# Low-dimensional systems and nanostructures



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- 1. Introduction semiconductor heterostructures (revison of solid state physics )
- 2. Nanotechnology
- 3. Quantum wells (1)
- 4. Quantum wells (2)
- 5. Quantum dots, Quantum wells in 1D, 2D and 3D
- 6. Optical transitions in nanostructures
- 7. Work on the article about quantum dots [TEST]
- 8. Carriers in heterostructures
- 9. Tunneling transport
- 10. Quantized conductance
- 11. Work on the article about the tunneling or conductance
- 12. Electric field in low-dimensional systems
- 13. Magnetic field in low-dimensional systems
- 14. Electric and magnetic fields in low-dimensional systems
- 15. Revision [Final TEST]

#### 1. Introduction – semiconductor heterostructures

Revision of solid state physics: Born-Oppenheimer approximation, Hartree-Fock method and one electron Hamiltonian, periodic potential, Bloch states, band structure, effective mass.

#### 2. Nanotechnology

Revision of solid state physics: tight-binding approximation, Linear Combination of Atomic Orbitals (LCAO).

Nanotechnology. Semiconductor heterostructures. Technology of low dimensional structures. Bandgap engineering: straddling, staggered and broken gap. Valence band offset.

#### 3. Quantum wells (1)

Infinite square quantum well. Finite square quantum well. Quantum well in heterostructures: finite square well with different effective masses in the well and barriers.

#### 4. Quantum wells (2)

Harmonic potential (parabolic well). Triangular potential. Wentzel – Krammers – Brillouin (WKB) method.

Band structure in 3D, 2D. Coulomb potential in 2D

#### 5. Quantum dots, Quantum wells in 1D, 2D and 3D

Quantum wells in 1D, 2D and 3D. Quantum wires and quantum dots. Bottom-up approach for low-dimensional systems and nanostructures. Energy gap as a function of the well width.

#### 6. Optical transitions in nanostructures

Time-dependent perturbation theory, Fermi golden rule, interband and intraband transitions in semiconductor heterostructures

#### 7. Work on the article about quantum dots

Students have to read the article (Phys. Rev. Lett., Nature, Science, etc.) and answer questions. Discussion.

#### 8. Carriers in heterostructures

Density of states of low dimensional systems. Doping of semiconductors. Heterojunction, p-n junction, metal-semiconductor junction, Schotky barrier

#### 9. Tunneling transport

Continuity equation. Potential step. Tunneling through the barrier. Transfer matrix approach. Resonant tunneling. Quantum unit of conductance.

#### **10.** Quantized conductance

Quantized conductance. Coulomb blockade, one-electron transistor.

#### 11. Work on the article about the tunneling or conductance

Students have to read the article (Phys. Rev. Lett., Nature, Science, etc.) and answer questions. Discussion.

#### 12. Electric field in low-dimensional systems

Scalar and vector potentials. Carriers in electric field: scalar and vector potential in Schrodinger equation. Schrodinger equation with uniform electric field. Local density of states. Franz-Kieldysh effect.

#### 13. Magnetic field in low-dimensional systems

Carriers in magnetic field. Schrodinger equation with uniform magnetic field – symmetric gauge, Landau gauge. Landau levels, degeneracy of Landau levels.

#### 14. Electric and magnetic fields in low-dimensional systems

Schrodinger equation with uniform electric and magnetic field. Hall effect. Shubnikov-de Haas effect. Quantum Hall effect. Fractional Quantum Hall Effect. Hofstadter butterfly. Fock-Darvin spectra

#### 15. Revision

Revision and preparing for the exam.

# Summary of the exercises

#### **1.** Introduction – semiconductor heterostructures

Schrodinger equation. Wave packet, Gaussian wavepacket.

#### 2. Nanotechnology

Tight-binding approximation: graphene bandctructure.

#### 3. Quantum wells (1)

Infinite square quantum well. Finite square quantum well. Finite square well with different effective masses in the well and barriers.

#### 4. Quantum wells (2)

Harmonic potential (parabolic well). Triangular potential. Wentzel – Krammers – Brillouin (WKB) method.

#### 5. Double quantum wells. Quantum dots.

Double quantum wells. Quantum dots (2D and 3D harmonic potential)

# Summary of the exercises

#### 6. Optical transitions in nanostructures

Interband and intraband transitions in semiconductor heterostructures. Continuity equation.

