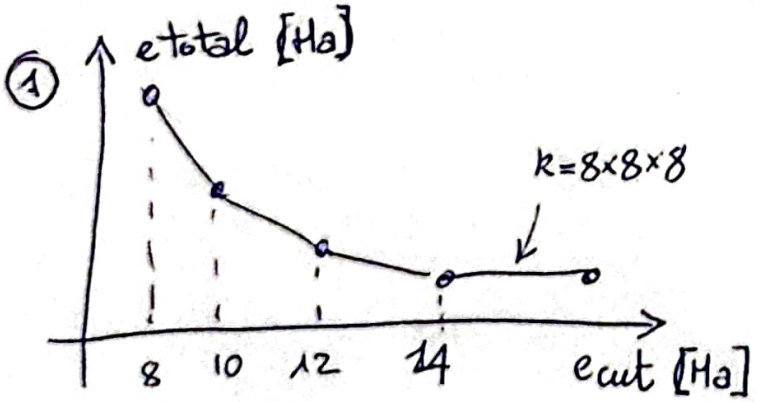
DFT - Steps, general results and analysis

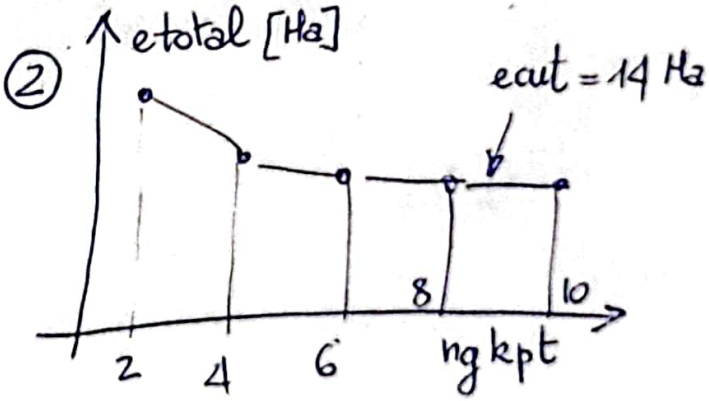
- Following and summarizing "ABINIT Hands-On" by Matteo Caguoud:

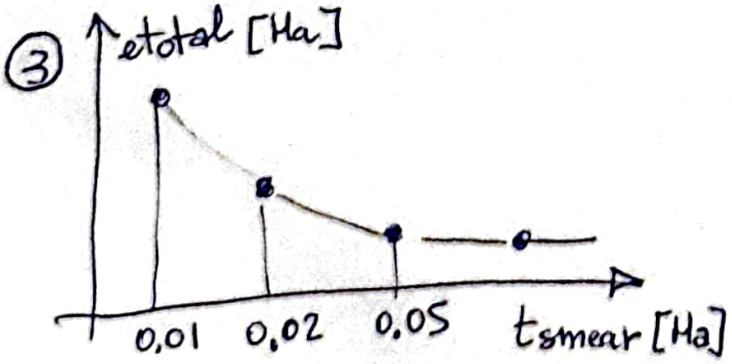
1) Find <u>convergence w.r.t. cut-off energy</u> (using multi-dataset mode) for a certain grid of k-points (pagg. 25-27)
2) Find <u>convergence w.r.t. number of k-points</u> (using multi-dataset mode) for the "optimized" cut-off energy
3) (only in metals, but doped diamond is conducting)
   → Find <u>convergence w.r.t. smearing-parameter.</u> (pagg. 28-29)

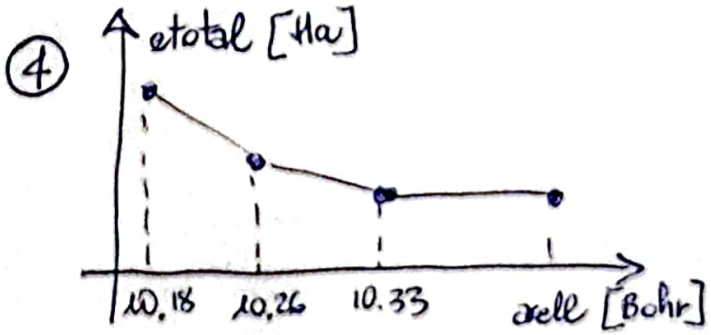
N.B. In principle these three convergences are not independent but...

