ASESMA-2023

Hands-on session - Phonons

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Introduction: Phonons

Normal mode frequencies, ω , and eigenvectors, $\mathbf{u}_{s\alpha}$ are determined by the secular equation:

$$\sum_{s',\beta} \tilde{D}_{s\alpha,s'\beta}(\mathbf{q})\, \tilde{\mathbf{u}}_{s'\beta}(\mathbf{q}) = \omega_{\mathbf{q}}^2\, \tilde{\mathbf{u}}_{s\alpha}(\mathbf{q})$$

where

$$\tilde{D}_{s\alpha,s'\beta}(\mathbf{q}) = \frac{1}{\sqrt{M_s M_{s'}}} \sum_{\mathbf{R},\mathbf{R}'} \frac{\partial^2 E_{tot}}{\partial \mathbf{u}_{s\alpha}(\mathbf{R}) \partial \mathbf{u}_{s'\beta}(\mathbf{R}')} e^{i\mathbf{q}(\mathbf{R}'-\mathbf{R})}$$

Interatomic force constants (IFC)

is the dynamical matrix.

This Matrix can be calculated from linear response and diagonalized to get phonon modes at $\mathbf{q}$.

Exercise 1: Phonons at Γ in non-polar materials

Go to the directory with the input files:

cd ~/ASESMA-2023/Day-5/Exercise1

In this directory you will find:

- *README.md* – File describing how to do the exercise
- *Si.scf.in* – Input file for the SCF ground-state calculation
- *Si.ph.in* – Input file for the phonon calculation at Γ
- *Si.dynmat.in* – Input file to impose the acoustic sum rule
- **reference** – Directory with the reference results

Exercise 1: Phonons at Γ in non-polar materials

```
&control
        calculation    = 'scf',
        restart_mode = 'from_scratch',
        prefix          = 'si',
        pseudo_dir='../pseudo/',
        outdir='../tmp/',
/
&system
        ibrav=2,
        celldm(1)=10.2625,
        nat=2,
        ntyp=1,
        ecutwfc=60.0,
        ecutrho=720.0,
/
&electrons
        mixing_beta=0.7,
        conv_thr=1d-10,
/
ATOMIC_SPECIES
Si 28.0855 Si.pbe-rrkj.UPF

ATOMIC_POSITIONS (alat)
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
K_POINTS automatic
4 4 4 1 1 1
```

Step 1. Perform a Self-Consistent Field ground-state calculation for silicon at the equilibrium structure using the pw.x program.

Si.scf.in

Input file for the SCF calculations

mpirun -np 4 pw.x -inp Si.scf.in > Si.scf.out

Input **Output**

Exercise 1: Phonons at Γ in non-polar materials

Step 2. Perform a phonon calculation at Γ using the ph.x program.

Si.ph.in → Input file for the phonon calculations

```
Phonons at Gamma
&inputph
  prefix = 'Si',
  tr2_ph = 1.0d-14,
  amass(1) = 28.0855,
  epsil = .true.
  outdir = './tmp'
  fildyn = 'Si.dyn',
 /
 0.0  0.0  0.0
```

- The same prefix as in the SCF calculation
- Threshold for self-consistency
- Atomic mass
- To calculate the dielectric tensor and effective charges
- Directory for temporary files
- File containing the dynamical matrix
- Coordinates of the q point (Γ) in units of 2*pi/a in the Cartesian reference system