**7.** Carriers in heterostructures (1) Transfer matrix approach. Potential step.

**8. Carriers in heterostructures (2)** Tunneling through the barrier.

**9. Resonant tunneling** Resonant tunneling.

**10. Quantized conductance** Quantized conductance. Coulomb blockade.

**11. Local density of states** Local density of states.

# Summary of the exercises

#### **12.** Electric field in low-dimensional systems

Carriers in electric field: scalar and vector potential in Schrodinger equation.

#### 13. Magnetic field in low-dimensional systems

Schrodinger equation with uniform magnetic field – symmetric gauge, Landau gauge. Landau levels, degeneracy of Landau levels.

#### 14. Electric and magnetic fields in low-dimensional systems

Schrodinger equation with uniform electric and magnetic field. Conductivity and resistivity tensors

#### 15. Hall effect. Fock-Darvin spectrum

Hall effect. Fock-Darvin spectrum.

## Assessment criteria:

#### Homeworks

Discussion of scientific papers Tests to check the effective use of the skills acquired during the lecture Exam: final test and oral exam



"THE SMALLER IT ALL GETS, THE BIGGER WE GET."







Motoryzacja (Hummer H2 sport utility truck)



Budownictwo Samoczyszczący się beton



**Elektronika** Wyświetlacze OLED

iPod Nano





The \$585 suits that went on sale today (October 8, 2009) are treated with Titanium Dioxide, a chemical compound commonly used in cosmetics and toothpaste. According to company spokes-person Junko Hirohata, TiO2 has photocatalytic properties, meaning that it when exposed to light it breaks down organic materials.



#### Antiviral Business Suits Fight H1N1 Swine Flu With Science & Style



# Epoka NANO







# The uncertainty principle



# Band theory of solids



2017-06-05

# The band theory of solids.



Fig. 11.4. Room-temperature bandgap energy versus lattice constant of common elemental and binary compound semiconductors.

# Band theory of solids



Fig. 2.3 Development of the diamond band gap

W. R. Fahrner (Editor) Nanotechnology and Nanoelectronics

#### **Born – Oppenheimer approximation**



Max Born (1882-1970)



Jacob R. Oppenheimer (1904-1967)

 $u(\vec{z}, \vec{D})u(\vec{z}, \vec{D}) = cu(\vec{z}, \vec{D})$ 

### **Born – Oppenheimer approximation**

Full non-relativistic Hamiltonian of the system of nuclei and electrons:

$$\begin{split} H(\vec{r},\vec{R}) \Psi(\vec{r},\vec{R}) &= E \Psi(\vec{r},\vec{R}) \\ &= -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 - \sum_N \frac{\hbar^2}{2M_N} \nabla_N^2 - \frac{1}{4\pi\varepsilon_0} \sum_{N,i} \frac{Z_N e^2}{|\vec{r}_i - \vec{R}_N|} + \\ &+ \frac{1}{4\pi\varepsilon_0} \sum_{N < K} \frac{Z_N Z_K e^2}{|\vec{R}_N - \vec{R}_K|} + \frac{1}{4\pi\varepsilon_0} \sum_{i < j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} = \\ &= \hat{T}_e + \hat{T}_N + V(\vec{r},\vec{R}) + V_e(\vec{r}) + G(\vec{R}) \end{split}$$

Electron and nuclear (ions) subsystems coordinates are intermixed, separation of electronic and nuclear variables is impossible

Assumption: motion of atomic nuclei and electrons in a molecule can be separated **Born-Oppenheimer adiabatic approximation** 

### LCAO method

The solution of the equation of electron states requires numerical methods

$$H_{el}(\vec{r},\vec{R})\Psi_{el}^{k}(\vec{r},\vec{R}) = [\hat{T}_{e} + V(\vec{r},\vec{R}) + V_{e}(\vec{r})]\Psi_{el}^{k}(\vec{r},\vec{R}) = E_{el}^{k}(\vec{R})\Psi_{el}^{k}(\vec{r},\vec{R})$$

