Solutions for excercise sheet 6

Exercise 1: Superconductivity in MgB_2

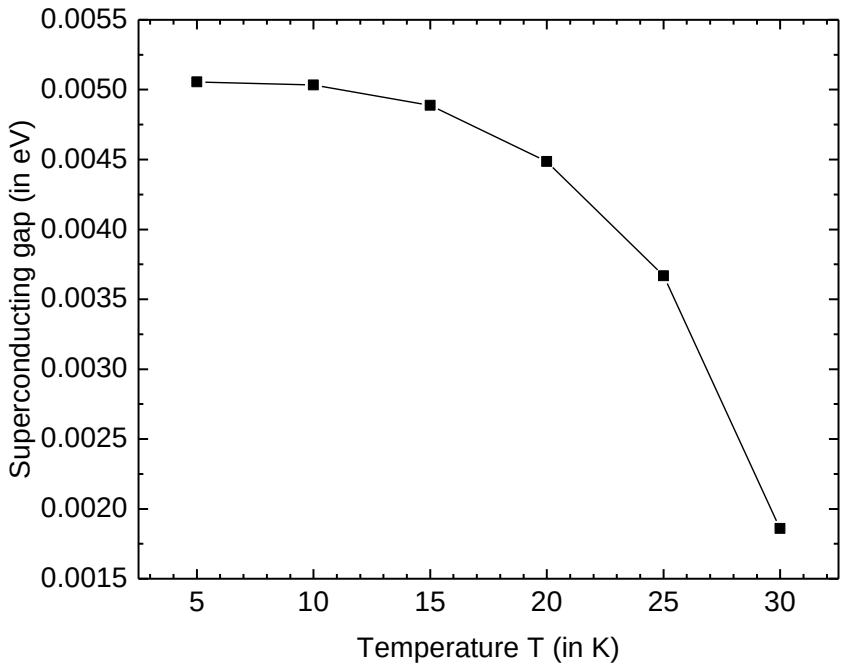
(a) Nothing to plot

(b) Nothing to plot.

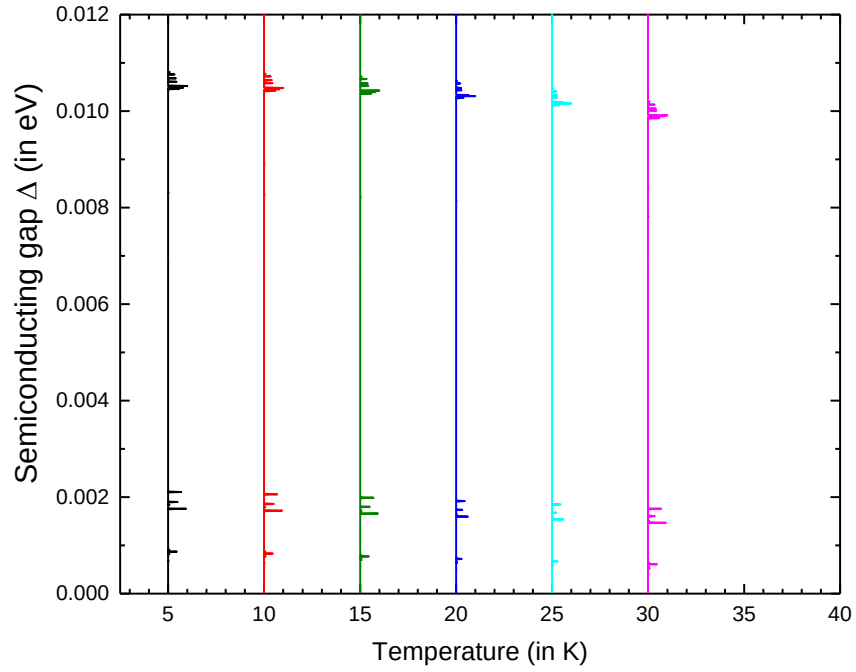
(c)