mpirun -np 4 ph.x -inp Si.ph.in > Si.ph.out

Exercise 1: Phonons at Γ in non-polar materials

Dynamical matrix file **Si.dyn** :

```
     Dielectric Tensor:

          13.806378036722           0.000000000000          -0.000000000000
          -0.000000000000          13.806378036722           0.000000000000
          -0.000000000000           0.000000000000          13.806378036722

Effective Charges E-U: Z_{alpha}{s,beta}
     atom #     1
          -0.075668487215           0.000000000000           0.000000000000
           0.000000000000          -0.075668487215           0.000000000000
           0.000000000000           0.000000000000          -0.075668487215
     atom #     2
          -0.075668487215           0.000000000000           0.000000000000
           0.000000000000          -0.075668487215          -0.000000000000
           0.000000000000          -0.000000000000          -0.075668487215
     Diagonalizing the dynamical matrix

     q = (    0.000000000   0.000000000   0.000000000 )
 **************************************************************************
     freq (    1) =       0.078830 [THz] =       2.629478 [cm-1]
(  0.429342 -0.000000 -0.450832  0.000000 -0.335285  0.000000 )
(  0.429342 -0.000000 -0.450832  0.000000 -0.335285  0.000000 )
     freq (    2) =       0.078830 [THz] =       2.629478 [cm-1]
(  0.558725  0.000000  0.386983  0.000000  0.195117  0.000000 )
(  0.558725  0.000000  0.386983  0.000000  0.195117  0.000000 )
     freq (    3) =       0.078830 [THz] =       2.629478 [cm-1]
(  0.059092  0.000000 -0.383399  0.000000  0.591197  0.000000 )
(  0.059092  0.000000 -0.383399  0.000000  0.591197  0.000000 )
     freq (    4) =      15.292493 [THz] =     510.102675 [cm-1]
( -0.129158  0.000000  0.093954  0.000000  0.688833 -0.000000 )
(  0.129158  0.000000 -0.093954  0.000000 -0.688833  0.000000 )
     freq (    5) =      15.292493 [THz] =     510.102675 [cm-1]
( -0.295782  0.000000  0.626619  0.000000 -0.140928  0.000000 )
(  0.295782  0.000000 -0.626619  0.000000  0.140928  0.000000 )
     freq (    6) =      15.292493 [THz] =     510.102675 [cm-1]
( -0.629151  0.000000 -0.313880  0.000000 -0.075155  0.000000 )
(  0.629151 -0.000000  0.313880 -0.000000  0.075155  0.000000 )
 **************************************************************************
```

Dielectric constant and Born effective charges (BECs)

Exercise 1: Phonons at Γ in non-polar materials

Dynamical matrix file **Si.dyn** :

```
Diagonalizing the dynamical matrix

 q = (    0.000000000   0.000000000   0.000000000 )
 **************************************************************************
    freq (    1) =       0.078830 [THz] =       2.629478 [cm-1]
 ( 0.429342 -0.000000 -0.450832  0.000000 -0.335285  0.000000 )
 ( 0.429342 -0.000000 -0.450832  0.000000 -0.335285  0.000000 )
    freq (    2) =       0.078830 [THz] =       2.629478 [cm-1]
 ( 0.558725  0.000000  0.386983  0.000000  0.195117  0.000000 )
 ( 0.558725  0.000000  0.386983  0.000000  0.195117  0.000000 )
    freq (    3) =       0.078830 [THz] =       2.629478 [cm-1]
 ( 0.059092  0.000000 -0.383399  0.000000  0.591197  0.000000 )
 ( 0.059092  0.000000 -0.383399  0.000000  0.591197  0.000000 )
    freq (    4) =      15.292493 [THz] =     510.102675 [cm-1]
 ( -0.129158  0.000000  0.093954  0.000000  0.688833 -0.000000 )
 ( 0.129158  0.000000 -0.093954  0.000000 -0.688833  0.000000 )
    freq (    5) =      15.292493 [THz] =     510.102675 [cm-1]
 ( -0.295782  0.000000  0.626619  0.000000 -0.140928  0.000000 )
 ( 0.295782  0.000000 -0.626619  0.000000  0.140928  0.000000 )
    freq (    6) =      15.292493 [THz] =     510.102675 [cm-1]
 ( -0.629151  0.000000 -0.313880  0.000000 -0.075155  0.000000 )
 ( 0.629151 -0.000000  0.313880 -0.000000  0.075155  0.000000 )
 **************************************************************************
```

Acoustic modes

Optical modes

Exercise 1: Phonons at Γ in non-polar materials

Acoustic sum rule at Γ

Problems with the frequency of the acoustic phonon mode at Γ and with effective charges.