One of methods: LCAO-MO with Hartree-Fock approximation – **self-consistent field method** (iterative method), *n*-electron wave function as Slater determinant, trivially satisfies the antisymmetric property of the exact solution:

$$\Psi_{el}^{k}(\vec{r}_{1},\vec{r}_{2},\vec{r}_{3},\dots,s_{1},s_{2},s_{3},\dots) = \frac{1}{\sqrt{n!}} \begin{vmatrix} \varphi_{1}^{sp}(\vec{r}_{1},s_{1}) & \varphi_{1}^{sp}(\vec{r}_{2},s_{2}) & \dots & \varphi_{1}^{sp}(\vec{r}_{n},s_{n}) \\ \varphi_{2}^{sp}(\vec{r}_{1},s_{1}) & \varphi_{2}^{sp}(\vec{r}_{2},s_{2}) & \dots & \varphi_{2}^{sp}(\vec{r}_{n},s_{2}) \\ \dots & \dots & \dots & \dots \\ \varphi_{n}^{sp}(\vec{r}_{1},s_{1}) & \varphi_{n}^{sp}(\vec{r}_{2},s_{2}) & \dots & \varphi_{n}^{sp}(\vec{r}_{n},s_{n}) \end{vmatrix}$$

Each of the single-electron spin-orbital  $\varphi_n^{sp}(\vec{r}_n, s_n)$  must be different – two spin-orbital can for instance share the same orbital function, but then theirs spins are different

$$\varphi_n^{sp}(\vec{r}_n, s_n) = \varphi_n^{sp}(\vec{r}_n) \begin{bmatrix} 0\\1 \end{bmatrix} \text{ or } \varphi_n^{sp}(\vec{r}_n) \begin{bmatrix} 1\\0 \end{bmatrix}$$

#### Hartree approximation (one-electron)

$$\Psi_{el}^k(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots) = \varphi_1(\vec{r}_1) \cdot \varphi_2(\vec{r}_2) \cdot \varphi_3(\vec{r}_3) \cdot \dots \cdot \varphi_n(\vec{r}_n)$$

We assume that an average potential from other ions and electrons acts on each electron:

$$\left(\sum_{i} \frac{p_i^2}{2m} + \sum_{i} V_i(\vec{r}_i)\right) \Psi_{el}^k(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots) = E_{tot}^k \Psi_{el}^k(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots)$$

Thus

$$\left(\frac{p_i^2}{2m} + V_i(\vec{r}_i)\right)\varphi_i(\vec{r}_i) = E_i\varphi_i(\vec{r}_i)$$

If every potential is the same  $V_1(\vec{r_1}) \approx V_2(\vec{r_2}) \approx \cdots \approx V_n(\vec{r_n}) \approx V(\vec{r})$  we get  $\sum_i E_i = E_{tot}$ One-electron Schrödinger equation:

$$\left(\frac{p^2}{2m} + V(\vec{r})\right)\varphi_i(\vec{r}_i) = E_i\varphi_i(\vec{r}_i)$$

This time *i* is the set of quantum numbers of one-electron quantum states  $\varphi_i(\vec{r_i})$  of energies  $E_i$ . One-electron states are subject to the Pauli exclusion principle.

A significant change in the number of electrons in a given band, leads to the change of  $V(\vec{r})$ and of the one –particle spectra! (for instance energy gap renormalization )

### **Bloch theorem**

#### **Assumptions:**

Motionless atoms, crystal (periodic) lattice . One-electron Hartree approximation

 $\Psi_{el}^k(\vec{r}_1,\vec{r}_2,\vec{r}_3,\dots) = \varphi_1(\vec{r}_1) \cdot \varphi_2(\vec{r}_2) \cdot \varphi_3(\vec{r}_3) \cdot \dots \cdot \varphi_n(\vec{r}_n)$ 

or Hartree-Fock approximation (Slater determinant).

Self-consistent field method – the multi-electron issue is reduced to the solution of one-electron problem in a potential of all other electrons and atoms



$$\left(\frac{p^2}{2m} + V(\vec{r})\right) \varphi_n(\vec{r}_n) = E_n \varphi_n(\vec{r}_n)$$
 "One-electron" Schrödinger equation

Effective potential, periodic potential of the crystal lattice, the same for all electrons.

$$V(\vec{r}) = V\left(\vec{r} + \vec{R}\right)$$

### **Bloch theorem**

Crystal lattice:

