Aalto University
School of Science

Extras based on homeworks, questions, etc…

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9.3.2015

Interacting vs. non-interacting electrons

- Non-interacting electrons mostly assumed in this course
  - With Pauli exclusion principle (FD statistics)
- When more than one electron, we are still solving one-electron Schrödinger: $\nabla^2\Psi(r) + V\Psi(r) = E\Psi(r)$ and filling the ”excited” states with electrons.
- Instead of: $\nabla^2\Psi(r) + V\Psi(r) + \frac{1}{|r_1 - r_2|} = E\Psi(r)$

  for interacting electrons

- Electrons always in eigenstates: infinite lifetime, no e-e scattering.
- In ”reality” we have quasiparticle excitations with finite lifetime (due to e-e scattering)

p vs v vs k

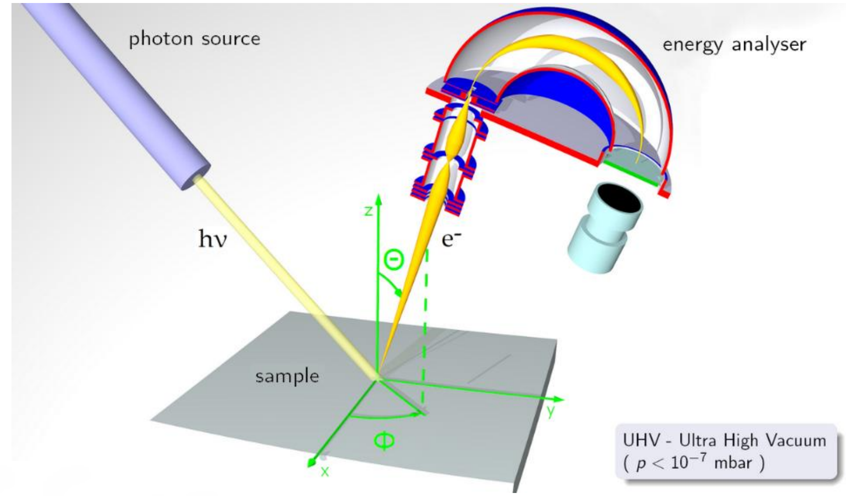
- As mentioned both the periodic part and phase factor contribute to momentum expectation value.

- $\langle p \rangle = m\langle v \rangle = m v_g$, shown here (slides 20-22)
  - Not effective mass times velocity

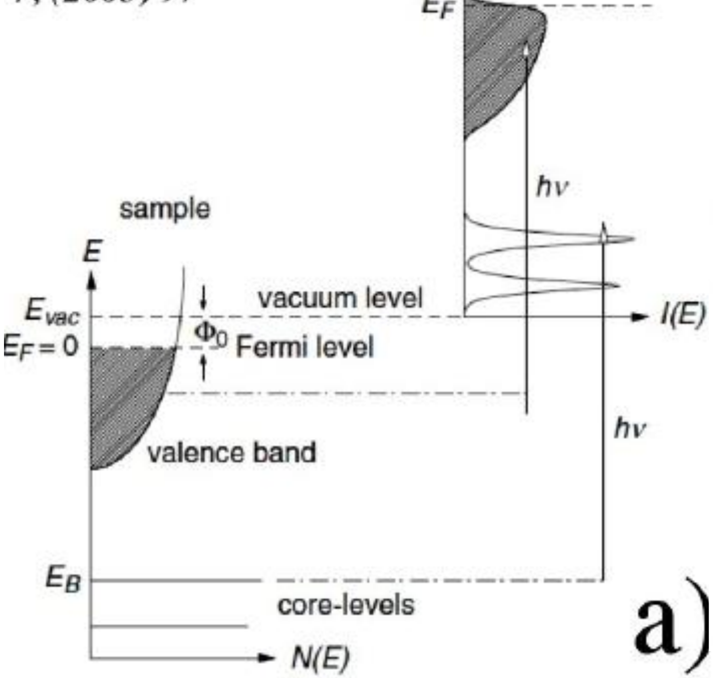
- k is conserved in lattice (modulo G), but p is not! See proof (slide 4)