Because of the numerical inaccuracies the interatomic force constants and effective charges do not strictly satisfy the acoustic sum rule (ASR).

ASR comes directly from the continous translational invariance of the crystal. If we translate the whole solid by a uniform displacement, the forces acting on the atoms must be zero.

As a consequence

For each α, β and i: $\sum_{\mathbf{L},j} C_{\alpha i,\beta j}(\mathbf{R_L}) = 0$ $\sum_{j} Z^*_{j,\alpha\beta} = 0$

As a consequence, the frequencies of the acoustic modes must be zero.

Exercise 1: Phonons at Γ in non-polar materials

Acoustic sum rule at Γ

Reasons for numerical inaccuracies:

- Insufficiently accurate SCF thresholds (in pw.x and/or ph.x)
- XC energy is computed in real space. More problematic for GGA than in LDA, For US pseudopotentials it could require large *ecutrho*.
- K-points sampling not accurate enough (especially, BECs and dielectric constant required denser k-point sampling).

Exercise 1: Phonons at Γ in non-polar materials

Acoustic sum rule at Γ

The acoustic sum rule (ASR) can however be imposed after the phonon calculations.
To do this we use the dynmat.x program that imposes the ASR on the elements of the dynamical matrix and diagonalize it.

The input file is Si.dynmat.in :

```
&input
  fildyn = 'Si.dyn',
  asr = 'simple',
 /
```

→ File containing the dynamical matrix

→ A way to impose the acoustic sum rule (simple, crystal, one-dim, zero-dim)

```
mpirun -np 4 dynmat.x -inp Si.dynmat.in > Si.dynmat.out
```

Exercise 1: Phonons at Γ in non-polar materials

The program dynmat.x produces the file dynmat.out which contains the new acoustic frequencies, which are exactly equal to zero.

```
     q =   0.0000      0.0000      0.0000
**********************************************************************
   freq (    1) =       0.000000 [THz] =       0.000000 [cm-1]
(  0.000000   0.000000     0.707107   0.000000     0.000000   0.000000   )
(  0.000000   0.000000     0.707107   0.000000     0.000000   0.000000   )
   freq (    2) =       0.000000 [THz] =       0.000000 [cm-1]
( -0.707107   0.000000     0.000000   0.000000     0.000000   0.000000   )
( -0.707107   0.000000     0.000000   0.000000     0.000000   0.000000   )
   freq (    3) =       0.000000 [THz] =       0.000000 [cm-1]
(  0.000000   0.000000     0.000000   0.000000     0.707107   0.000000   )
(  0.000000   0.000000     0.000000   0.000000     0.707107   0.000000   )
   freq (    4) =      15.292290 [THz] =     510.095902 [cm-1]
(  0.000000   0.000000     0.707107   0.000000     0.000000   0.000000   )
(  0.000000   0.000000    -0.707107   0.000000     0.000000   0.000000   )
   freq (    5) =      15.292290 [THz] =     510.095902 [cm-1]
(  0.000000   0.000000     0.000000   0.000000    -0.707107   0.000000   )
(  0.000000   0.000000     0.000000   0.000000     0.707107   0.000000   )
   freq (    6) =      15.292290 [THz] =     510.095902 [cm-1]
( -0.707107   0.000000     0.000000   0.000000     0.000000   0.000000   )
(  0.707107   0.000000     0.000000   0.000000     0.000000   0.000000   )
**********************************************************************
```