 $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \qquad n_i \in \mathbb{Z}$ For periodic functions with the lattice period  $\vec{R}$  $f(\vec{r}) = f(\vec{r} + \vec{R})$  a good base in the Fourier series expansion are functions  $g(\vec{r}) = \exp(i\vec{G}\vec{r})$  which depend on the reciprocal lattice vectors:

$$\vec{G} = m_1 \vec{a}_1^* + m_2 \vec{a}_2^* + m_3 \vec{a}_3^*, \qquad m_i \in \mathbb{Z}$$



$$\vec{a}_i \vec{a}_j^* = 2\pi \delta_{ij}$$

 $\exp[i\vec{G}(\vec{r}+\vec{R})] =$  $= \exp[i\vec{G}\vec{r}] \cdot \exp[i\vec{G}\vec{R}] = \exp[i\vec{G}\vec{r}] \exp[2\pi (n_1m_1 + n_2m_2 + n_3m_3)] = \exp(i\vec{G}\vec{r})$ 

therefore  $g(\vec{r}) = g(\vec{r} + \vec{R})$  and finally we get:

$$V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} \exp(i\vec{G}\vec{r})$$

### **Bloch theorem**

Periodic potenetial we can expand as a Fourier series:

$$V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} \exp(i\vec{G}\vec{r})$$

The wavefunction can be represented as a sum of plane waves of different wavelengths satisfying periodic boundary conditions :

$$\varphi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} \exp\left(i\vec{k}\vec{r}\right)$$

Schrödinger equation:

$$\left(\frac{\hat{p}^2}{2m} + V(\vec{r})\right)\varphi(\vec{r}) = E \ \varphi(\vec{r})$$

$$\sum_{\vec{k}} \frac{\hbar^2 \vec{k}^2}{2m} C_{\vec{k}} \exp(i\vec{k}\vec{r}) + \sum_{\vec{k},\vec{G}} C_{\vec{k}} V_{\vec{G}} \exp[i(\vec{k}+\vec{G})\vec{r}] = E \sum_{\vec{k}} C_{\vec{k}} \exp(i\vec{k}\vec{r})$$

This is an equation for *E* and  $C_{\vec{k}}$  for all vectors  $\vec{k}, \vec{r}$  and  $\vec{G}$ .



See also: Ibach, Luth "Solid State Physics"

### **Bloch theorem**

$$\sum_{\vec{k}} \frac{\hbar^2 \vec{k}^2}{2m} C_{\vec{k}} \exp(i\vec{k}\vec{r}) + \sum_{\vec{k},\vec{G}} C_{\vec{k}} V_{\vec{G}} \exp[i(\vec{k} + \vec{G})\vec{r}] = E \sum_{\vec{k}} C_{\vec{k}} \exp(i\vec{k}\vec{r})$$

The sum is over all  $\vec{k}$ ,  $\vec{G}$ , therefore:

$$\sum_{\vec{k},\vec{G}} C_{\vec{k}} V_{\vec{G}} \exp[i(\vec{k} + \vec{G})\vec{r}] = \dots \vec{k} + \vec{G} \to \vec{k} \dots$$
$$= \sum_{\vec{k},\vec{G}} C_{\vec{k}-\vec{G}} V_{\vec{G}} \exp[i\vec{k}\vec{r}]$$

We get Schrödinger equation in a form:

$$\sum_{\vec{k}} \exp(i\vec{k}\vec{r}) \left[ \left( \frac{\hbar^2 \vec{k}^2}{2m} - E \right) C_{\vec{k}} + \sum_{\vec{G}} C_{\vec{k}-\vec{G}} V_{\vec{G}} \right] = 0$$

That must be met for each vector  $\vec{r}$ .

### **Bloch theorem**

$$\sum_{\vec{k}} \exp(i\vec{k}\vec{r}) \left[ \left( \frac{\hbar^2 \vec{k}^2}{2m} - E \right) C_{\vec{k}} + \sum_{\vec{G}} C_{\vec{k}-\vec{G}} V_{\vec{G}} \right] = 0$$

for each vector  $\vec{r}$ .

Thus, for each vector  $\vec{k}$  we got equation for coefficients  $C_{\vec{k}}$  and E:

$$\left(\frac{\hbar^2 \vec{k}^2}{2m} - E\right) C_{\vec{k}} + \sum_{\vec{G}} C_{\vec{k} - \vec{G}} V_{\vec{G}} = 0$$



Try to plot the mattrix of this equation

In this equation for  $C_{\vec{k}}$  also coefficients shifted by  $\vec{G}$  like  $C_{\vec{k}-\vec{G}_1}$ ,  $C_{\vec{k}-\vec{G}_2}$ ,  $C_{\vec{k}-\vec{G}_3}$  appear (but others do not, even when we started for any  $\vec{k}$ !).

