

Reminders/Introduction: Quantum Mechanics

- Electron described by wave function as basis variable

$$\psi(x, y, z, t)$$

- Square of the wave function describes probability

$$\psi^* \psi$$

- In practice: Solve Schrödinger equation to find wave function

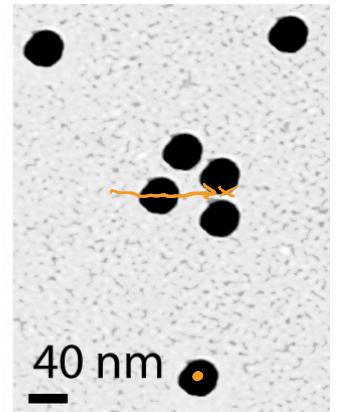
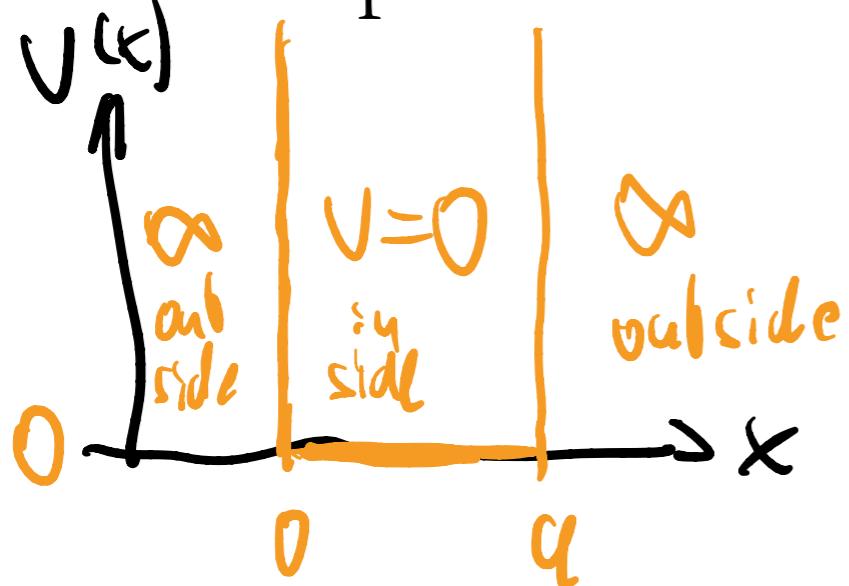
$$\hat{H}\psi(x, y, z, t) = i\hbar \frac{\partial}{\partial t} \psi(x, y, z, t)$$
$$= E \psi$$

free electron: $V=0 \rightarrow \frac{d^2\psi}{dx^2} + \left(\frac{2m}{\hbar^2} E \right) \psi = 0$

= k^2

Solution of the Schrödinger Equation: Infinite 1D Well

- infinite well potential looks like this:



↪ solution: outside = 0 $\rightarrow \psi = 0$

inside: free electron

$$\psi(x) = A \exp(i k x) + B \exp(-i k x)$$

↪ boundary $\psi(0) = 0 \rightarrow B = -A$

$$\rightarrow \psi(x) = A [\exp(i k x) - \exp(-i k x)] = 2A i \sin(kx)$$

Solution of the Schrödinger Equation: Infinite 1D Well

$$\psi(x) = 2Ai \sin(kx)$$

$$k^2 \equiv \frac{2m}{\hbar^2} E$$

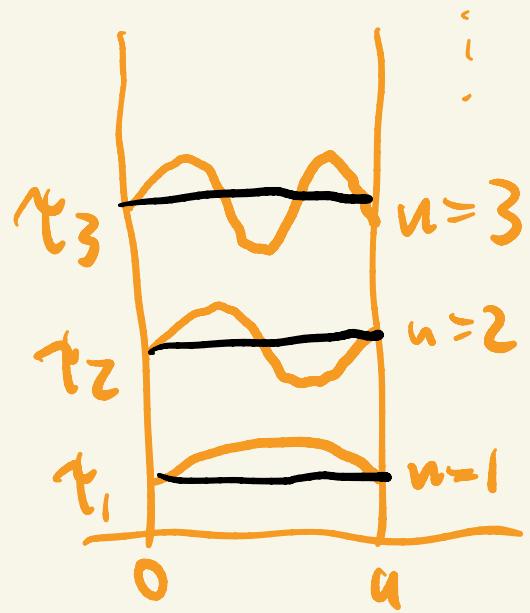
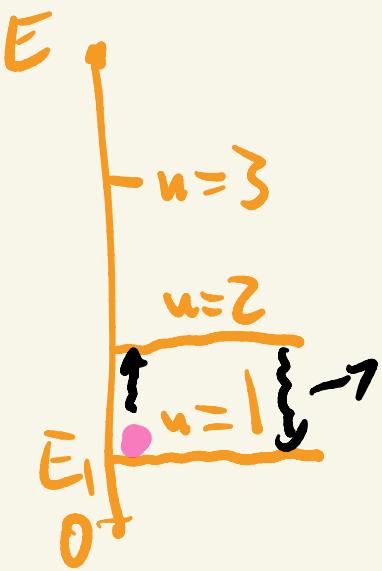
- still have to determine k by fulfilling: $\psi(a) = 0 = 2Ai \sin(ka)$

- this requires: $ka = n\pi \rightarrow k = \frac{n\pi}{a}$

$$\rightarrow \psi(x) = 2Ai \sin\left(\frac{n\pi x}{a}\right) \quad n > 0, \text{ integer}$$

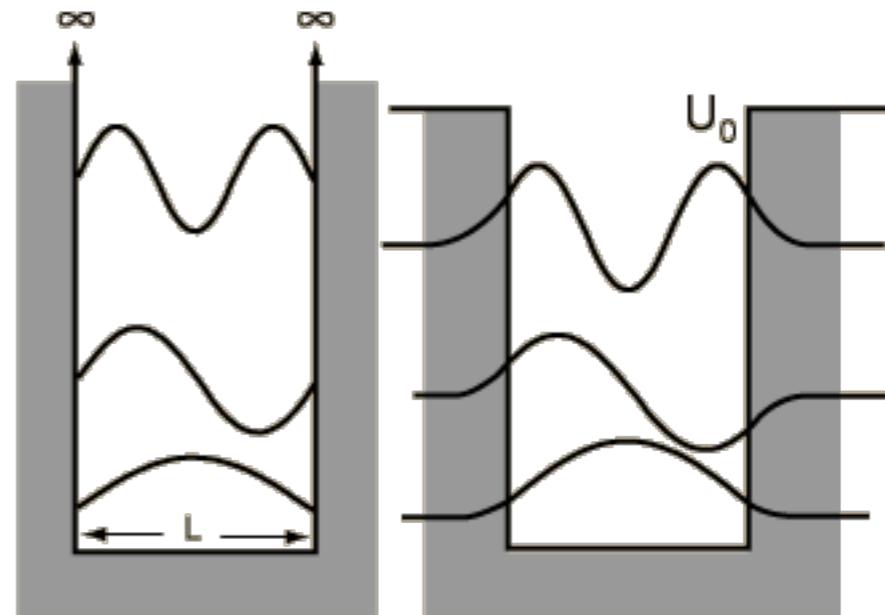
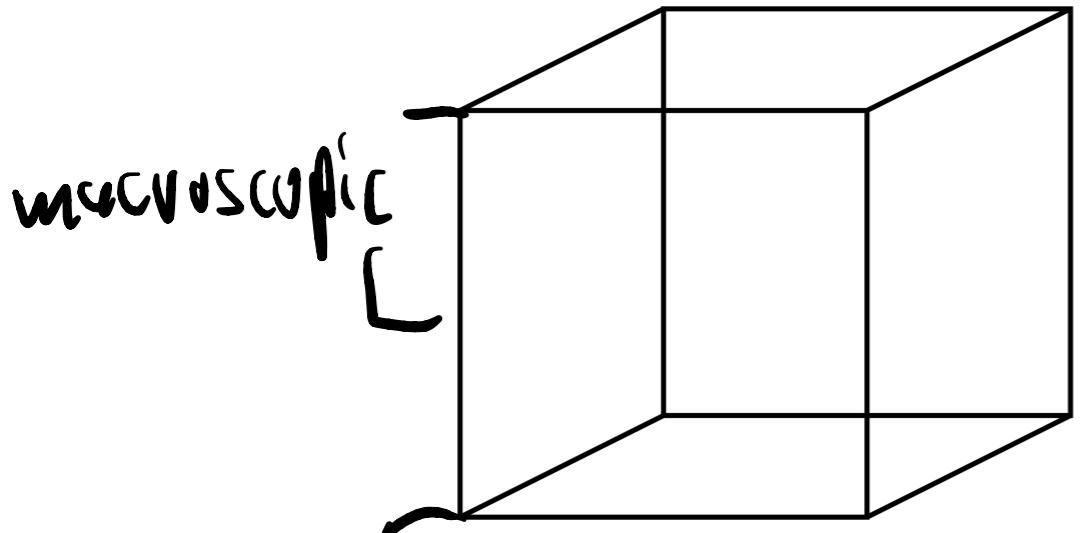
↳ normalization determines A