Exercise 2: Phonons at Γ in polar materials

Polar materials in the **q = 0** limit: a macroscopic electric field appears as a consequence of the long-range character of the Coulomb interaction (incompatible with Periodic Boundary Conditions).
A non-analytic term must be added to Interatomic Force Constants at **q= 0**:

$$\tilde{C}_{s\alpha,s'\beta}(\mathbf{q}) = \tilde{C}^{\text{analytic}}_{s\alpha,s'\beta}(\mathbf{q}) + \frac{4\pi}{\Omega}\frac{(\mathbf{q}\cdot\boldsymbol{Z}^{\star}_{s})_{\alpha}(\mathbf{q}\cdot\boldsymbol{Z}^{\star}_{s'})_{\beta}}{\mathbf{q}\cdot\epsilon_{\infty}\cdot\mathbf{q}}$$

Effective charges $\boldsymbol{Z}^{\star}_{s}$ are related to polarization P induced by a lattice distortion:

$$Z^{\star}_{s,\alpha\beta} = \Omega\frac{\partial \mathrm{P}_{\alpha}}{\partial u_{s\beta}}$$

Dielectric tensor $\epsilon^{\alpha\beta}_{\infty}$ is related to polarization **P** induced by an electric field **E** :

$$\epsilon^{\alpha\beta}_{\infty} = \delta_{\alpha\beta} + 4\pi\left.\frac{\partial \mathrm{P}_{\alpha}}{\partial \mathrm{E}_{\beta}}\right|_{u_s(q=0)=0}$$

All of the above can be calculated from (mixed) second order derivatives of the total energy.

Exercise 2: Phonons at Γ in polar materials

Go to the directory with the input files:

cd ~/ASESMA-2023/Day-5/Exercise2

In this directory you will find:

- *README.md* – File describing how to do the exercise
- *AlAs.scf.in* – Input file for the SCF ground-state calculation
- *AlAs.ph.in* – Input file for the phonon calculation at Γ
- *AlAs.dynmat.in* – Input file to impose the acoustic sum rule
- **reference** – Directory with the reference results

Exercise 2: Phonons at Γ in polar materials

AlAs.ph.in

```
Phonons at Gamma
&inputph
  prefix = 'AlAs',
  tr2_ph = 1.0d-14,
  Amass(1) = 26.98,
  Amass(2) = 74.92,
  epsil = .true.
  outdir = './tmp'
  fildyn = 'AlAs.dyn',
 /
 0.0  0.0  0.0
```

Step 1. Perform a Self-Consistent Field ground-state calculation for the polar semiconductor AlAs.

```
mpirun -np 4 pw.x -inp AlAs.scf.in > AlAs.scf.out
```

Step 2. Perform a phonon calculation at Gamma for AlAs.

```
mpirun -np 4 ph.x -inp AlAs.ph.in > AlAs.ph.out
```

Exercise 2: Phonons at Γ in polar materials

In the file ph.AlAs.out you will find information about the dielectric tensor and effective charges:

Dielectric constant in cartesian axis

```
(     13.743997537      0.000000000      0.000000000 )
(      0.000000000     13.743997537      0.000000000 )
(      0.000000000      0.000000000     13.743997537 )
```

Effective charges (d Force / dE) in cartesian axis

```
     atom     1   Al Mean Z*:      1.88275
  Ex  (      1.88275      -0.00000       0.00000 )
  Ey  (      0.00000       1.88275       0.00000 )
  Ez  (     -0.00000      -0.00000       1.88275 )
     atom     2   As Mean Z*:     -3.23400
  Ex  (     -3.23400       0.00000      -0.00000 )
  Ey  (      0.00000      -3.23400      -0.00000 )
  Ez  (     -0.00000       0.00000      -3.23400 )
```

Diagonalizing the dynamical matrix

```
  q = (    0.000000000   0.000000000   0.000000000 )
 **************************************************
  freq (    1) =       0.151928 [THz] =       5.067777 [cm-1]
  freq (    2) =       0.151928 [THz] =       5.067777 [cm-1]
  freq (    3) =       0.151928 [THz] =       5.067777 [cm-1]
  freq (    4) =      11.258171 [THz] =     375.532153 [cm-1]
  freq (    5) =      11.258171 [THz] =     375.532153 [cm-1]
  freq (    6) =      11.258171 [THz] =     375.532153 [cm-1]
 **************************************************
```

