Response-function: Phonon band structures and thermodynamical properties

Tutorial Response-function 2

This lesson aims at showing how to get the following physical properties, for periodic solids:

- Interatomic forces constants
- Phonon band structures
- Thermodynamical properties

This lesson should take about 1 hour.

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3. Analysis of the derivative databases (the ANADDB utility)
4. The computation of interatomic force constants
5. The efficient computation of phonon band structures
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1. Generation of the derivative databases

Before beginning, you might consider to work in a different subdirectory as for the other lessons. Why not create "Work_rf2" in ~abinit/tests/tutorespfn/Input?

This tutorial starts by the generation of a database, that is quite time-consuming. We suggest you to start immediately this computation...

Copy the files ~abinit/tests/tutorespfn/Input/trf2_1.files and ~abinit/tests/tutorespfn/Input/trf2_1.in in "Work_rf2".

Issue now:

1. `abinit < trf2_1.files >& log &`

It takes about 15 minutes to be completed on a PC 2.8 GHz...

In order to do interatomic force constant calculations, and to compute associated phonon band structure and thermodynamical properties, you should first have some theoretical background. Let us assume that you have read the litterature relative to the first lesson on response functions. You
might find additional material, related to the present section, in the following references:


If you haven't read parts of these references, you should take the time to get and read them now.

In short, the idea is that, in order to compute properties for which the phonon frequencies are needed in all the Brillouin zone, one can use an elaborate Fourier interpolation, so that only few dynamical matrices need to be computed directly. Others will be computed by interpolation.

Let us have a look at the input file trf2_1.in . The calculation is done for AlAs, the same crystalline material as for the previous lesson on response functions. Many input parameters are also quite similar, both at the level of the description of the unit cell, as for the choice of cut-off energy and k point grid.

Still, this input file is rather complex : in one single run, one produces the (Derivative Databases) DDBs needed for the rest of this tutorial. So, it starts with a ground-state calculation (dataset 1), followed by the computation of the response to the d/dk perturbation (dataset 2), and the response to electric fields, and phonons at Gamma (dataset 3). Datasets 4 to 10 generate the dynamical matrices at 7 q wavevectors, other than Gamma. At present (v4.6), one can only compute one q point per dataset, that is why so many datasets are needed.

Also, the values of these q wavevectors are not determined automatically. They must correspond to the q wavevectors needed by the ANADDB utility (see later), that is, they should form a reduced set of symmetry-inequivalent wavevectors, corresponding to a regularly spaced grid. In principle, they ought not include the Gamma point, but it is recommended to have it in the set, in order for the Fourier interpolation not to introduce errors at that important point. In order to minimize the number of preliminary non-self-consistent calculations, it is advised to take a q point mesh that is adjusted to the k point mesh used for the electronic structure : all q wavevectors should connect two k point wavevectors from this grid.

Such a set of q wavevectors can be generated straightforwardly by running a GS calculation with kptopt=1, nshiftk=1, shiftk=0 0 0 (to include gamma) and taking the output kpt set file as this qpt set. One might set nstep=1 and nline=1, so only one iteration runs. The input file ~abinit/tests/tutorespfn/Input/trf2_2.in is precisely an input file that can be used to generate such a set of k points. Copy it in the present Work_rf2 directly, as well as the accompanying ~abinit/tests/tutorespfn/Input/trf2_2.files. Examine these files, then run this calculation (it is very rapid - it won't hurt the trf2_1 job). The following k point set is obtained:

<table>
<thead>
<tr>
<th>kpt</th>
<th>0.00000000E+00</th>
<th>0.00000000E+00</th>
<th>0.00000000E+00</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2.50000000E-01</td>
<td>0.00000000E+00</td>
<td>0.00000000E+00</td>
</tr>
<tr>
<td></td>
<td>5.00000000E-01</td>
<td>0.00000000E+00</td>
<td>0.00000000E+00</td>
</tr>
<tr>
<td></td>
<td>2.50000000E-01</td>
<td>2.50000000E-01</td>
<td>0.00000000E+00</td>
</tr>
<tr>
<td></td>
<td>5.00000000E-01</td>
<td>2.50000000E-01</td>
<td>0.00000000E+00</td>
</tr>
<tr>
<td></td>
<td>-2.50000000E-01</td>
<td>2.50000000E-01</td>
<td>0.00000000E+00</td>
</tr>
<tr>
<td></td>
<td>5.00000000E-01</td>
<td>5.00000000E-01</td>
<td>0.00000000E+00</td>
</tr>
<tr>
<td></td>
<td>-2.50000000E-01</td>
<td>5.00000000E-01</td>
<td>2.50000000E-01</td>
</tr>
</tbody>
</table>

It is, as promised, the same as the q point set in the trf2_1.in file.
Now, it might be worth to examine in some detail one of the Derivative Database that has been created by the trf2_1 run. We suppose that the file trf2_1o_DS3_DDB has already been created. It corresponds to the third dataset, namely the response to q=0 and electric field. Edit this file, and read the 6.5 section of the respfn_help.html file. Examine the trf2_1o_DS3_DDB file carefully.

Seven other similar files will be generated by the trf2_1 run, containing the same header, but a different 2DTE block. It will be the duty of the MRGDDB utility, next section, to gather all these information.

Now, there might be two possibilities: either the trf2_1 run is finished, and you can continue the tutorial with the section 2 about the MRGDDB utility, or the run is not finished. In the latter case, instead of waiting for trf2_1 to be finished, we suggest you to pursue with section 3. You will use as DDB file the one that can be found in ~abinit/tests/tutorespfn/Refs, with the name trf2_3.ddb.out, instead of the one that would result from the section 2. Copy this file to the present directory, then go to section section 3 of this tutorial. You might come back to section 2 afterwards.

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### 2. Manipulation of the derivative databases (the MRGDDB utility)

The use of the MRGDDB utility is described in its help file. Please, read it carefully now.

Use MRGDDB to create the merge DDB from the eight DDB's corresponding to datasets 3 to 10 of the trf2_1 job, containing the dynamical matrices for the 8 q points, as well as the response to the electric field (dielectric tensor and Born effective charges). Including also the one from dataset 1 won't hurt (it contains the forces and stresses), but is not needed for the computation of phonon band structure, interatomic force constants, and thermodynamical properties. Name the new DDB trf2_3.ddb.out.

File ~abinit/tests/tutorespfn/Input/trf2_3.in is an example of input file for MRGDDB. You can copy it in the Work_rf2 directory, and run the merge as follows:

```bash
mrgddb < trf2_3.in
```

It takes less than one second on a typical PC.

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### 3. Analysis of the derivative databases (the ANADDB utility)

An introduction to the use of the ANADDB utility is described in its help file. Please, read it carefully now.

This ANADDB utility is able to perform many different tasks, each governed by a selected set of input variables, with also some input variables common to many of the different tasks. The list of tasks to be done in one run is governed by different flags. Here is the list of flags:

- `dieflag`
- `elaflag`
- `elphflag`

Tips for ABINIT users and developers - https://wiki.abinit.org/
Please, take some time to read the description of each of these flags. Note that some of these flags might be required to allow to run another task.

In this tutorial, we will focus on the flags ifcflag and thmflag

4. The computation of interatomic force constants

You can copy the files ~abinit/tests/tutorespfn/Input/trf2_4.in and ~abinit/tests/tutorespfn/Input/trf2_4.files to the Work_rf2 directory.

Edit the file trf2_4.in. Note that ifcflag is activated. Related input variables can be split in three groups.

The first group of variables define the grid of q wavevectors:

- brav
- nagpt
- nqshft
- q1shft

Unfortunately, the names of input variables and their meaning is not exactly the same as the names used to generate the k points in ABINIT. This is a shame, a remnant of history ... Please read carefully the documentation that describes these input variables.

The second group of variables allows to impose some known constraint on the dynamical matrices and Born effective charges before proceeding with the analysis:

- asr
- chneut

Please, read carefully the explanation for these input variables.

