Recap of exercise 1

Convergence testing

Total energy vs cut-off energy

k-point sampling

ENCUT

$H\Psi = E\Psi \longrightarrow H_{KS}\phi = E_{KS}\phi$

fully interacting system

non-interacting system w/ same density as the i.a. system

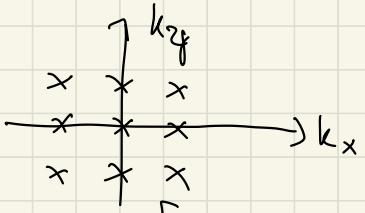
E_{kin} can be evaluated more easily

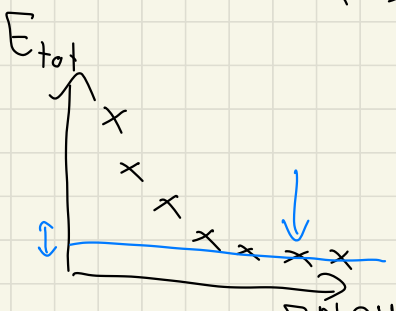
$$\phi_{\vec{k},i}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} C_{\vec{k},i}\, e^{i(\vec{k}+\vec{K})\vec{r}}$$

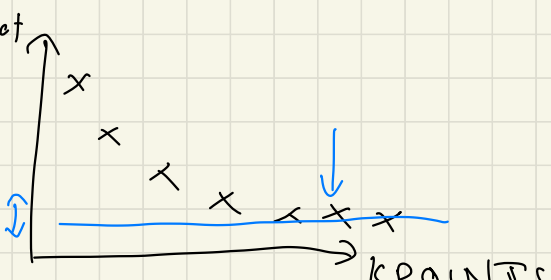
$$ENCUT \equiv E_{cutoff} \propto k^2_{cutoff}$$

KPOINTS

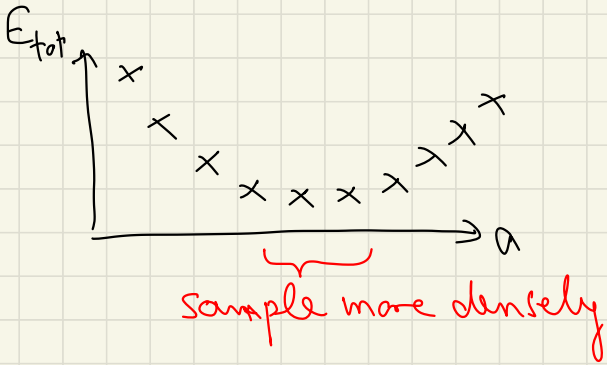
Determines BZ sampling density

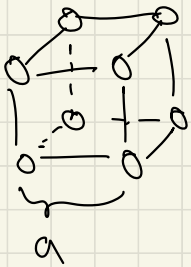






Geometric optimization



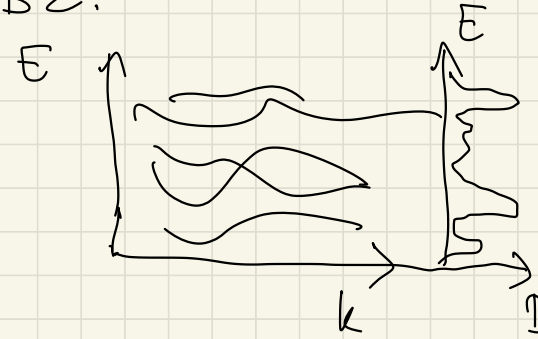


In practice for noncubic systems: Structural relaxation for:

- Unit-cell volume
- Unit-cell shape
- Internal atomic coordinates

Bandstructure & DOS

Kohn-Sham energies plotted for different locations in the BZ.



1 DAV: xxx
2 DAV: xxx
⋮
1 F= xxx

} scf loops of the iterative solution of the KS equations