No LO-TO splitting

Exercise 2: Phonons at Γ in polar materials

Step 3. Impose Acoustic Sum Rule and add the non-analytic LO-TO splitting using the dynmat.x program.

```
&input
  fildyn = 'AlAs.dyn',
  amass(1) = 26.98,
  amass(2) = 74.92,
  asr = 'simple',
q(1) = 1.0, q(2) = 0.0, q(3) = 0.0
/
```

Direction in the Brillouin zone along which we want to compute the LOTO splitting

check the output file

```
# mode    [cm-1]    [THz]      IR
    1     -0.00   -0.0000   0.0000
    2     -0.00   -0.0000   0.0000
    3     -0.00   -0.0000   0.0000
    4    375.51   11.2574   7.6126
    5    375.51   11.2574   7.6126
    6    410.55   12.3080   7.6126
```

LO-TO splitting

```
mpirun -np 4 dynmat.x < AlAs.dynmat.in > AlAs.dynmat.out
```

Exercise 3: Phonons dispersion in non-polar materials

Go to the directory with the input files:

cd ~/ASESMA-2023/Day-5/Exercise3

In this directory you will find:

- *README.md* – File describing how to do the exercise
- *Si.scf.in* – Input file for the SCF ground-state calculation
- *Si.ph.in* – Input file for the phonon calculation at Γ
- *Si.q2r.in* – Input file for calculation of Interatomic Force Constants
- *Si.matdyn.in* – Input file for Fourier Interpolation for various q points
- *Si.plotband.in* – Input file for plotting a phonon dispersion
- **reference** – Directory with the reference results

Exercise 3: Phonons dispersion in non-polar materials

Step 1. Perform a SCF calculation for silicon at the equilibrium structure using the pw.x program.

```
mpirun -np 4 pw.x -inp Si.scf. in > Si.scf.out
```

```
Phonons on uniform q-grid
&inputph
  prefix = 'Si',
  tr2_ph = 1.0d-14,
  amass(1) = 28.0855,
  ldisp = .true.,
  nq1 = 4,
  nq2 = 4,
  nq3 = 4,
 outdir = './tmp'
  fildyn = 'Si.dyn',
 /
```

Step 2. Perform a phonon calculation on a uniform grid of q points using the ph.x program.

```
mpirun -np 4 ph.x -inp Si.ph.in > Si.ph.out
```

Option for the calculation on a grid
Uniform grid of q points

$$\mathbf{q}_{ijk} = \frac{i-1}{\mathrm{nq1}}\mathbf{G}_1 + \frac{j-1}{\mathrm{nq2}}\mathbf{G}_2 + \frac{k-1}{\mathrm{nq3}}\mathbf{G}_3$$

Exercise 3: Phonons dispersion in non-polar materials

4x4x4 = 64 q-points => Use of symmetry => 8 non-equivalent q points
The file Si.dyn0 contains a list of the non-equivalent q points (8, in this case).

```
      4   4   4    (q-grid)
      8            (number of non-equivalent q-points)
q1 =  0.0000000000000000E+00   0.0000000000000000E+00   0.0000000000000000E+00
q2 = -0.2500000000000000E+00   0.2500000000000000E+00  -0.2500000000000000E+00
q3 =  0.5000000000000000E+00  -0.5000000000000000E+00   0.5000000000000000E+00
q4 =  0.0000000000000000E+00   0.5000000000000000E+00   0.0000000000000000E+00
q5 =  0.7500000000000000E+00  -0.2500000000000000E+00   0.7500000000000000E+00
q6 =  0.5000000000000000E+00   0.0000000000000000E+00   0.5000000000000000E+00
q7 =  0.0000000000000000E+00  -0.1000000000000000E+01   0.0000000000000000E+00
q8 = -0.5000000000000000E+00  -0.1000000000000000E+01   0.0000000000000000E+00
```

The phonon code ph.x generates a file for every non-equivalent q point (Si.dyn1, Si.dyn2, ..., Si.dyn8), which contain information about dynamical matrices, phonon frequencies and atomic displacements

Exercise 3: Phonons dispersion in non-polar materials

Step 3. Calculation of the Interatomic Force Constants (IFC) using the q2r.x program.