$$E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$



Solids: Free-electron gas model

- Free-electron gas model of a solid looks like:



- found for 1D infinite well:

$$E = \frac{\hbar^2 k^2}{2m}$$

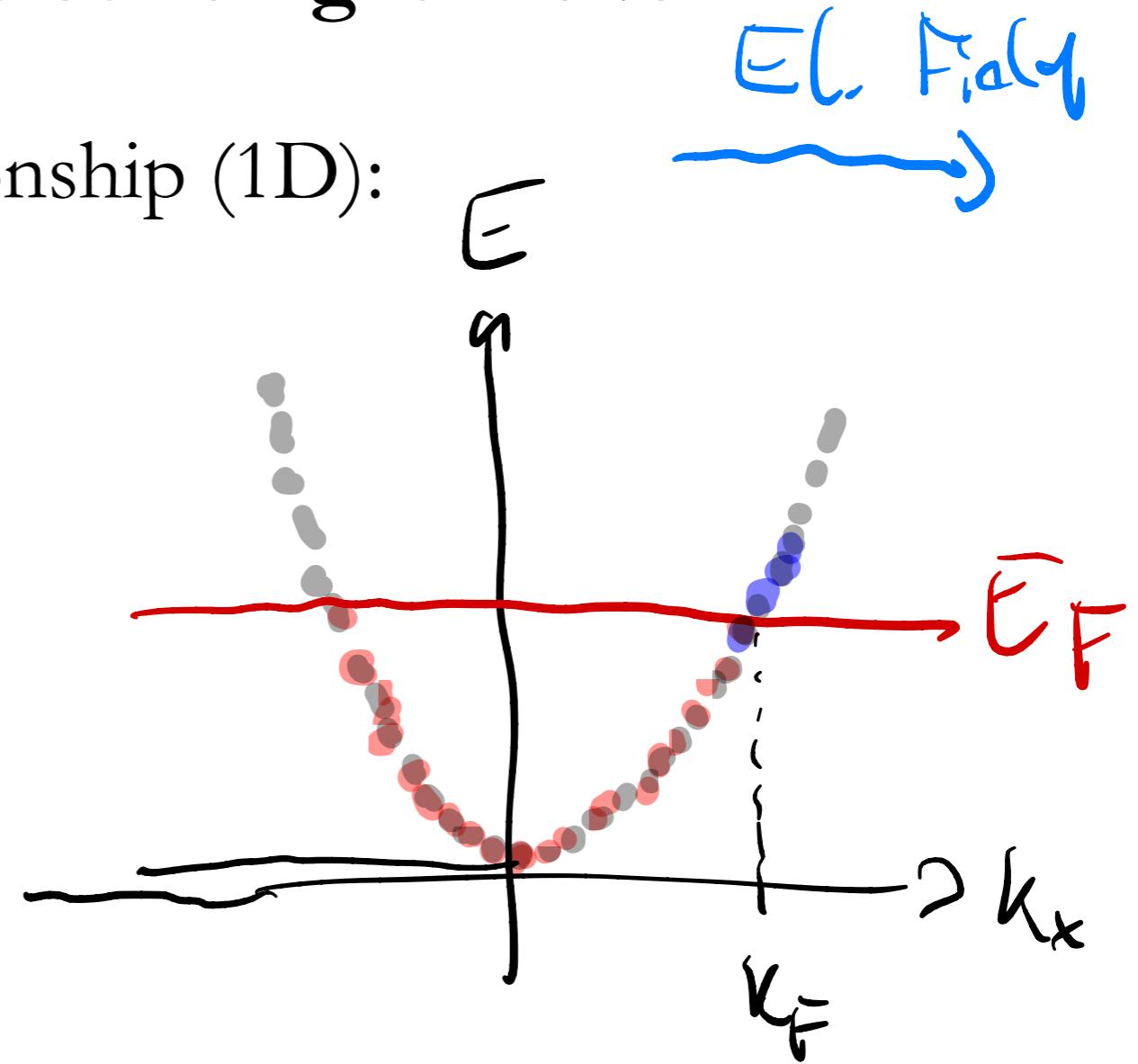
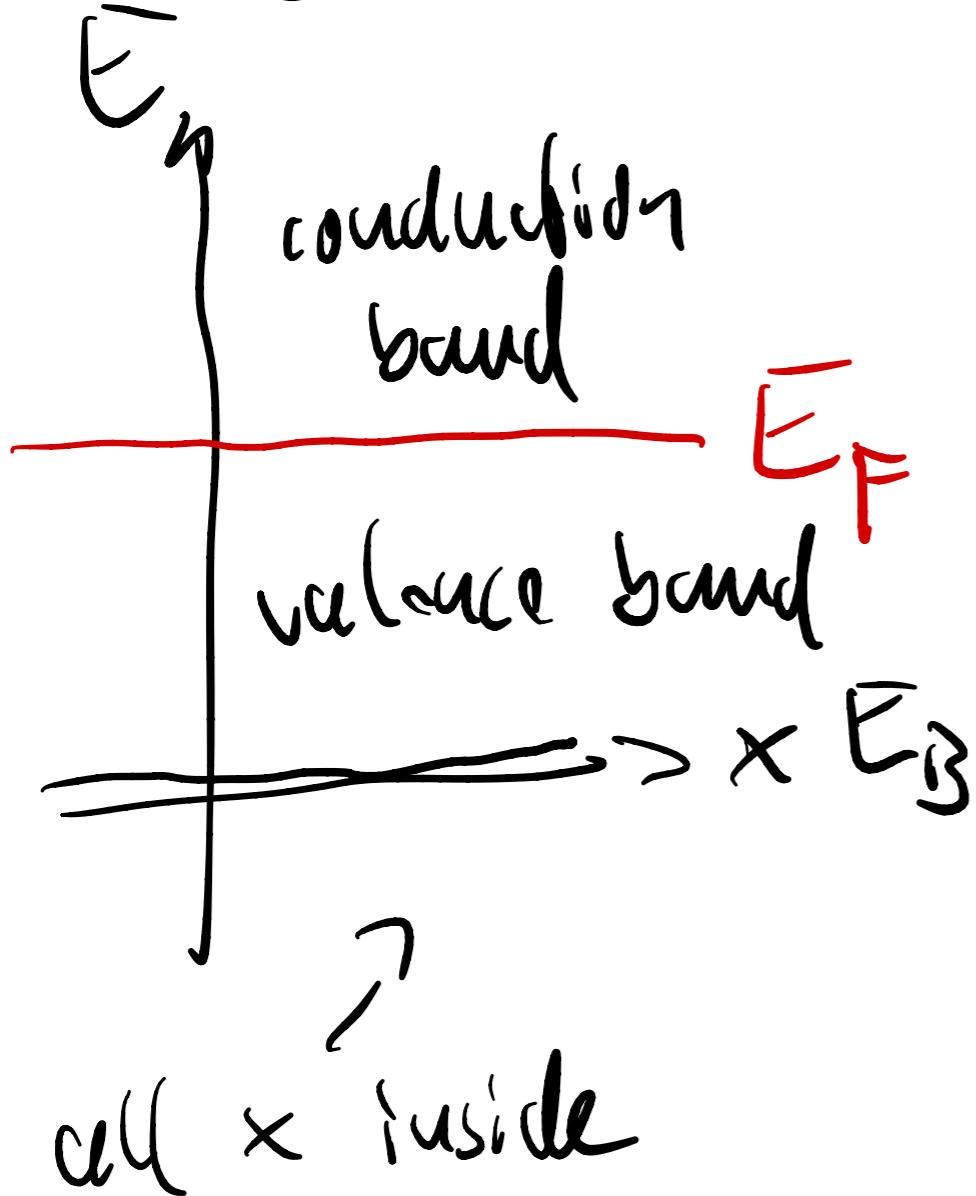
$$k^2 = \frac{v^2 \pi^2}{L^2}$$