Finally, a third group of variables is related specifically to the analysis of the Interatomic Force Constants:

- dipdip
- ifcana
- ifcout
- naticf
- atific

Here also, spend some time to read the associated documentation.

Now, you should issue:
anaddb < trf2_4.files > trf2_4.log

It will last only a few seconds.

The file trf2_4.out contains the list of interatomic force constants, as well as some analysis. Edit this file.

Try to find the following paragraph:

Analysis of interatomic force constants

Are given: column(1-3), the total force constant
then column(4-6), the Ewald part
then column(7-9), the short-range part

Column 1, 4 and 7 are related to the displacement of the generic atom along x,
column 2, 5 and 8 are related to the displacement of the generic atom along y,
column 3, 6 and 9 are related to the displacement of the generic atom along z.

The interatomic force constants are output for the nuclei specified by the input variable atifc. Here, only atom 1 is considered. The IFCs with respect to the other nuclei is given, by order of increasing distance. For each pair of nuclei involving atom 1, there is first the output of the IFCs in cartesian coordinates, as well as their decomposition into an Ewald and a short-range part, then, the analysis with respect to a local system of coordinate. The latter is chosen such as to diagonalize the IFC tensor, in case of the self-force constant, and in the other cases, the first vector is the vector joining the two nuclei, in order to decompose the IFC into a longitudinal and a transverse component.

5. The efficient computation of phonon band structures

You can copy the files ~/abinit/tests/tutorespfn/Input/trf2_5.in and ~/abinit/tests/tutorespfn/Input/trf2_5.files to the Work_rf2 directory.

Edit the file trf2_5.in. Note that ifcflag is again activated. Indeed, in order to compute a phonon band structure using the Fourier interpolation, the IFCs are required. This is why the two first groups of variables, needed to generate the IFCs are still defined. The third group of variables is now restricted to dipdip only.

Then, come the input variables needed to define the list of q wavevectors in the band structure:

- eivec: flag to turn on the analysis of phonon eigenvectors
- nph1l: number of q-points for phonon interpolation
- qph1l: list of q-points for phonon interpolation
- nph2l: number of q-directions for LO-TO correction
- qph2l: list of q-directions for LO-TO correction

Now, you should issue:
anaddb < trf2_5.files > trf2_5.log

It will last only a few seconds.

The file trf2_5.out contains the list of eigenvalues, for all the needed q-wavevectors. You can edit it, and have a look at the different sections of the file. Note that the interatomic force constants are computed (they are needed for the Fourier interpolation), but not printed.

Please, edit also the other output file, named trf2_5_B2EPS.freq. It contains the frequencies, in a format suitable for graphical output, using the program band2eps (the latter should be more documented, and will not be described in the present tutorial).

You can copy the files ~abinit/tests/tutorespfn/Input/trf2_6.in and ~abinit/tests/tutorespfn/Input/trf2_6.files to the Work_rf2 directory, then issue

band2eps < trf2_6.files > trf2_6.log

The file trf2_6.out.eps has been produced. It is an .eps file (eps stand for Encapsulated PostScript). You can use the program ghostview to visualize it. The command to issue will depend on the way you have configured your machine, but the following might perhaps do the work:

gv trf2_6.out.eps

You should see a nice phonon band structure for AlAs. Well, not so nice, after all, because there are two strange dips for the highest phonon band, at the Gamma point. This is due to the lack of LO-TO splitting for the ANADDDB treatment of the first list of vector. The correct phonon band structure is presented here. You can correct the LO-TO splitting by the following little hack.

Edit the file trf2_5_B2EPS.freq, and note that the value of the frequency, in the sixth column, has a discontinuity exactly for the Gamma point (the three first columns give the k point coordinates), that is, at lines 1 and 31:

```
0.000000D+00  0.000000D+00  0.000000D+00  0.156855D-02  0.156855D-02
0.156855D-02
```

Replace these values (sixth column, line 1 and 31) by the correct value, including the LO-TO splitting, that you can find in the file trf2_5.out, at the end, second list of vector. That is, the lines 1 and 31 should now read:

```
0.000000D+00  0.000000D+00  0.000000D+00  0.156855D-02  1.730353E-03
0.156855D-02
```

Now, run again band2eps. Your phonon band structure should be perfect!