Fourier transforms of IFC's :

$$\tilde{C}_{s\alpha,s'\beta}(\mathbf{q}_{ijk}) = \frac{\partial^2 E_{tot}}{\partial \tilde{\mathbf{u}}^*_{s\alpha}(\mathbf{q}_{ijk}) \partial \tilde{\mathbf{u}}_{s'\beta}(\mathbf{q}_{ijk})}$$

α, β are Cartesian components, and s, s' are atomic indices.

$$\tilde{C}_{s\alpha,s'\beta}(\mathbf{q}_{ijk}) \longrightarrow C_{s\alpha,s'\beta}(\mathbf{R}_{lmn}) = \frac{1}{N_{\mathbf{q}}} \sum_{i,j,k} \tilde{C}_{s\alpha,s'\beta}(\mathbf{q}_{ijk}) e^{i\mathbf{q}_{ijk}\cdot\mathbf{R}_{lmn}}$$

Fourier transforms of IFC's on a grid of q points nq1 x nq2 x nq3 in reciprocal space

IFC's in a supercell nq1 x nq2 x nq3 in real space

Exercise 3: Phonons dispersion in non-polar materials

Input file Si.q2r.in :

```
&input
  fildyn = 'Si.dyn',
  zasr = 'simple',
flfrc = 'Si444.fc',
 /
```

fildyn → Dynamical matrices from the phonon calculation

zasr → A way to impose the acoustic sum rule

flfrc → Output file of the interatomic force constants

The denser the grid of q points, the larger the vectors R for which the Interatomic Force Constants are calculated.

To perform the calculation:

```
mpirun -np 4 q2r.x -inp Si.q2r.in > Si.q2r.out
```

Exercise 3: Phonons dispersion in non-polar materials

Step 4. Calculate phonons at generic q' points using IFC by means of the code matdyn.x

$$C_{s\alpha,s'\beta}(\mathbf{R}_{lmn}) \xrightarrow{\tilde{C}_{s\alpha,s'\beta}(\mathbf{q}') = \sum_{l,m,n} C_{s\alpha,s'\beta}(\mathbf{R}_{lmn}) e^{-i\mathbf{q}'\cdot\mathbf{R}_{lmn}}} \tilde{C}_{s\alpha,s'\beta}(\mathbf{q}')$$

IFC's on a grid in real space — Fourier interpolation — Fourier transforms of IFC's at generic q' points in reciprocal space

Input file Si.matdyn.in :

mpirun -np 4 matdyn.x -i Si.matdyn.in > Si.matdyn.out

```
&input
  asr = 'simple',
  amass(1) = 28.0855,
  flfrc = 'Si444.fc',
  flfrq = 'Si.freq'
 /
396
   0.000000   0.000000   0.000000   0.000000
   0.012658   0.000000   0.000000   0.012658
```

- asr = 'simple', → Acoustic sum rule
- amass(1) = 28.0855, → Atomic mass
- flfrc = 'Si444.fc', → File with IFC's
- flfrq = 'Si.freq' → Output file with the frequencies
- 396 → Number of q points
- 0.000000 0.000000 0.000000 0.000000 / 0.012658 0.000000 0.000000 0.012658 → Coordinates of q points

Exercise 3: Phonons dispersion in non-polar materials

Step 5. Plot the phonon dispersion using the plotband.x program and gnuplot.