- in 2D: $E = \frac{\hbar^2}{2m} (k_x^2 + k_y^2)$

- in 3D: $E = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2)$

Solids: Free-electron gas model

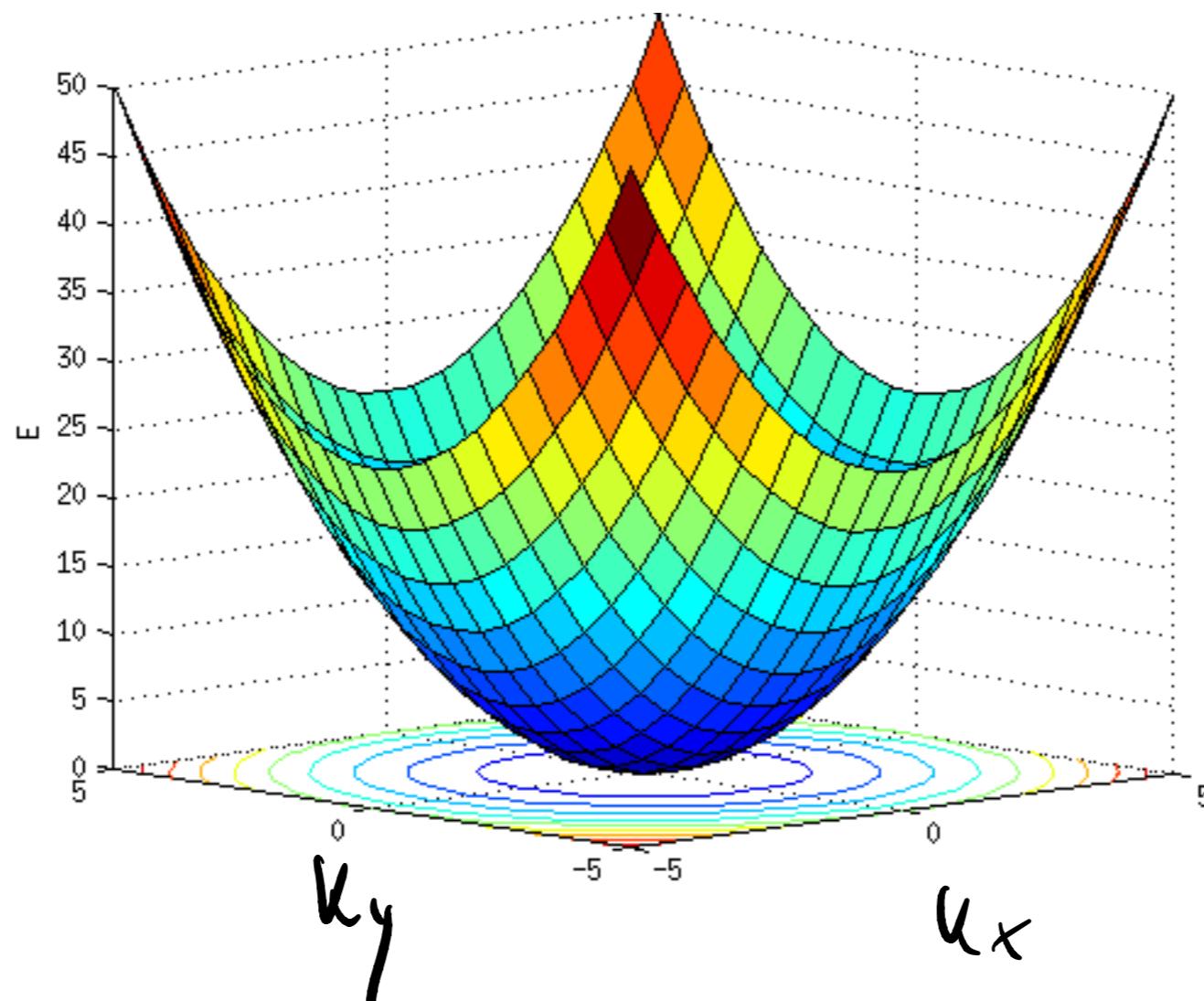
- energy-momentum relationship (1D):



momentum: $p = \hbar k$

Solids: Free-electron gas model

- energy-momentum relationship (2D):