This equation couples those expansion coefficients  $\varphi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} \exp(i\vec{k}\vec{r})$ , whose  $\vec{k}$  - values differ from one another by a reciprocal lattice vector  $\vec{G}$ .



### **Bloch theorem**

$$\left(\frac{\hbar^2 \vec{k}^2}{2m} - E\right) C_{\vec{k}} + \sum_{\vec{G}} C_{\vec{k}-\vec{G}} V_{\vec{G}} = 0$$

We do not need to solve these equations for all vectors  $\vec{G}$  – we can find a solution in **one** unit cell of the reciprocal lattice and copy it *N* times (*N* – number of unit cells)!

Thus we can find eigenvalues  $E \to E_{\vec{k}} \to E(\vec{k})$  corresponding to the wave-function  $\varphi_{\vec{k}}(\vec{r})$  represented as a superposition of plane waves whose wave vectors  $\vec{k}$  differ only by reciprocal lattice vectors  $\vec{G}$ .



Wave vector  $\vec{k}$  is a good quantum number according to which the energy eigenvalues and quantum states may be indexed. Thus the function  $\varphi(\vec{r})$  is the superposition of  $\varphi_{\vec{k}}(\vec{r})$  of energies  $E(\vec{k})$ 

$$\varphi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} \exp(i\vec{k}\vec{r}) = \dots = \sum_{\substack{\vec{k} \text{ Brillouin}\\zone}} \varphi_{\vec{k}}(\vec{r})$$

(later on we introduce coefficient n for different solutions of  $E_{\vec{k}}$  corresponding to the same  $\vec{k}$ )

### **Bloch theorem**

Wave-function which is the solution of the Schrodinger equation  $\varphi_{\vec{k}}(\vec{r})$  is represented as a superposition of plane waves whose wave vectors  $\vec{k}$  differ only by reciprocal lattice vectors  $\vec{G}$  and it has energies  $E_{\vec{k}} = E(\vec{k})$ :

$$\varphi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} \exp\left[i\left(\vec{k}-\vec{G}\right)\vec{r}\right]$$

Each vector  $\vec{k} - \vec{G}$  can enumerate states; it is convenient to choose the shortest vector (which belongs to the first Brillouin zone).



$$\varphi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} e^{i(\vec{k}-\vec{G})\vec{r}} = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} e^{-i\vec{G}\vec{r}} e^{i\vec{k}\vec{r}} =: u_{\vec{k}}(\vec{r})e^{i\vec{k}\vec{r}}$$

The function  $u_{\vec{k}}(\vec{r})$  is a Fourier series over reciprocal lattice points  $\vec{G}$ , and thus has the periodicity of the lattice.



### **Bloch theorem**

Bloch waves whose wave vectors differ by a reciprocal lattice vector are IDENTICAL!



 $\vec{k}_1 - \vec{k}_2 = \vec{G}$ 

### **Bloch theorem**

$$\varphi_{n,\vec{k}}(\vec{r}) = u_{n,\vec{k}}(\vec{r}) e^{i\vec{k}\vec{r}}$$
Bloch wave,  
Bloch function
Bloch envelope

The solution of the one-electron Schrödinger equation for a periodic potential has a form of modulated plane wave:  $u = (\vec{r}) = u = (\vec{r} + \vec{R})$ 

$$u_{n,\vec{k}}(\vec{r}) = u_{n,\vec{k}}(\vec{r} + \vec{R})$$



We introduced coefficient n for different solutions corresponding to the same  $\vec{k}$  (*index*).  $\vec{k}$ -vector is an element of the *first Brillouin zone*.

$$u_{n,\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} e^{i\vec{G}\vec{r}}$$

### **Brillouin zones**

 $\vec{a}_i^* \vec{a}_j = 2\pi \delta_{ij}$ 

$$m_i \in \mathbb{Z}$$

 $\mathbb{Z}$ 

2-D square lattice



 $\vec{a}_i^*\vec{a}_j=2\pi\delta_{ij}$ 

### **Brillouin zones**

$$ec{R} = n_1 ec{a}_1 + n_2 ec{a}_2 + n_3 ec{a}_3,$$
  
 $ec{G} = m_1 ec{a}_1^* + m_2 ec{a}_2^* + m_3 ec{a}_3^*,$ 

$$m_i \in \mathbb{Z}$$
  
 $m_i \in \mathbb{Z}$ 

 $n \in \mathbb{Z}$ 

2-D square lattice







### **Brillouin zones**

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \qquad n_i \in \mathbb{Z} \vec{G} = m_1 \vec{a}_1^* + m_2 \vec{a}_2^* + m_3 \vec{a}_3^*, \qquad m_i \in \mathbb{Z}$$