Input file Si.plotband.in :

```
Si.freq
0 600
freq.plot
freq.ps
0.0
100.0 0.0
```

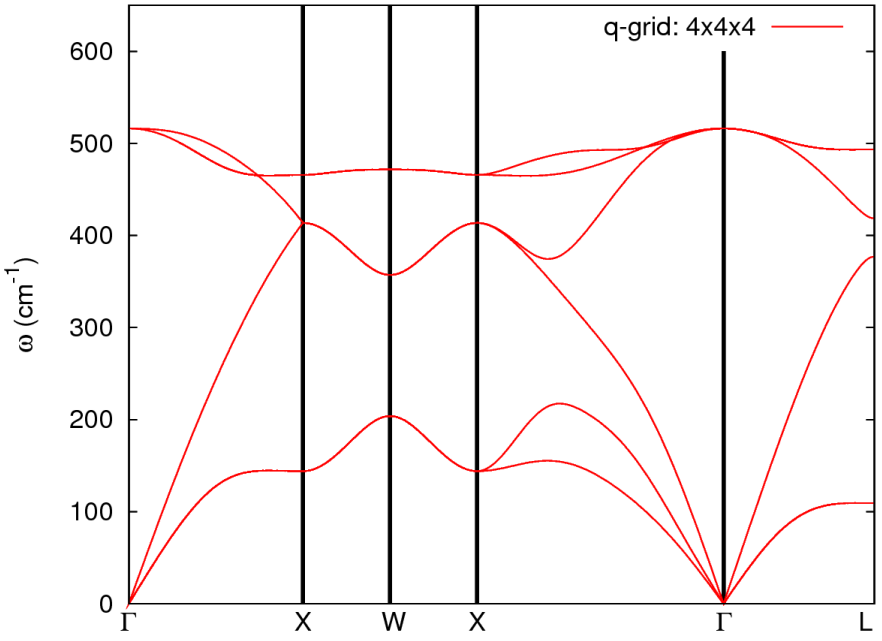
→ Input file with the frequencies at various q' points
→ Range of frequencies for a visualization
→ Output file with frequencies which will be used for plot
→ Plot of the dispersion (we will produce another one)
→ Fermi level (needed only for band structure plot)
→ Freq. step and reference freq. on the plot freq.ps

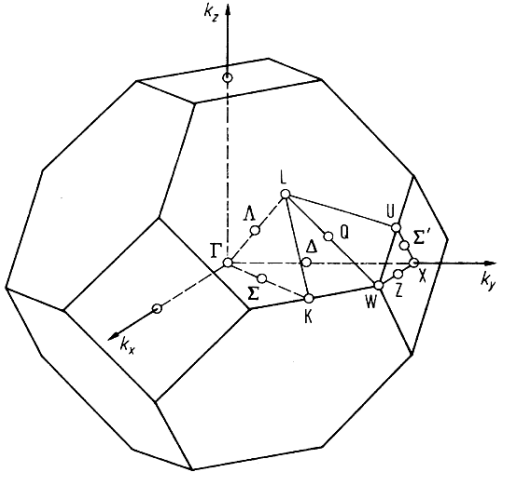
plotband.x < Si.plotband.in > Si.plotband.out

Use gnuplot and the file plot_dispersion.gp in order to plot the phonon dispersion of silicon (look at the file experimental_data.dat for the experimental reference).
You will get a postscript file phonon_dispersion.eps which you can visualize.

Exercise 3: Phonons dispersion in non-polar materials

Phonon dispersion of silicon along some high-symmetry directions in the Brillouin zone (file phonon_dispersion.eps):





Exercise 3: Phonons dispersion in non-polar materials

How to determine whether the quality of the Fourier interpolation is satisfactory? Compare with the direct calculation (no interpolation)!

