Comp session of

Phonon evaluation

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 Helmholtz 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

outputs

gaas.wfc : wavefunction data

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

gaas.save : eigen values of KS orbitals

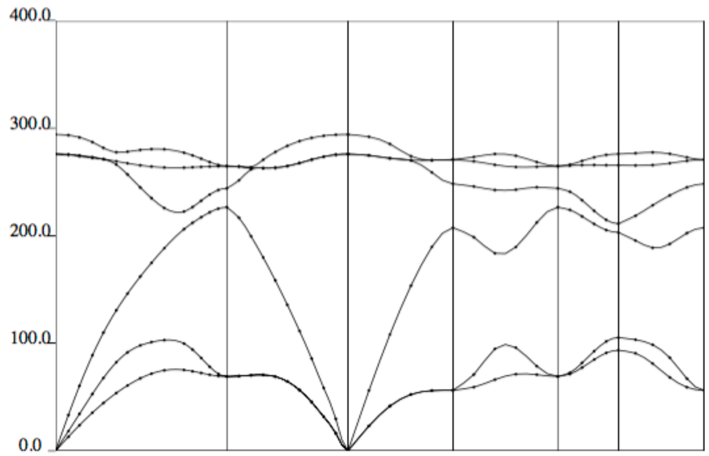
Getting smooth q-dep.

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

'discrete q-pt' evaluation $\xrightarrow{\text{ph.x}}$ Fourier Tr. to 'r'

$\xrightarrow{\text{q2r.x}}$ 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

outputs

gaas.dyn1,2,... : force constants of sampling q point

q2r.x

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

1) Go to '3_q2r/' directory

2) copy the force constants of sampling q points

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

3) Follow the instruction shown by Ichibha

outputs

gaas444.fc : force constants of real space space

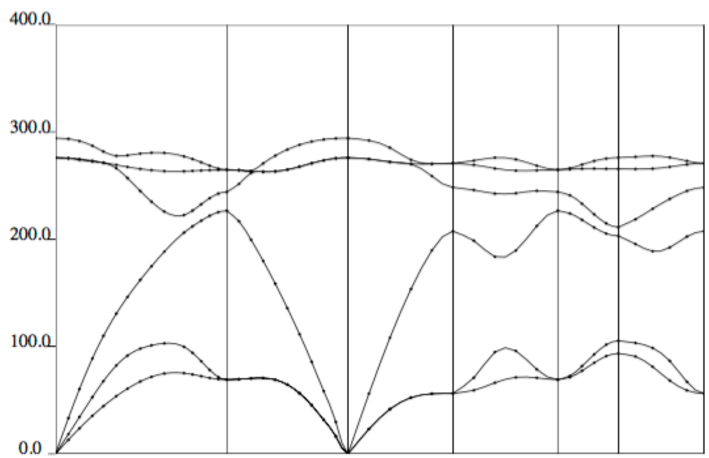
Getting smooth q-dep.

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

'discrete q-pt' evaluation **ph.x** ➔ Fourier Tr. to 'r'

q2r.x ➔ again inv-Fourier Tr. to 'q'

➔ '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

outputs

PHDOS.out : phonon DOS data

fqha.x

fqha.x : evaluating Helmholtz 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

outputs

gaas.thermal : Helmholtz free energy

matdyn.x/dispersion

matdyn.x : calculating phonon DOS, <u>dispersion</u>

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

outputs

matdyn.modes : force constants of picked up q points

gaas.freq : frequencies of picked up 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

outputs

gaas-phdisp.ps : phonon dispersion graph image
gaas-phdisp.xmgr : phonon dispersion data

fin

ph.x

For each $\vec{q}$ point, mode frequency $\omega_{\vec{q}}$ is given as eigen values of this eigen equation

$$\omega_{\vec{q}}^2 \tilde{U}_{i,\vec{q}}^{\alpha}\left(\omega_{\vec{q}}\right) = \sum_{j,\beta} D_{ij}^{\alpha\beta}\left(\vec{q}\right) \tilde{U}_{j,\vec{q}}^{\beta}\left(\omega_{\vec{q}}\right) \qquad (1)$$

Here,

$$D_{ij}^{\alpha\beta}\left(\vec{q}\right) \equiv \frac{1}{\sqrt{m_i}\sqrt{m_j}} \sum_{J'} \frac{\partial^2 E_{tot}}{\partial u_{0,i}^{\alpha}\, \partial u_{J',j}^{\beta}} \cdot e^{i\vec{q}\cdot\left(\vec{R}_{J'}-\vec{R}_0\right)} \qquad (2)$$

This matrix is calculated in a few sampling $\vec{q}$ points

Following process, we'll get $D_{ij}^{\alpha\beta}\left(\vec{q}\right)$ for arbitrary $\vec{q}$

q2r.x

$$D_{ij}^{\alpha\beta}(\vec{q}) \equiv \frac{1}{\sqrt{m_i}\sqrt{m_j}} \sum_{J'} \frac{\partial^2 E_{tot}}{\partial u_{0,i}^{\alpha}\, \partial u_{J',j}^{\beta}} \cdot e^{i\vec{q}\cdot\left(\vec{R}_{J'}-\vec{R}_0\right)} \qquad (3)$$

Fourier transform

$$\frac{1}{\sqrt{m_i}\sqrt{m_j}} \frac{\partial^2 E_{tot}}{\partial u_{0,i}^{\alpha}\, \partial u_{J,j}^{\beta}} = \frac{\Omega}{(2\pi)^3} \int D_{ij}^{\alpha\beta}(\vec{q})\, e^{-i\vec{q}\cdot\left(\vec{R}_J-\vec{R}_0\right)}\, d\vec{q} \qquad (4)$$

is approximated by

$$\frac{1}{\sqrt{m_i}\sqrt{m_j}} \frac{\partial^2 E_{tot}}{\partial u_{0,i}^{\alpha}\, \partial u_{J,j}^{\beta}} \simeq \frac{1}{N_{sample}} \sum_{\vec{q}'} D_{ij}^{\alpha\beta}(\vec{q}')\, e^{-i\vec{q}'\cdot\left(\vec{R}_J-\vec{R}_0\right)} \qquad (5)$$

Here, N_{sample} is number of sampling $\vec{q}$ points

matdyn.x

substitute

$$\frac{1}{\sqrt{m_i}\sqrt{m_j}}\frac{\partial^2 E_{tot}}{\partial u_{0,i}^{\alpha}\,\partial u_{J,j}^{\beta}} \simeq \frac{1}{N_{sample}}\sum_{\vec{q}'} D_{ij}^{\alpha\beta}\left(\vec{q}'\right) e^{-i\vec{q}'\cdot\left(\vec{R}_J-\vec{R}_0\right)} N_{sample} \quad (5)$$

into

$$D_{ij}^{\alpha\beta}\left(\vec{q}\right) \equiv \frac{1}{\sqrt{m_i}\sqrt{m_j}}\sum_{J}\frac{\partial^2 E_{tot}}{\partial u_{0,i}^{\alpha}\,\partial u_{J,j}^{\beta}}\cdot e^{i\vec{q}\cdot\left(\vec{R}_J-\vec{R}_0\right)} \quad (2)$$

finally, you can get

$$D_{ij}^{\alpha\beta}\left(\vec{q}\right) = \sum_{J}\sum_{\vec{q}'} D_{ij}^{\alpha\beta}\left(\vec{q}'\right)\cdot e^{i\left(\vec{q}-\vec{q}'\right)\cdot\left(\vec{R}_J-\vec{R}_0\right)} \quad (6)$$