2-D square lattice

![](_page_37_Picture_5.jpeg)

### **Brillouin zones**

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \qquad n_i \in \mathbb{Z} \vec{G} = m_1 \vec{a}_1^* + m_2 \vec{a}_2^* + m_3 \vec{a}_3^*, \qquad m_i \in \mathbb{Z}$$

2-D hexagonal lattice

![](_page_38_Figure_4.jpeg)

### **Brillouin zones**

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \qquad n_i \in \mathbb{Z} \vec{G} = m_1 \vec{a}_1^* + m_2 \vec{a}_2^* + m_3 \vec{a}_3^*, \qquad m_i \in \mathbb{Z}$$

![](_page_39_Figure_3.jpeg)

![](_page_39_Picture_4.jpeg)

### **Brillouin zones**

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \qquad n_i \in \mathbb{Z} \vec{G} = m_1 \vec{a}_1^* + m_2 \vec{a}_2^* + m_3 \vec{a}_3^*, \qquad m_i \in \mathbb{Z}$$

Brillouin zone in 1D

![](_page_40_Figure_4.jpeg)

Brillouin zone in 2D, oblique lattice.

![](_page_40_Figure_6.jpeg)

![](_page_40_Figure_7.jpeg)

Brillouin zone for face centered cubic (fcc) lattice. The limiting zone walls comes from reciprocal lattice points (2,0,0) square and (1,1,1) hexagonal.

http://oen.dydaktyka.agh.edu.pl/dydaktyka/fizyka/c\_teoria\_pasmowa/2.php

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### **Brillouin zones**

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \qquad n_i \in \mathbb{Z} \vec{G} = m_1 \vec{a}_1^* + m_2 \vec{a}_2^* + m_3 \vec{a}_3^*, \qquad m_i \in \mathbb{Z}$$

*bcc* lattice

![](_page_41_Figure_4.jpeg)

![](_page_41_Picture_5.jpeg)

heksagonal lattice

Ibach, Luth

# Potencjał periodyczny

![](_page_42_Figure_1.jpeg)

Yu, Cardona Fundametals of semiconductors

Fig. 2.2. (a) The crystal structure of diamond and zinc-blende (ZnS). (b) the fcc lattice showing a set of primitive lattice vectors. (c) The reciprocal lattice of the fcc lattice shown with the first Brillouin zone. Special high-symmetry points are denoted by  $\Gamma$ , X, and L, while high-symmetry lines joining some of these points are labeled as  $\Lambda$  and  $\Delta$ 

2017-06-05

# Fermi surfaces of metals

![](_page_43_Picture_1.jpeg)

![](_page_43_Picture_2.jpeg)

Fig.13 Fermi surface of aluminum

![](_page_43_Picture_4.jpeg)

![](_page_43_Picture_5.jpeg)

Fig.12 Fermi surface of calcium

Fig. 11 In the three noble metals the free electron sphere bulges out in the [111] directions to make contact with the hexagonal zone faces.

http://physics.unl.edu/tsymbal/teaching/SSP-927/Section%2010\_Metals-Electron\_dynamics\_and\_Fermi\_surfaces.pdf

### **Bloch theorem**

![](_page_44_Figure_2.jpeg)

Example: electron in a constant potential

$$H = -\frac{\hbar^2}{2m} \,\Delta + V$$

substituting  $\varphi_{n,\vec{k}}(\vec{r}) = 1 \, e^{i \vec{k} \vec{r}}$ 

The solution is

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

The momentum operator  $\hat{p} = -i\hbar \nabla$  acting on  $\varphi_{n,\vec{k}}(\vec{r})$ 

 $\hat{p}\varphi_{n,\vec{k}}(\vec{r}) = \hbar k \ \varphi_{n,\vec{k}}(\vec{r})$ . The solutions of the Schrödinger equation with a constant potential are eigenfunctions of the momentum operator. The momentum is well defined, the eigenvalue of the momentum operator is  $\hat{p} = \hbar k$  (this defines the sense of  $\vec{k}$ -vector).