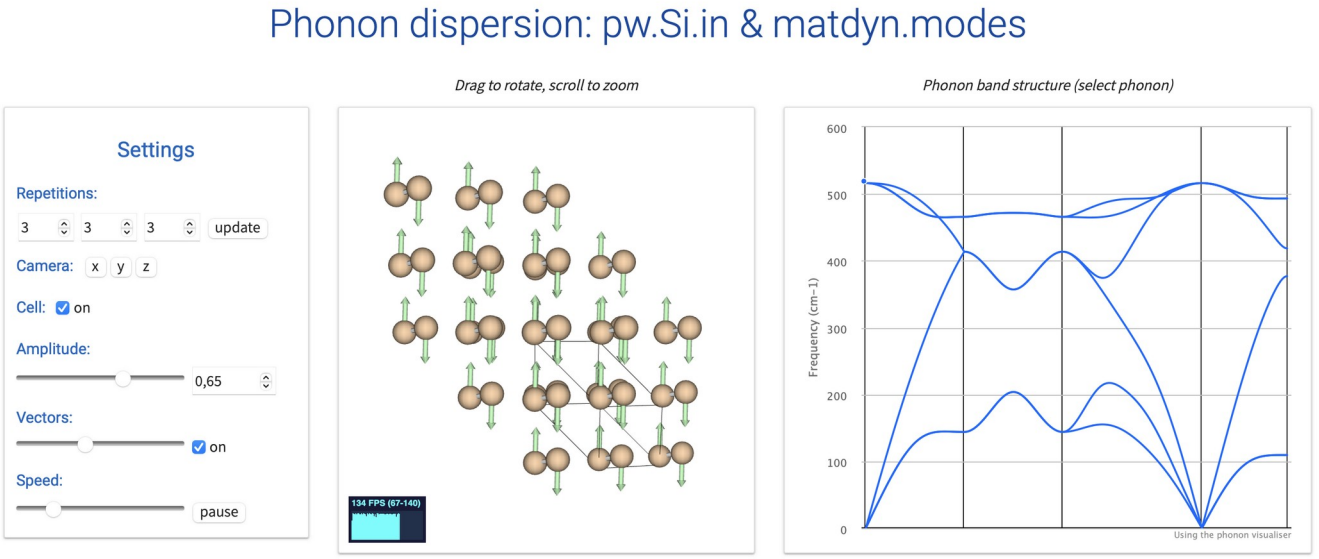
Homework-1: Perform a direct phonon calculation (no interpolation) at several q' points and make a comparison with the phonon frequencies obtained from the Interpolation. Use exercise1 as an example. Some q' points along the Gamma-X high symmetry line are listed in the file reference/q_points_direct_calc.txt

Homework-2: Perform a phonon dispersion calculation for several q-points grids (eg. 2x2x2, 4x4x4, and 6x6x6) and compare the dispersions. Do they converge?

Phonon modes visualizer

The phonon modes are not always easy to visualize, especially if we are not at Γ. An online phonon visualizer is very helpful in this regard.

https://www.materialscloud.org/work/tools/interactivephonon



Exercise 4: Phonons dispersion in polar materials

Go to the directory with the input files:

cd ~/ASESMA-2023/Day-5/Exercise4

In this directory you will find:

- *README.md* – File describing how to do the exercise
- *AlAs.scf.in* – Input file for the SCF ground-state calculation
- *AlAs.ph.in* – Input file for the phonon calculation at Γ
- *AlAs.q2r.in* – Input file for calculation of Interatomic Force Constants
- *AlAs.matdyn.in* – Input file for Fourier Interpolation for various q points
- *AlAs.plotband.in* – Input file for plotting a phonon dispersion
- **reference** – Directory with the reference results

Exercise 4: Phonons dispersion in polar materials

Step 1. Perform a SCF calculation for silicon at the equilibrium structure using the pw.x program.

```
mpirun -np 4 pw.x -inp AlAs.scf.in > AlAs.scf.out
```

Step 2. Perform a phonon calculation on a uniform grid of q points using the ph.x program.

```
mpirun -np 4 ph.x -inp AlAs.ph.in > AlAs.ph.out
```

Step 3. Calculation of the Interatomic Force Constants (IFC) using the q2r.x program.

```
mpirun -np 4 q2r.x -inp AlAs.q2r.in > AlAs.q2r.out
```

Step 4. Calculate phonons at generic q' points using IFC by means of the code matdyn.x

```
mpirun -np 4 matdyn.x -i AlAs.matdyn.in > AlAs.matdyn.out
```