

# PHYS-636 General aspects of the electronic structure of crystals

Yevtushynsky Daniil

Cursus	Sem.	Type
Physics		Obl.

Language of English teaching Credits 2 Session Oral Exam Workload 60h Hours 28 28 Courses Number of positions

#### Remark

Next time: Fall 2017

#### **Summary**

The course is aimed at giving a general understanding and building a feeling of what electronic states inside a crystal are.

#### Content

The core notion is the electronic band dispersion: how it is formed, how it defines the charge dynamics, how it is modified upon perturbing the Hamiltonian and accounting for additional electronic interactions.

## Formation of the electronic band structure, single particle in the periodic potential

Tracking the formation of the electronic band structure with different models

Singling out common aspects of the electronic states in the periodic potential

Similarity of the electronic states in the periodic crystal to the free electronic states in vacuum Packets of plane waves and Bloch waves

- the form of the wave function and band dispersion in the crossover to the classical picture

Band structure as a basis for understanding electronic properties of materials

#### Multiple electrons inside a crystal

Band filling, Fermi surface, electron count Mean-field approximation Photoemission

- essence of electron spectroscopy
- spectrum of a matrix in mathematics
- photoemission process, conservation of energy and momentum; photoemission as a projection of the initial state to the (single-particle) plane waves

Examples of the electronic structure for real materials from angle-resolved photoemission spectroscopy (ARPES)

## Response of the particle in the periodic potential to the external perturbation

Electron distribution at finite temperatures, Fermi function Heat capacity and plasma frequency

Electrical transport, response to external electrical and magnetic field

- Bloch wave packet in the applied field
- electron scattering, mean free path, lifetime
- derivation of the expressions for the electrical conductivity, Hall coefficient and magnetoresistance based on the electronic band dispersion

Measured and calculated Hall coefficient

- band structure obtained in the theoretical calculation
- band structure from experimental ARPES measurements
- magnetoresistance, Seebeck coefficient, other transport coefficients

## Symmetry breaking

Impurity states Surface states

Additional static periodic potential, charge-density-wave

- electron susceptibility, Fermi surface nesting, examples from ARPES



#### **Band hybridization**

Chain of atoms with two energy levels Two adjacent chains of atoms Introducing off-diagonal elements to the Hamiltonian

#### Interacting electronic systems

Electron-phonon interactions Superconductivity

- Bose-Einstein condensation
- basic understanding of electron pairing
- BCS theory
- materials with record critical temperatures

Electron-electron interactions

- many-body problem in classical physics
- success and breakdown of the mean field theory
- Wigner crystal, Mott insulator, localization of electrons in solids
- electron-electron scattering, electronic self energy

Fermi liquid theory Spectral function

ARPES studies of the interacting electronic systems

## Keywords

electronic structure, band structure, electronic spectrum, spectral function, electronic interactions, angle-resolved photoemission spectroscopy (ARPES)

## **Learning Prerequisites**

## Required courses

general course of quantum mechanics solid state physics

## **Expected student activities**

understand the electronic states inside the periodic crystal and their response to the external perturbations