![](_page_44_Figure_10.jpeg)

### **Bloch theorem**

#### Przykład:

Electron motion in a periodic potential.

$$V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} \exp(i\vec{G}\vec{r})$$

The solution is:

$$\psi_{n,\vec{k}}(\vec{r}) = u_{n,\vec{k}}(\vec{r}) e^{i\vec{k}\vec{r}}$$

Thus:

$$u_{n,\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} e^{i\vec{G}\vec{r}}$$

![](_page_45_Figure_9.jpeg)

Applying  $\hat{p} = -i\hbar \nabla$  we get  $\hat{p}\psi(\vec{r}) = -i\hbar (i \vec{k} + \nabla u_{n,\vec{k}})e^{i\vec{k}\vec{r}} \neq \hbar \vec{k}\psi(\vec{r}).$ 

Momentum of the Bloch function is not well defined!

 $\hbar \vec{k}$  is so-called quasi-momentum or crystal momentum.

### **Bloch theorem**

#### Przykład:

Electron motion in a periodic potential.

$$V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} \exp(i\vec{G}\vec{r})$$

The solution is:

$$\psi_{n,\vec{k}}(\vec{r}) = u_{n,\vec{k}}(\vec{r}) e^{i\vec{k}\vec{r}}$$

Thus:

$$u_{n,\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} e^{i\vec{G}\vec{r}}$$

If our crystal has a finite size set of vectors k is finite (though enormous!). for instance, we can assume periodic boundary conditions and then:

$$\vec{k}_i = 0, \pm \frac{2\pi}{L_i}, \pm \frac{4\pi}{L_i}, \pm \frac{6\pi}{L_i}, \dots, \pm \frac{2\pi n_i}{L_i}$$

![](_page_46_Picture_11.jpeg)

### **Bloch theorem**

Bloch functions whose wave vectors differ by a reciprocal lattice vector, are the same!

$$\psi_{n,\vec{k}+\vec{G}}(\vec{r}) = \psi_{n,\vec{k}}(\vec{r})$$
  
**Proof:**  
 $\vec{G} = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$ 

$$\begin{split} \psi_{n,\vec{k}+\vec{G}}(\vec{r}) &= u_{n,\vec{k}+\vec{G}}(\vec{r}) \, e^{i(\vec{k}+\vec{G})\vec{r}} \\ &= \sum_{\vec{G}'} C\big(\vec{k}+\vec{G}-\vec{G}'\big) e^{-i\vec{G}'\vec{r}} \, e^{i(\vec{k}+\vec{G})\vec{r}} = \cdots \\ &= \sum_{\vec{G}''} C\big(\vec{k}-\vec{G}''\big) e^{-i\vec{G}''\vec{r}} \, e^{i(\vec{k})\vec{r}} = \, \psi_{n,\vec{k}}(\vec{r}) \end{split}$$

What about energies?

$$\left(\frac{\vec{p}^2}{2m_0} + V(\vec{r})\right)\psi_{n,\vec{k}}(\vec{r}) = E(n,\vec{k}) \ \psi_{n,\vec{k}}(\vec{r})$$

$$\left(\frac{\vec{p}^2}{2m_0} + V(\vec{r})\right)\psi_{n,\vec{k}+\vec{G}}(\vec{r}) = E\left(n,\vec{k}+\vec{G}\right)\,\psi_{n,\vec{k}+\vec{G}}(\vec{r})$$

### **Bloch theorem**

Bloch functions whose wave vectors differ by a reciprocal lattice vector, are the same!

$$\psi_{n,\vec{k}+\vec{G}}(\vec{r}) = \psi_{n,\vec{k}}(\vec{r})$$
  
**Proof:**  
 $\vec{G} = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$ 

$$\begin{split} \psi_{n,\vec{k}+\vec{G}}(\vec{r}) &= u_{n,\vec{k}+\vec{G}}(\vec{r}) \, e^{i(\vec{k}+\vec{G})\vec{r}} \\ &= \sum_{\vec{G}'} C\left(\vec{k}+\vec{G}-\vec{G}'\right) e^{-i\vec{G}'\vec{r}} \, e^{i(\vec{k}+\vec{G})\vec{r}} = \cdots \\ &= \sum_{\vec{G}''} C\left(\vec{k}-\vec{G}''\right) e^{-i\vec{G}''\vec{r}} \, e^{i(\vec{k})\vec{r}} = \psi_{n,\vec{k}}\left(\vec{r}\right) \end{split}$$

What about energies?