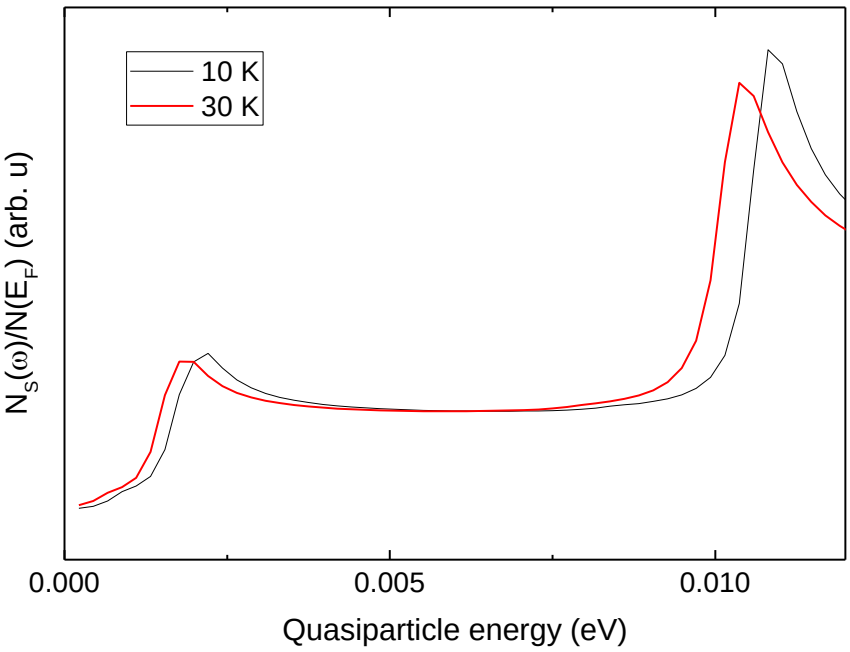
```
Finish reading .ephmat files
lambda_max =              2.8312452   lambda_k_max =              1.1057338
Electron-phonon coupling strength =    0.8459062
Estimated Allen-Dynes Tc =      21.9155879 K for muc =    0.16000
Estimated BCS superconducting gap =       0.0033238 eV
WARNING WARNING WARNING
The code will crash for tempsmax much larger than Allen-Dynes Tc
```

(d) Superconducting band gap in isotropic approximation:



(e) (if you obtain some error for these calculations, run them without using the restart mechanism, i.e. using the input file from (b) and only changing `liso` and `laniso`.)





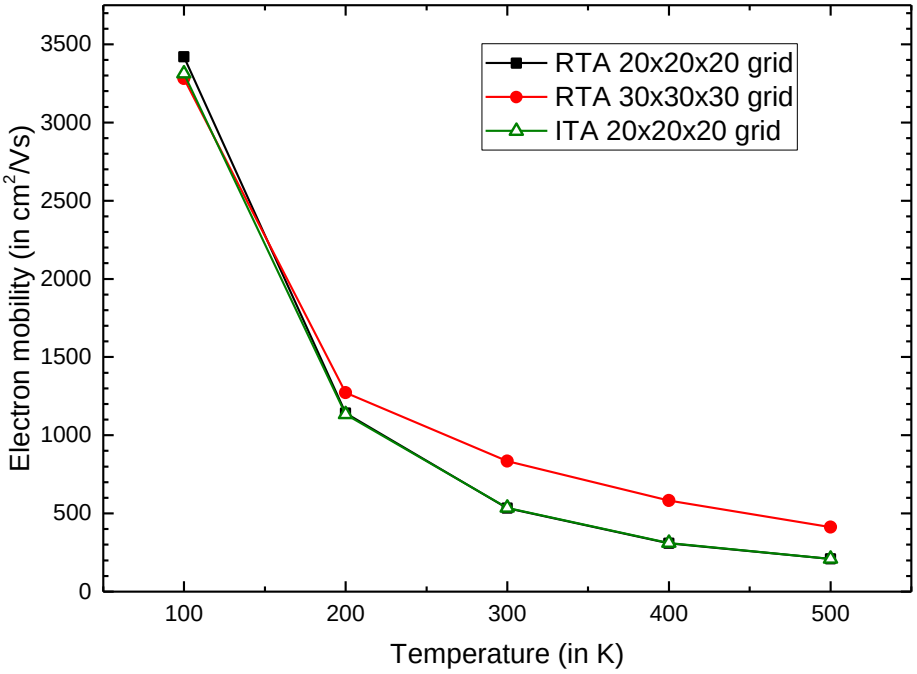
Exercise 2: Electron and hole mobility in silicon

