Practical session of

Phonon evaluation

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Download template

- Open this URL by firefox

https://www.dropbox.com/s/l3lb571e77w7vt9/files.zip?dl=0

- Pick up the downloaded file 'files.zip' on your Desktop.

(File includes all the I/O for phonon calc.)

- Unzip the file to get ~/Desktop/files

Confirm your contents

```
% pwd
/Users/maezono/Desktop/files

% ls
1_scf/          4_phdos/    7_disp_phband/          As.pbe-n-van.UPF*
2_phonon/       5_freeE/    8_phonon_separated/     Ga.pbe-n-van.UPF*
3_q2r/          6_phband/       9_dynmat/
```

Each folder contains step-by-step

procedure of phonon calculations

Procedure

overview

pw.x : evaluating wavefunction 1_scf/

ph.x/q2r.x : evaluating the 2nd. order force constant

2_phonon/, 3_q2r/

matdyn.x : calculating phonon DOS, dispersion

4_phdos/, 6_phband/

fqha.x : evaluating Free energy

5_freeE/

plotband.x : making phonon dispersion graph

7_disp_phband/

pw.x

pw.x: evaluating wavefunction

1) Go to '1_scf/' directory

2) Follow the instruction shown by Ichibha

pw.x

Execute pw.x

% pw.x < input.in > out.o &

outputs

gaas.wfc : wavefunction data

gaas.wfc1,2,...,N : wave function data for parallel processing

gaas.save : eigen values of KS orbitals

Getting smooth q-dep.

q2r.x/Fourier transform from 'q to r'

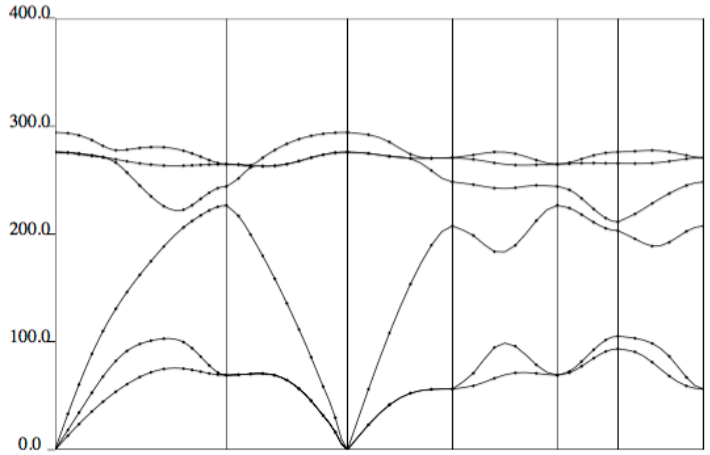
q2r.x

'discrete q-pt' evaluation → Fourier Tr. to 'r' (continuous)

matdyn.x

→ again inv-Fourier Tr. to 'q'

'continuous q-pt' interpolation



ph.x

ph.x/q2r.x: evaluating the 2nd. order force constant

1) Go to '2_phonon/' directory

2) copy wavefunction from 1_scf

```
cp ../1_scf/gaas.* .
```

3) Follow the instruction shown by Ichibha

Execute ph.x

```
% ph.x < input.in > out.o
```

ph.x

Phonon calculation takes much time...

Let us use the 'pre-cooked' files. (~20min.)

[c.f., ~15 sec. for SCF]

- Kill the process,

  ctrl+c

- Copy the 'pre-cooked' output files

  cp ../9_dynmat/* .

outputs

gaas.dyn0 : inequivalent q points

gaas.dyn1,2,... : Force constants on each discrete q-point

q2r.x

ph.x/q2r.x: evaluating the 2nd. order force constant

1) Go to '3_q2r/' directory

2) copy the force constants of sampling q points

%cp ../2_phonon/gaas.dyn* .

3) Execute q2r.x [take a look!]

% q2r.x < input.in > out.o

outputs

gaas444.fc : Force constants in real space

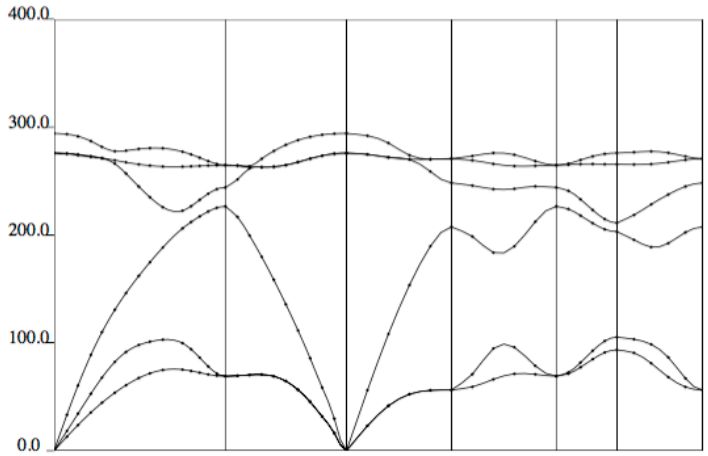
Getting smooth q-dep.

q2r.x

'discrete q-pt' evaluation → Fourier Tr. to 'r'

→ again inv-Fourier Tr. to 'q'

matdyn.x 'continuous q-pt' interpolation



matdyn.x /DOS

matdyn.x : calculating phonon DOS, dispersion

1) Go to '4_phdos/' directory

2) copy the force constants of sampling real space

```
cp ../3_q2r/gaas444.fc .
```

3) Follow the instruction shown by Ichibha

matdyn.x /DOS

1) Execute matdyn.x [take a look!]

% matdyn.x < input.in > out.o

Phonon DOS is written in PHDOS.out

2) make figure of phonon DOS

gnuplot plot.gv [script to generate plot/take a look!]

3) display the figure

gs gaas-phdos.eps

fqha.x

fqha.x : evaluating Free energy

1) Go to '5_freeE/' directory

2) Get the phonon DOS

```
cp ../4_phdos/PHDOS.out .
```

3) Follow the instruction shown by Ichibha

fqha.x

1) Execute fqha.x [take a look!]

%fqha.x < input.in > out.o

→ Free energy is written in gaas.thermal

2) Generate plot of Free energy

% gnuplot plot.gv [script to generate plot/take a look!]

3) Display the plot

% gs gaas-phdos.eps

matdyn.x/dispersion

matdyn.x : calculating phonon DOS, dispersion

1) Go to '6_phband/' directory

2) copy the force constants of sampling real space

%cp ../3_q2r/gaas444.fc .

3) Follow the instruction shown by Ichibha

matdyn.x/dispersion

Execute matdyn.x

% matdyn.x < input.in > out.o

outputs

gaas.freq : frequencies at selected q-points

matdyn.modes : force constants at selected q-points

plotband.x

plotband.x : making phonon dispersion graph

1) Go to '7_disp_phband/' directory

2) Copy the phonon dispersion data

```
%cp ../6_phband/gaas.freq .
```

3) Follow the instruction shown by Ichibha

plotband.x

1) Execute plotband.x

% plotband.x < input.in > out.o

outputs

gaas-phdisp.ps : phonon dispersion [PS image]

gaas-phdisp.xmgr : phonon dispersion [Xmgrace input]

2) Display the plot

% gs gaas-phdisp.ps

Fin