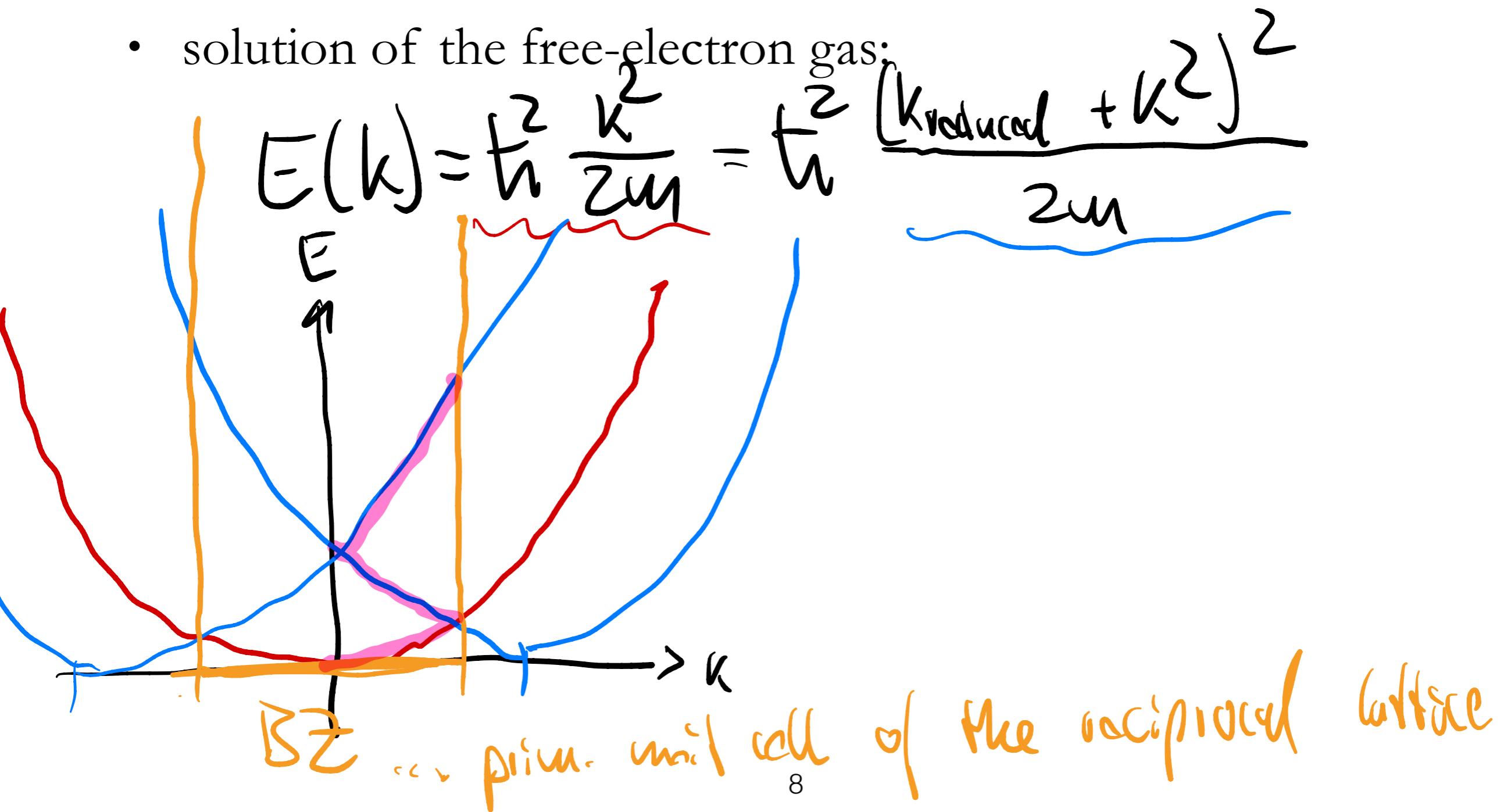


Towards a Band Theory of Solids: Periodic Potential

- we assume: all atoms sit on equilibrium positions
- this leads to a *periodic* lattice of atoms (potential for electrons)

Towards a Band Theory of Solids: Periodic Potential

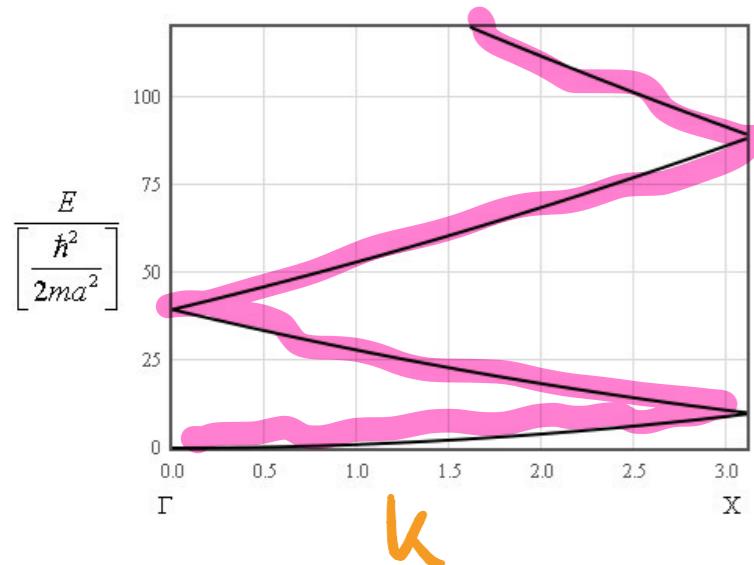
- we assume: all atoms sit on equilibrium positions
- this leads to a *periodic* lattice of atoms (potential for electrons)
- Bloch theorem (for all periodic potentials)
- solution of the free-electron gas:



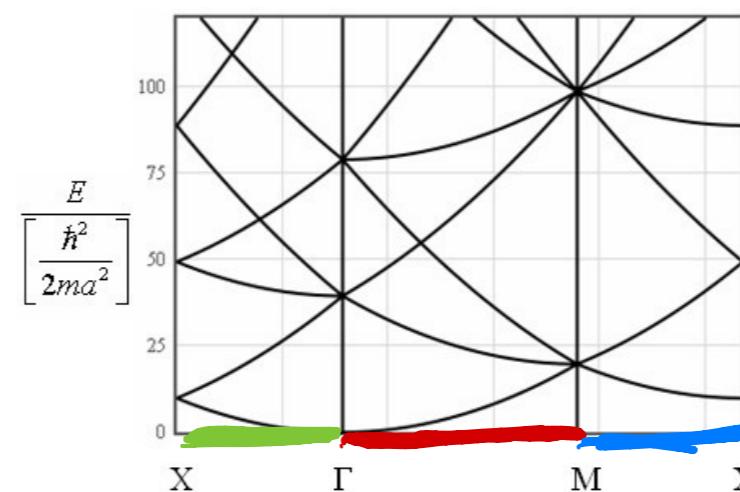
Towards a Band Theory of Solids: Empty Lattice Approximation

- lattice is periodic, but no atoms are present
- plot solutions for different lattice types: don't show periodicity

1D

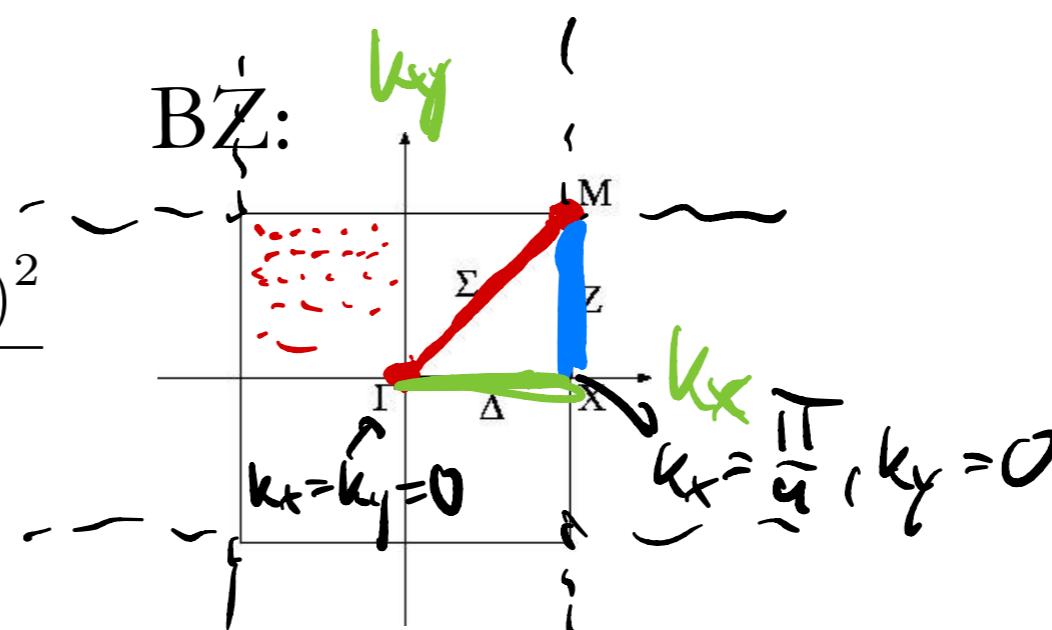


2D (square)