$$\begin{pmatrix} \frac{\vec{p}^2}{2m_0} + V(\vec{r}) \end{pmatrix} \psi_{n,\vec{k}}(\vec{r}) = E(n,\vec{k}) \ \psi_{n,\vec{k}}(\vec{r})$$

$$\begin{pmatrix} \frac{\vec{p}^2}{2m_0} + V(\vec{r}) \end{pmatrix} \psi_{n,\vec{k}+\vec{G}}(\vec{r}) = E(n,\vec{k}+\vec{G}) \ \psi_{n,\vec{k}+\vec{G}}(\vec{r})$$

$$\Rightarrow E(n,\vec{k}) = E(n,\vec{k}+\vec{G})$$

Energy eigenvalues are a periodic function of  $\vec{k}$  (wave vectors of Bloch function).

2017-06-05

### The nearly free-electron approximation

$$E(n,\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m}$$

![](_page_49_Figure_4.jpeg)

### The nearly free-electron approximation

$$E(n,\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m} = E(n,\vec{k}+\vec{G}) = \frac{\hbar^2 (\vec{k}+\vec{G})^2}{2m}$$

![](_page_50_Figure_4.jpeg)

### The nearly free-electron approximation

$$E(n,\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m} = E(n,\vec{k}+\vec{G}) = \frac{\hbar^2 (\vec{k}+\vec{G})^2}{2m}$$

![](_page_51_Figure_4.jpeg)

### The nearly free-electron approximation

$$E(n,\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m} = E(n,\vec{k}+\vec{G}) = \frac{\hbar^2 (\vec{k}+\vec{G})^2}{2m}$$

![](_page_52_Figure_4.jpeg)

### The nearly free-electron approximation

$$E(n,\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m} = E(n,\vec{k}+\vec{G}) = \frac{\hbar^2 (\vec{k}+\vec{G})^2}{2m}$$

![](_page_53_Figure_4.jpeg)

### The nearly free-electron approximation

Energy of the plane wave in empty space as the function of wave vector:

$$E(n,\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m} = E(n,\vec{k}+\vec{G}) = \frac{\hbar^2 (\vec{k}+\vec{G})^2}{2m}$$

Reduced Brilloin zone. On the border of the Brillouin zone energies are degenerated

![](_page_54_Figure_5.jpeg)

![](_page_55_Figure_1.jpeg)

![](_page_56_Figure_1.jpeg)

 $a_r$ 

 $a_{\star}$ 

![](_page_57_Figure_1.jpeg)

### The nearly free-electron approximation

The appropriate expressions for a perturbation calculation of the influence of a small potential

$$V(x) = V_0 \cos\left(\frac{2\pi}{a}x\right)$$
(1D)  
"small potential"

Small potential inluence on the borders of the Brilloun zone:

$$V(x) = V_0 \cos\left(\frac{2\pi}{a}x\right) = \frac{V_0}{2} \left(e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x}\right)$$

$$\int \frac{\pi}{a_x} k_x = hkl = 000, 100, 100, 200, 200, -\frac{\pi}{a_x} \frac{\pi}{a_x} k_x$$

L

I I

I I

![](_page_59_Figure_1.jpeg)

![](_page_60_Figure_1.jpeg)

![](_page_61_Figure_1.jpeg)

![](_page_62_Figure_1.jpeg)

### The electronic band structure

- It is convenient to present the energies only in the 1st Brillouin zone.
- The electron state in the solid state is given by the wave vector of the 1st Brillouin zone, band number and a spin.

![](_page_63_Figure_3.jpeg)

### **Bloch theorem**

 $\hat{p}\psi(\vec{r}) = -i\hbar \left(i\,\vec{k} + \nabla u_{n,\vec{k}}\right) e^{i\vec{k}\vec{r}} \neq \hbar\vec{k}\psi(\vec{r}).$ 

 $\hbar \vec{k}$  is so-called quasi-momentum or crystal momentum.

If we consider interactions with other quasi-particles (electrons, phonons, magnons etc.) existing in the crystal and real particles penetrating through the crystal (e.g. photons, neutron) the momentum conservation law must be replaced by the **quasi-momentum conservation law** :

$$\sum_{i} \hbar \vec{k}_{i} + \sum_{i} \vec{p}_{i} = \sum_{i} \hbar \vec{k}_{i}' + \sum_{i} \vec{p}_{i}' + \hbar \vec{G}$$

The energy conservation is always the same:

$$\sum_{i} E_{i} = \sum_{i} E_{i}'$$