# 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



### **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



### **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 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



Brillouin zone in 2D, oblique lattice.





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





heksagonal lattice

Ibach, Luth

# Potencjał periodyczny



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  $\Delta$ 

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# Fermi surfaces of metals





Fig.13 Fermi surface of aluminum





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**



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).



### **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:

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



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:

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



### **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).

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### The nearly free-electron approximation

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



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



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### 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







 $a_r$ 

 $a_{\star}$ 



### 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:

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

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

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### 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.



### **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:

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