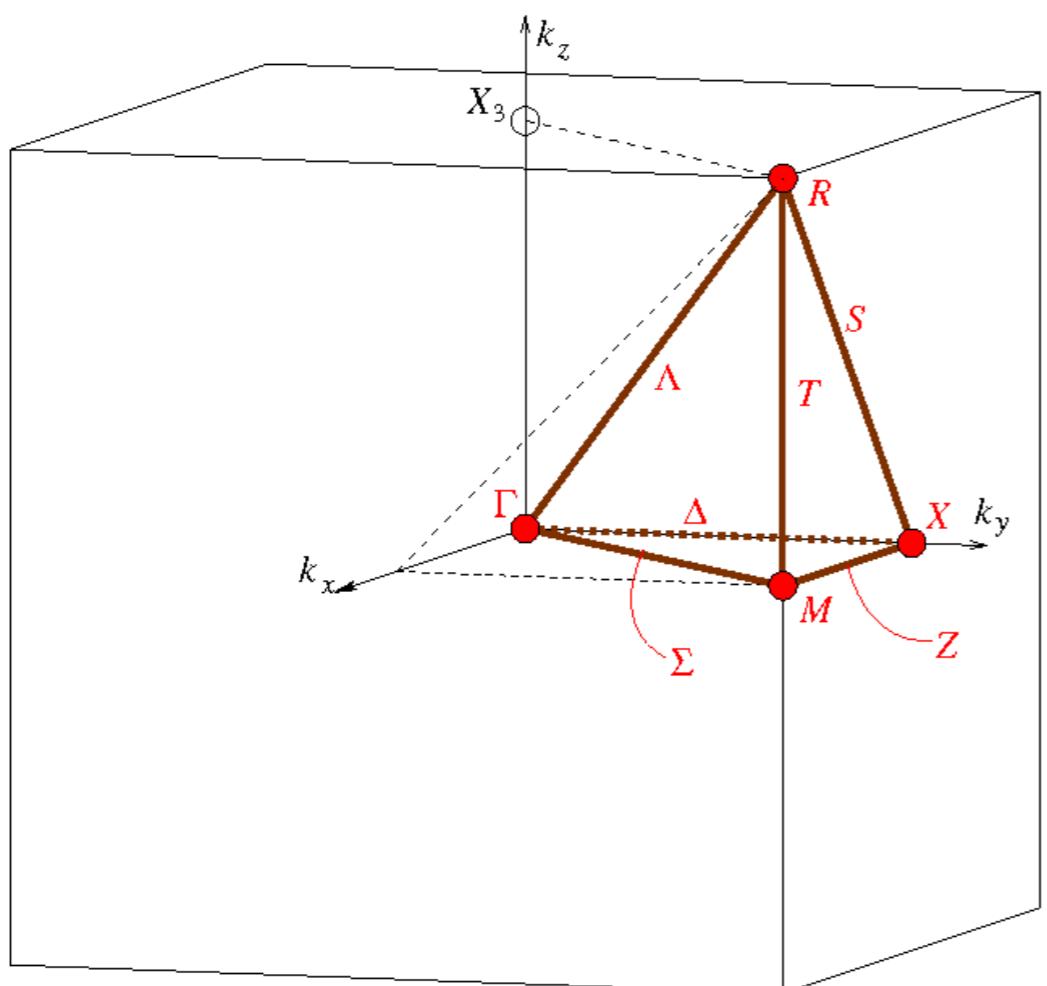
(c) <http://lamp.tu-graz.ac.at/~hadley/ss1/empty/empty.php>

$$E(\mathbf{k}) = \hbar^2 \frac{\mathbf{k}^2}{2m} = \hbar^2 \frac{(\mathbf{k}_{\text{reduced}} + \mathbf{K})^2}{2m}$$