4) Reform <u>structural relaxation</u> (pagg. 31.-34)









5) ELECTRONIC PROPERTIES

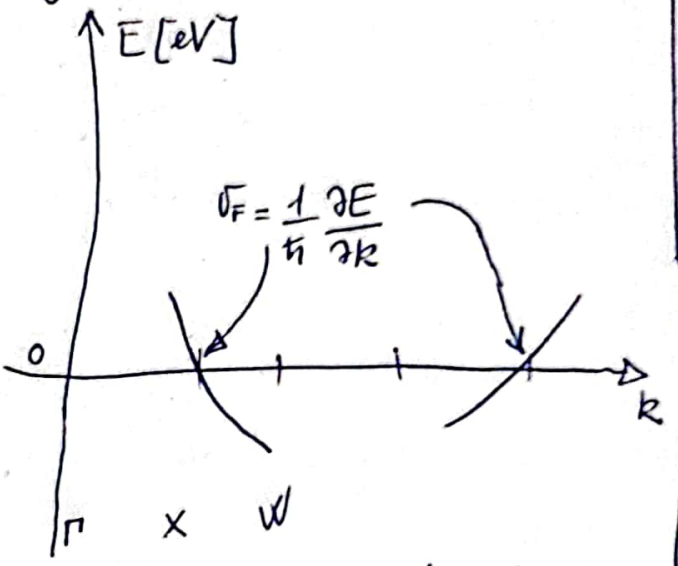
- Band structure (eventually adding Spin-Orbit Coupling (SOC) in heavy metals) → (pagg. 35-42)

WHAT YOU CAN GET FROM BAND STRUCTURE?

a) Comparison ~~from~~ with results from literature

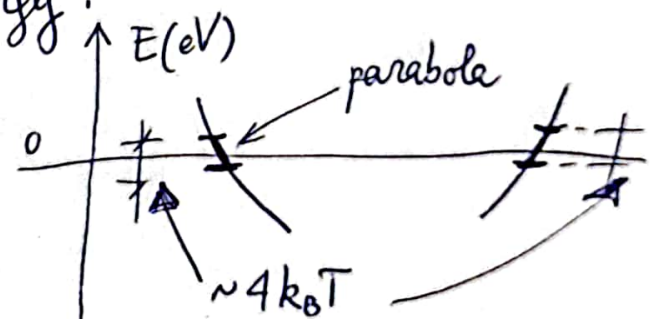
b) Calculation of the Fermi velocity in any point where a band crosses the Fermi energy

- $v_F = \frac{1}{\hbar}\left[\frac{\partial E(k)}{\partial k}\right]_{k=k_F}$



c) Calculation of the effective mass in any point where a band crosses the Fermi energy:

- fit by a quadratic (parabolic) behaviour a small region (of extension $\sim 4k_BT$) around the E_F of the band
- Then you can obtain the effective mass in that k point by:



$$m^*(k_F) = \frac{\hbar^2}{\left(d^2E/dk^2\right)_{k=k_F}}$$

d) The total (average) values of v_F and m^* on the Fermi surface, that can be used in other analyses on experimental values can be obtained, in first approximation, by a simple average of the different values found in the different k_F points