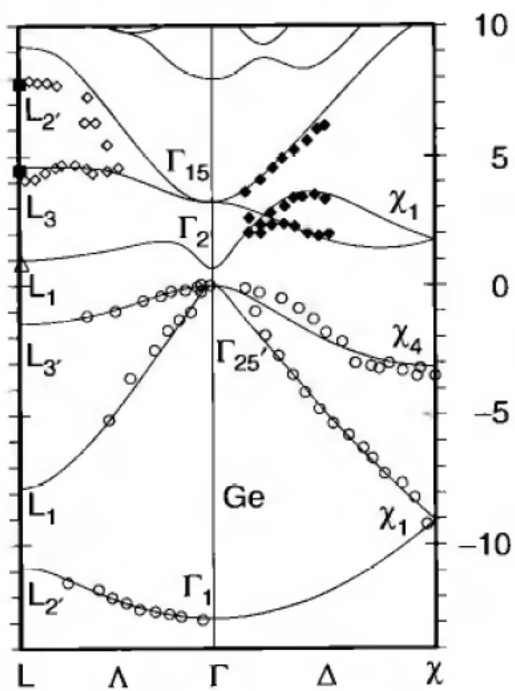
Measuring band structure

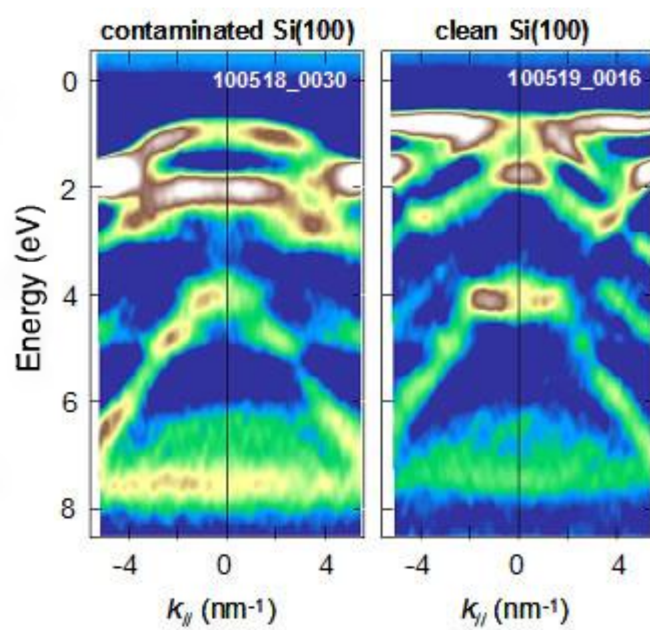
- Photoemission spectroscopy
- Angle-resolved (ARPES)



From F. Reinert and S. Hufner, New J. Phys. 7, (2005) 97

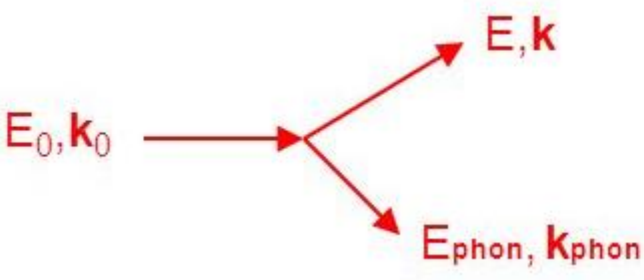






Measuring band structure or phonon dispersion

- Phonons by inelastic neutron scattering



Energy and momentum conservation:

$$E = E_0 - E_{phon}$$

$$\mathbf{k} = \mathbf{k}_0 - \mathbf{k}_{phon} + \mathbf{G}_{hkl}$$