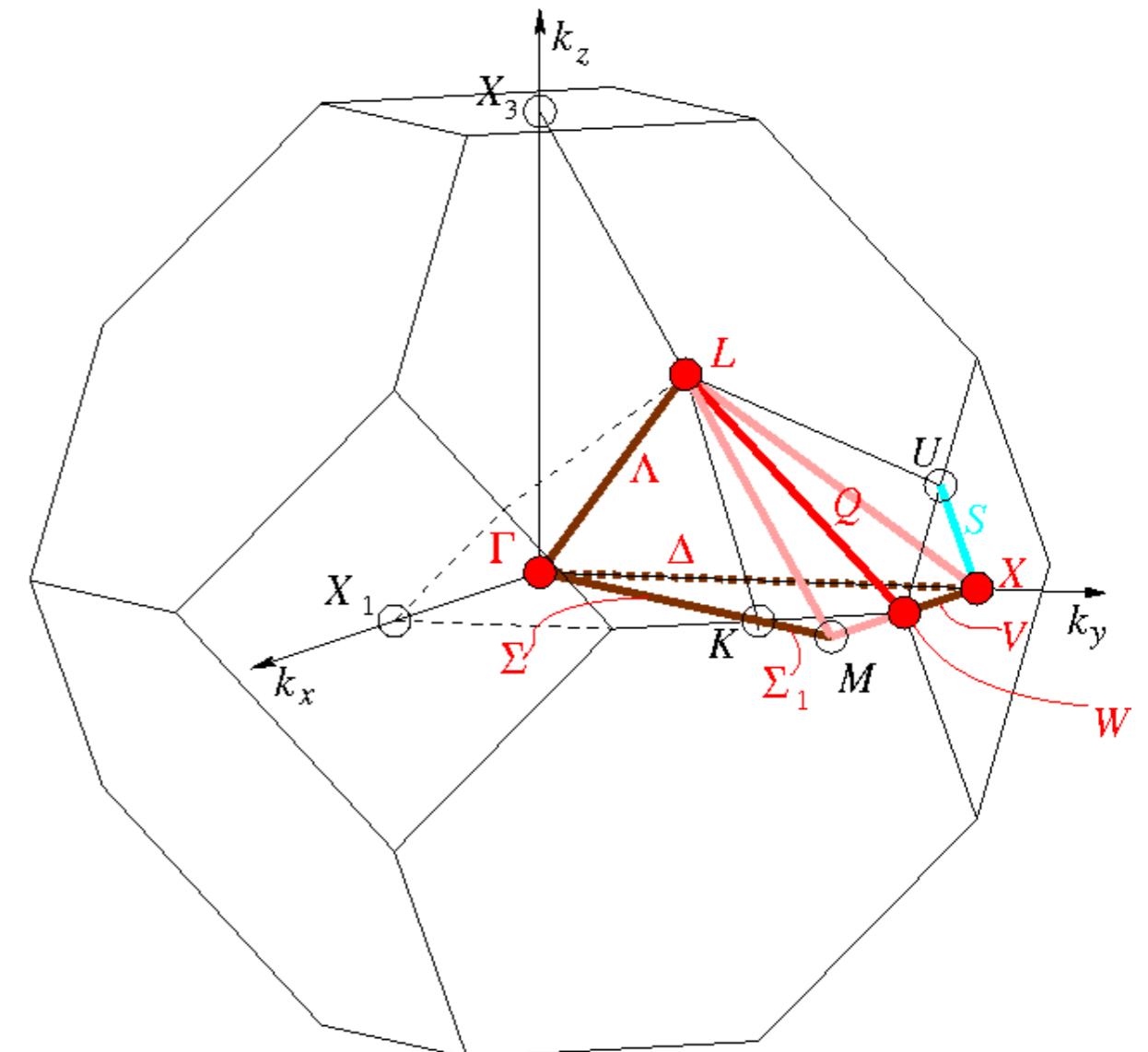


Towards a Band Theory of Solids: Reciprocal Lattice

- Wigner-Seitz cell of reciprocal lattice: Brillouin zone



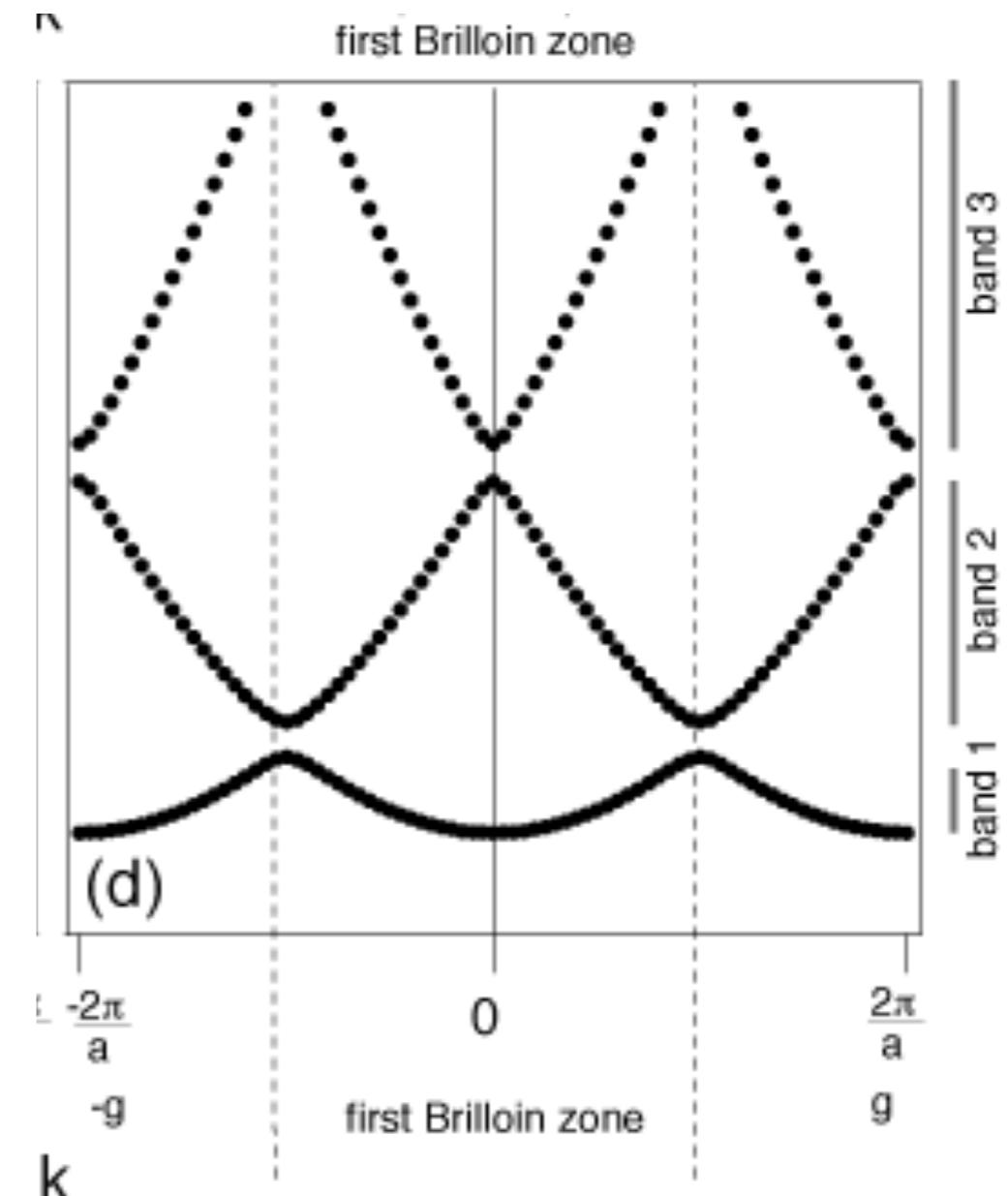
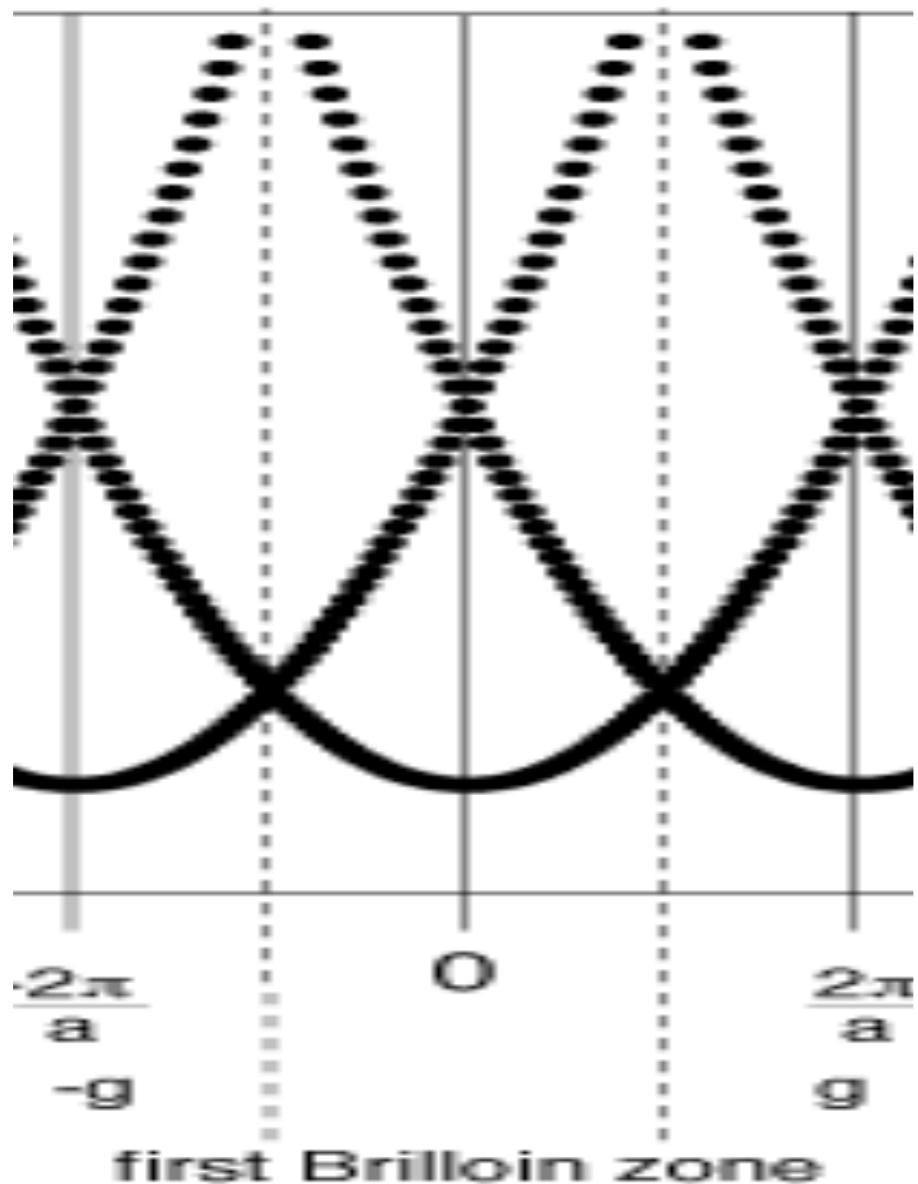
© bilbao crystallographic server
<http://www.cryst.ehu.es>