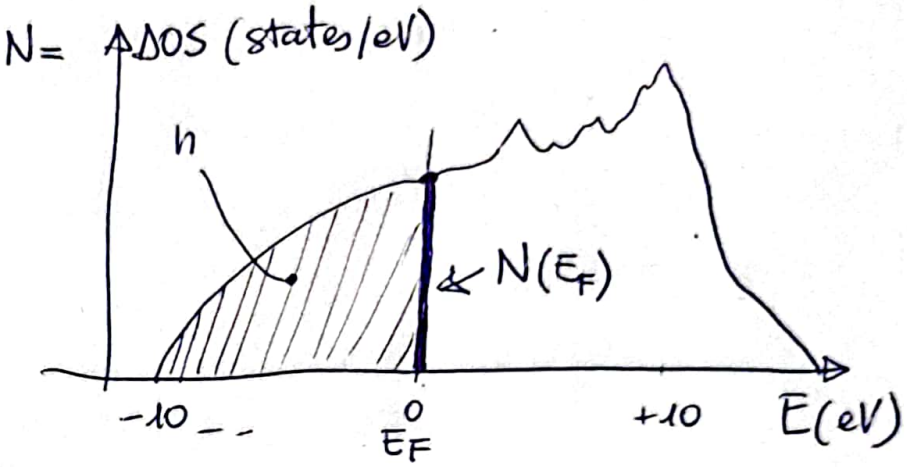
- Density of States → (pagg 41-47)

WHAT YOU CAN GET FROM DOS ?

a) Comparison with literature

b) Density of states at Fermi energy :

$N(E_F)$



c) Density of charge carriers n :

$$n = \int_{E_{min}}^{E_F} N(E)\, dE$$

n is very important for calculations and analysis of the transport properties (see Erik)

d) Comparison with n from literature ... but attention

→ most of the values of n present in the books are calculated in free electron model approximation

→ difference ? ...

- Fermi surface → (pagg. 46-47)

a) Comparison with literature

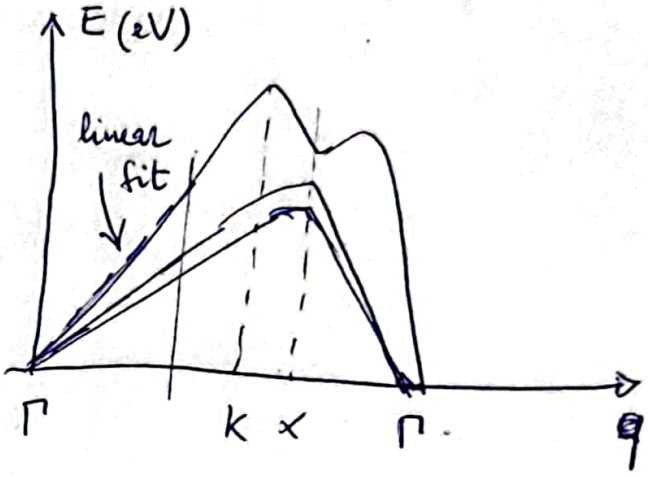
6) PHONON PROPERTIES

- **Dispersion relations** (phonon bands) → (pagg. 53-58)

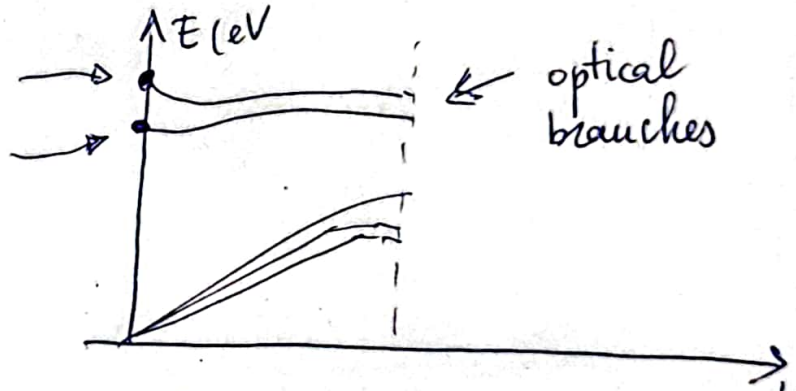
WHAT YOU CAN GET FROM DISPERSION RELATIONS

a) Comparison with literature

b) Speed of sound in directions of high symmetry → by a linear fit of the acoustic branches at energies close to zero i.e. at q vectors close to Γ



c) The energy values of optical branches at q=0 can give info on the energies of Raman peaks but attention → not all the modes are Raman active