(a) Nothing to plot

(b)&(c)&(d) The calculations only work if the 16 phonon wavevectors given at the end of the EPW input files are the same as the coordinates given in the file Si.dyn0. The coordinates depend on the definition of the lattice vectors of the unit cell used for the calculations. The ones given in the provided input files are the coordinates of the q-vectors obtained for the reference file Si.scf.in_ref (added to the zip file for this exercise). Also, the acoustic sum rule correction scheme in EPW apparently does not always work. You might have to delete the lines

```
lifc        = .true.
asr_typ     = 'crystal'
```

from the EPW input files for the calculations to run.

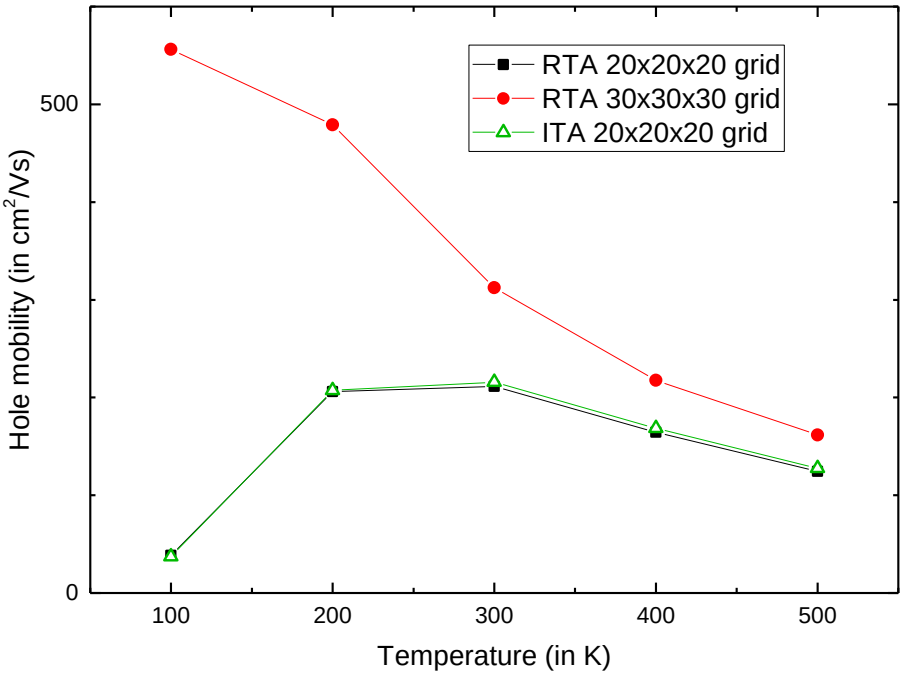


The hole mobilities for the ITA can be difficult to obtain. It might only work after a calculation of the electron mobilities (in the same folder). You might also need to use the restart feature, with the keywords

```
restart      = .true.
restart_freq = 50
selecqread   = .false.
```

(i.e. removing the "!" in front of these keywords) to trigger calculation of the hole mobilities instead of the electron mobilities.

The input file epw3.in_ref in the .zip-file was updated accordingly.


RTA 20x20x20 grid
RTA 30x30x30 grid
ITA 20x20x20 grid
Hole mobility (in cm²/Vs)
500
0
100
200
300
400
500
Temperature (in K)