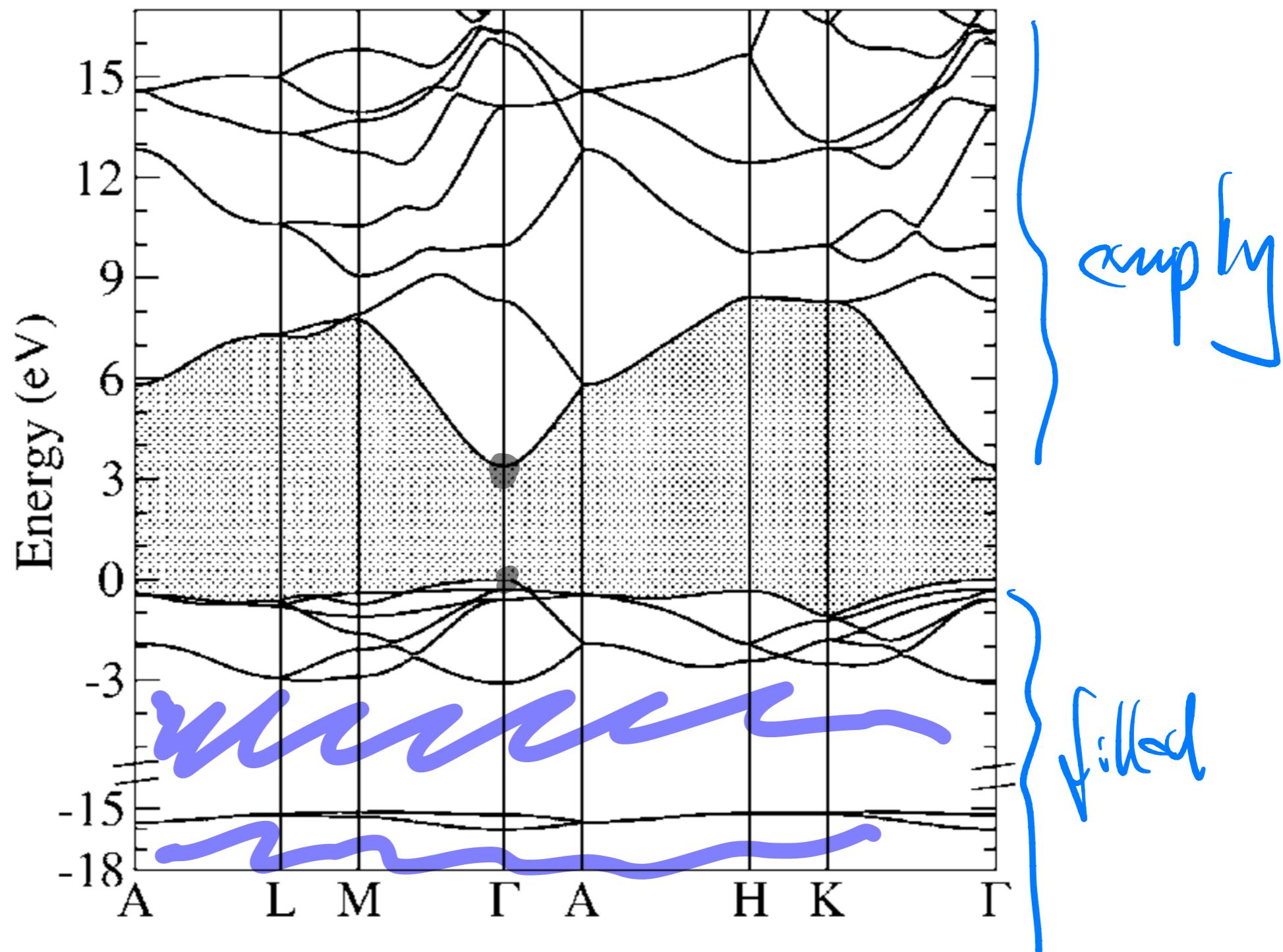
© bilbao crystallographic server
<http://www.cryst.ehu.es>

Towards a Band Theory of Solids: Nearly Free Electrons

- these results allow us to draw the following energy diagram for nearly free electrons