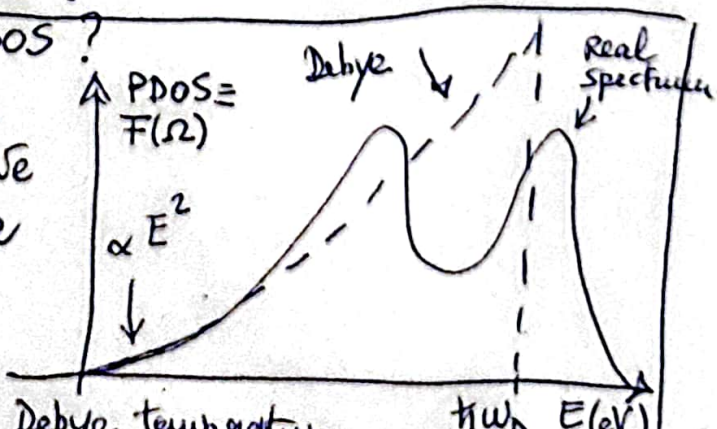


→ There are specific commands in ABINIT for the calculation of Raman and IR active-modes energies
↳ comparison with Raman spectra in doped diamond

- **Phonon DOS** → (pag. 58)

WHAT YOU CAN GET FROM PDOS?

a) By fitting the low-energy part ($E \leq E_{max}/10$) by a parabolic curve and then extending this parabola up to the value that produce the same integral of the true PDOS → Debye energy or Debye temperature → comparison with literature



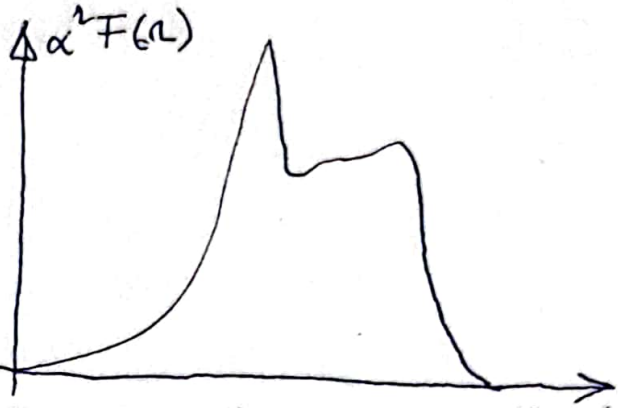
• Electron-phonon spectral function $\alpha^2F(\Omega)$ → (pagg 59-67)

WHAT YOU CAN GET FROM $\alpha^2F(\Omega)$?

a) comparison with literature

b) Thermodinamical electron-phonon coupling constant:

$$\lambda = 2\int_0^{\Omega_{max}} \frac{\alpha^2F(\Omega)}{\Omega} d\Omega$$



- Eventually you can compare this λ with the transport one λ_{tr} that you can obtain from the fit of the linear T dependence of resistivity at high T (see pagg. 42-45 of AEP lecture Notes - Chapt. 5)

$$\rho = \rho_0 + \frac{2\pi k_B}{e^2\hbar}\frac{m_{eff}}{n}\lambda_{tr} T$$

where $\frac{m_{eff}}{n}$ can be obtained from DFT band structure and DOS

Remember that λ and λ_{tr} are similar, but not identical because $\alpha^2F(\Omega)_{tr}$ is different from $\alpha^2F(\Omega)$ (due to the contribution of small-angle scattering in transport properties). λ and λ_{tr} are dimensionless and of order of 1.

c) Neglecting (as a first approximation) the previous difference, you can use $\alpha^2F(\Omega)$ (obtained from DFT) for the estimation of the measured resistivity by using eq. (1) at page 42 of Chapt. 5 of the notes.

d) If the metal is superconducting (as Nb), from λ you can obtain the critical temperature T_c by using the Allen-Dynes formula (pagg. 13 and 14 of Chapt. 6 of the AEP notes) and by fixing (from literature) the value of the repulsive Coulomb pseudo-potential μ^*.
This is automatically done by the routine of Abinit that calculates T_c