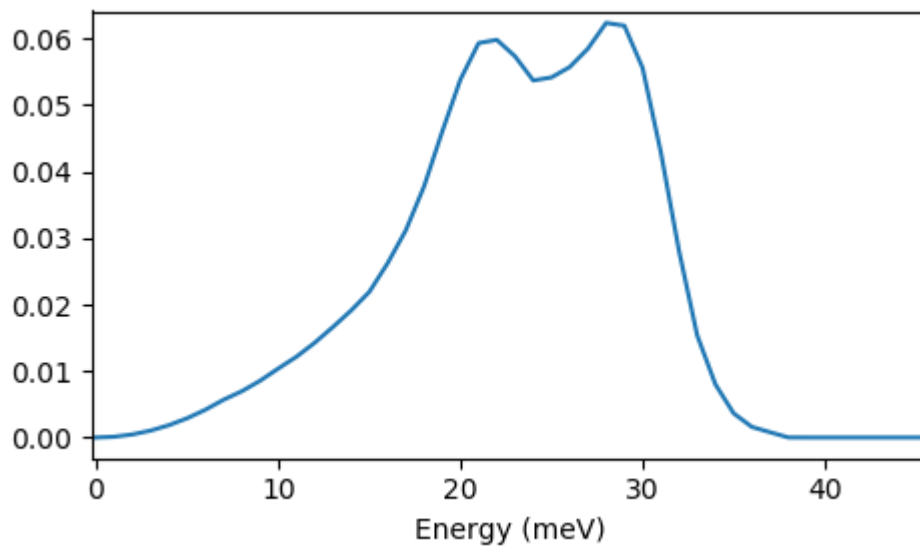
Plot the final result for DOS

In [87]:

```

dos = hh.load('work/final-dos.h5')
plt.figure(figsize=(5,3))
plt.plot(dos.E, dos.I)
plt.xlabel('Energy (meV)')
# plt.xlim(0, 30)
plt.tight_layout()

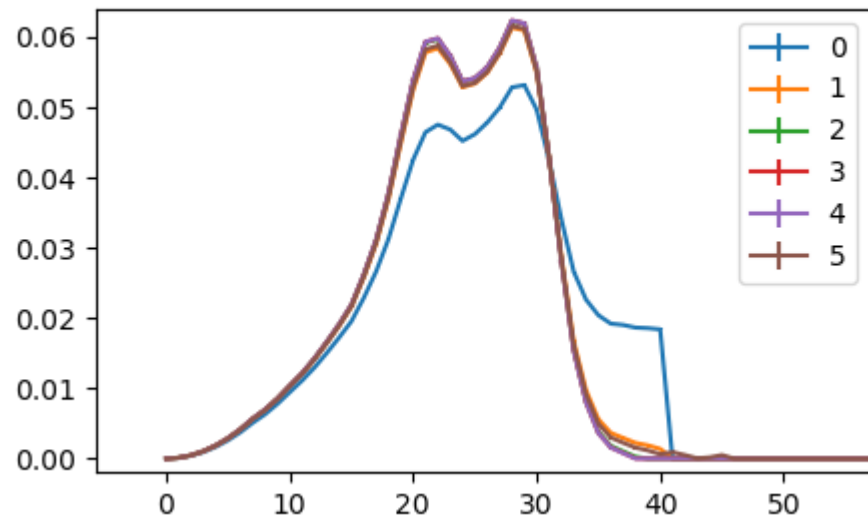
```



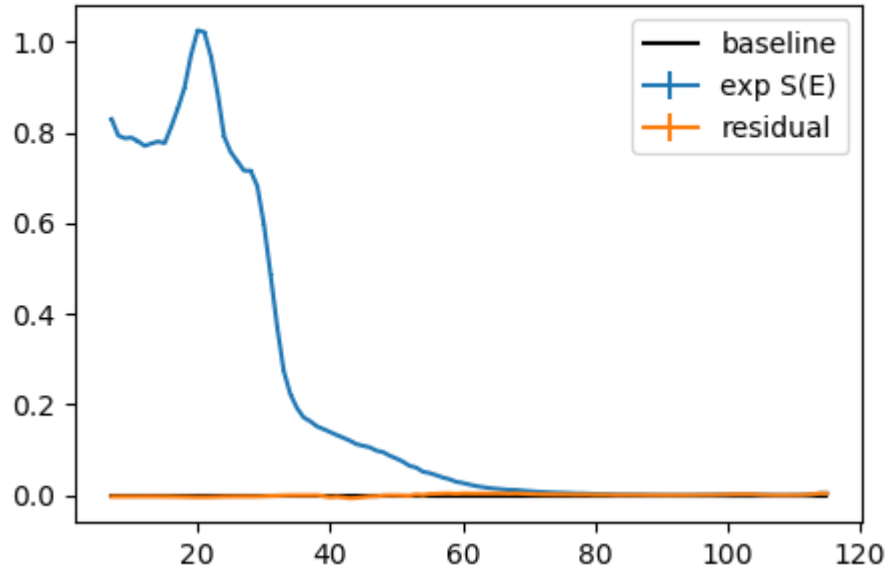
More plotting utils are available

In [29]: `from multiphonon.backward import plotutils as pu`

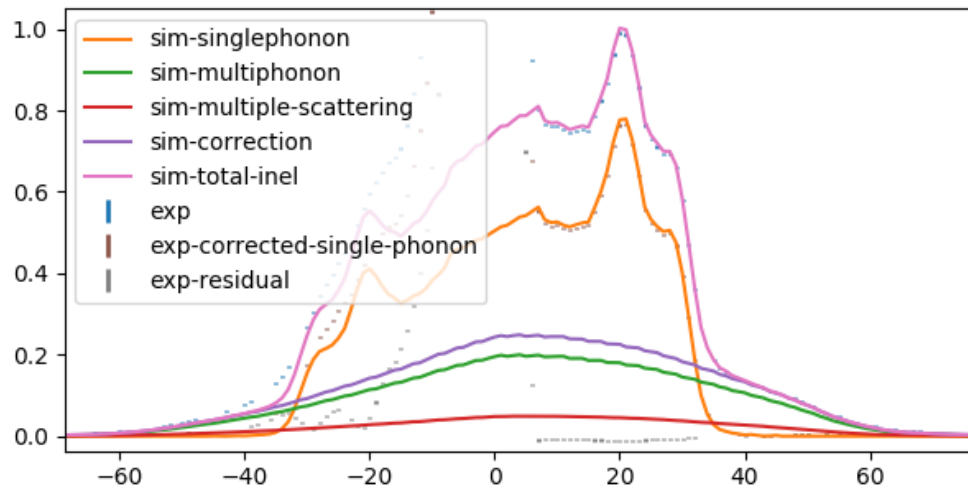
```
In [81]: plt.figure(figsize=(5,3))  
pu.plot_dos_iteration('work/')
```



```
In [80]: plt.figure(figsize=(6,4))  
pu.plot_residual('work/')
```



```
In [86]: plt.figure(figsize=(10, 4))  
pu.plot_intermediate_result_se('work/round-5')
```



```
In [ ]:
```