Of course, one should make a convergence study, on the k and q point grids (separately!), as well as on the energy cut-off, and also test LDA and GGA ... But this is left to the user!
6. Thermodynamical properties.

We will give only a very short example of the use of ANADDB to compute thermodynamical properties. This is because this part of ANADDB is likely the farthest from a clean, stable, usage. By exploring the input variables, the user should be able to produce figures and data like the ones for SiO2 quartz and stishovite, published in


You can copy the files ~/abinit/tests/tutorespfn/Input/trf2_7.in and
 ~/abinit/tests/tutorespfn/Input/trf2_7.files to the Work_rf2 directory, and have a look at them.
The same DDB as for trf2_4 and trf2_5 is used, namely trf2_3.ddb.out. The following additional input variables are present:

- thmflag
- ng2qpt
- ngrids
- q2sht
- nchan
- nchan
- thmtol
- ntemper
- temperinc
- tempermin

Examine the input file, the input variables, then run anaddb (as usual ...). Then, edit the output file. You should be able to find the crucial section:

<table>
<thead>
<tr>
<th>At</th>
<th>T</th>
<th>F(J/mol-c)</th>
<th>E(J/mol-c)</th>
<th>S(J/(mol-c.K))</th>
<th>C(J/(mol-c.K))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>20.0</td>
<td>8.1384756E+03</td>
<td>8.1463588E+03</td>
<td>3.9416450E-01</td>
<td>1.4169102E+00</td>
</tr>
<tr>
<td></td>
<td>40.0</td>
<td>8.1061319E+03</td>
<td>8.2368069E+03</td>
<td>3.2668767E+00</td>
<td>7.8985027E+00</td>
</tr>
<tr>
<td></td>
<td>60.0</td>
<td>7.9980215E+03</td>
<td>8.4576599E+03</td>
<td>7.6590737E+00</td>
<td>1.3992227E+01</td>
</tr>
<tr>
<td></td>
<td>80.0</td>
<td>7.7974376E+03</td>
<td>8.7915524E+03</td>
<td>1.2426435E+01</td>
<td>1.9325165E+01</td>
</tr>
<tr>
<td></td>
<td>100.0</td>
<td>7.5004823E+03</td>
<td>9.2274431E+03</td>
<td>1.7269608E+01</td>
<td>2.4175005E+01</td>
</tr>
<tr>
<td></td>
<td>120.0</td>
<td>7.1069991E+03</td>
<td>9.7544363E+03</td>
<td>2.2061977E+01</td>
<td>2.8411187E+01</td>
</tr>
<tr>
<td></td>
<td>140.0</td>
<td>6.6189292E+03</td>
<td>1.0359248E+04</td>
<td>2.6716563E+01</td>
<td>3.1955266E+01</td>
</tr>
<tr>
<td></td>
<td>160.0</td>
<td>6.0396228E+03</td>
<td>1.1028289E+04</td>
<td>3.1179165E+01</td>
<td>3.4847422E+01</td>
</tr>
<tr>
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<td>1.1749439E+04</td>
<td>3.5423425E+01</td>
<td>3.7183863E+01</td>
</tr>
<tr>
<td></td>
<td>200.0</td>
<td>4.6241912E+03</td>
<td>1.2512641E+04</td>
<td>3.9442249E+01</td>
<td>3.9069447E+01</td>
</tr>
</tbody>
</table>

There, one finds, the phonon free energy, the phonon internal energy, the phonon entropy and the phonon heat capacity.

Do not forget that we are working in the harmonic approximation; beyond some temperature, anharmonic effects will have a sizeable contributions.

The atomic temperature factors can also be computed. An example is presented in tests/v5, test 22.
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