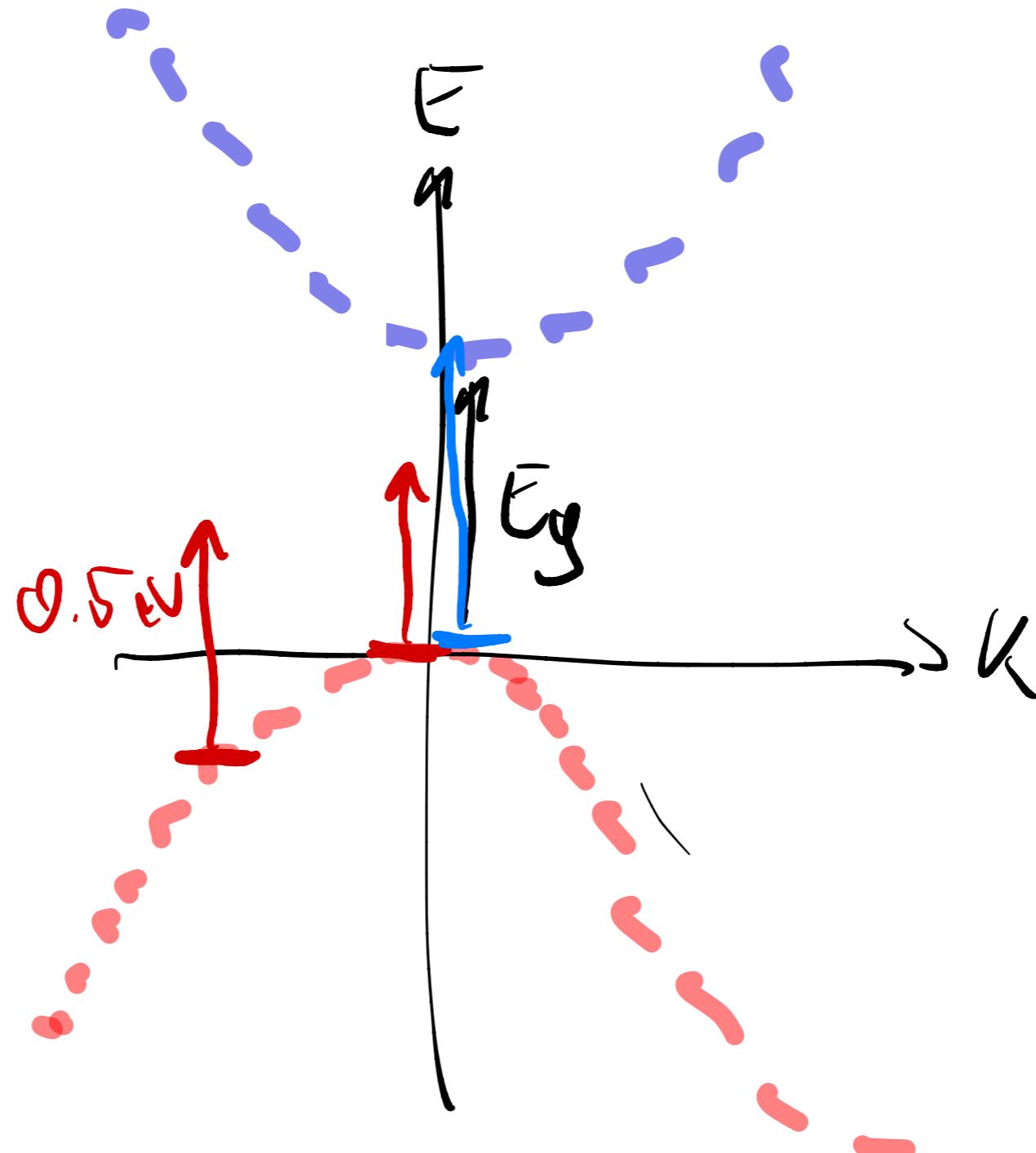


Band Structure for a real material



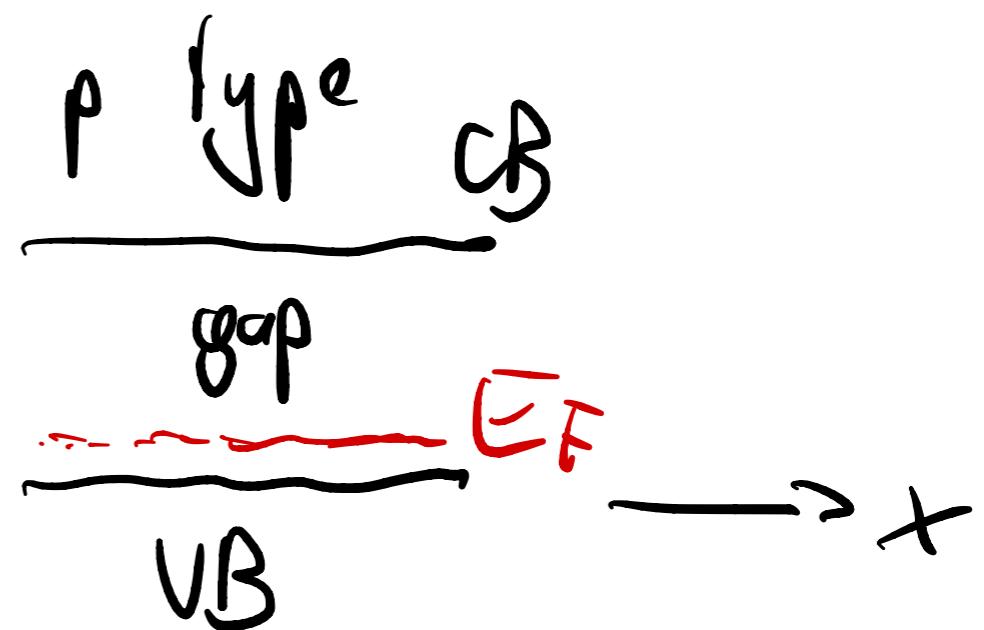
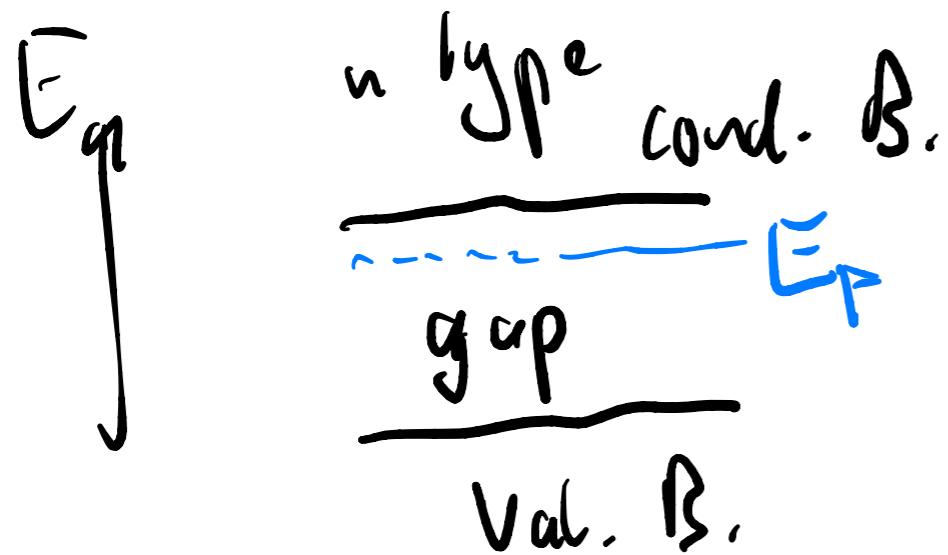
(c) Phys. Rev. B 73, 245212 (2006)

Semiconductors: Conductivity and Absorption



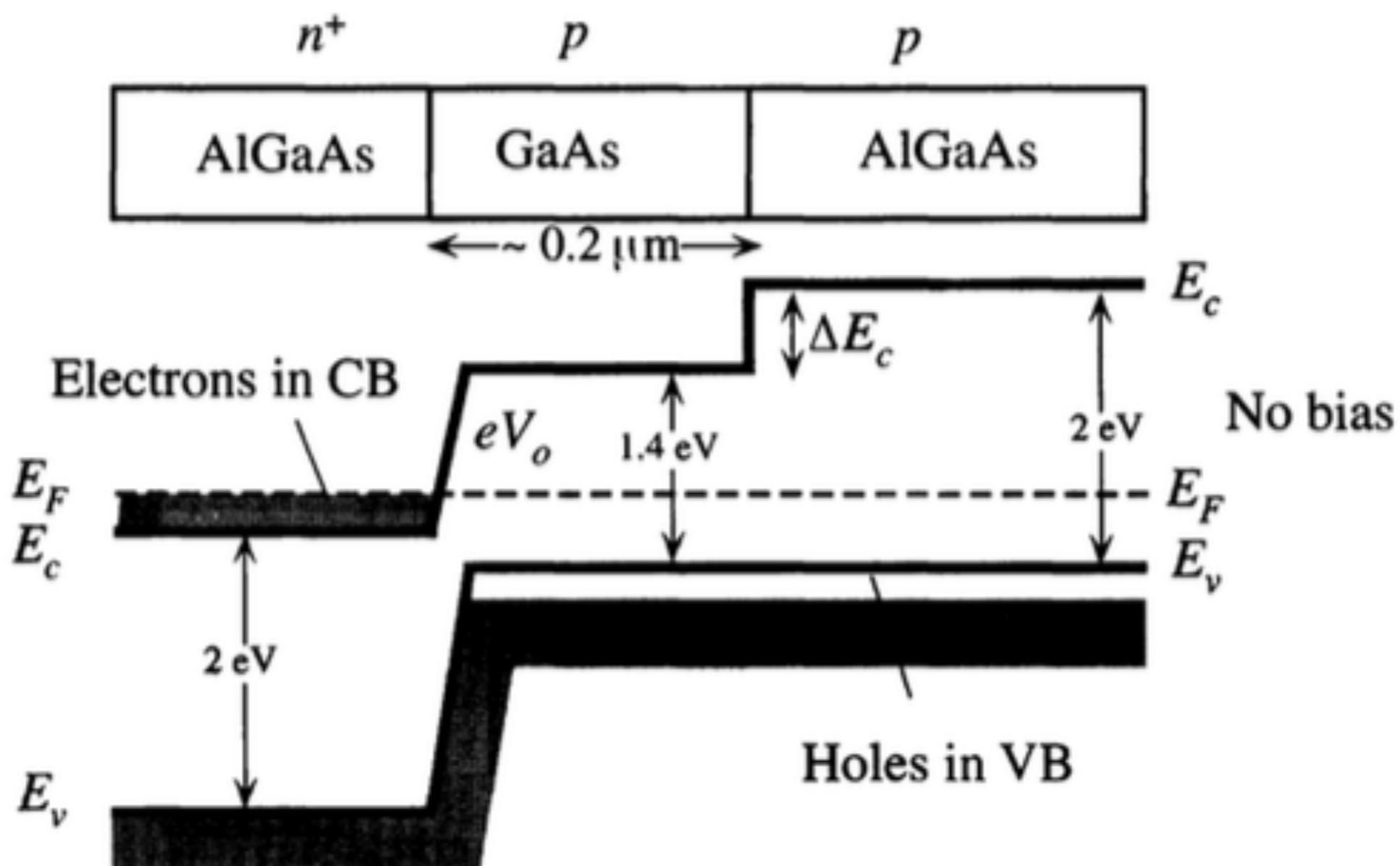
p-n junction: Energy Band diagram

- before contact:



- after contact:

Heterojunction LED:



Tasks:

- Plot existing data in colab (using colab sheet/files)
- Generate new colab sheet:
 - Connect to MP and download band structures for a few materials
 - Correct the band gap (optional)
 - Compute the branch-point energy
 - Include in your plot