# Phys 3080

# Solid state physics

## *Exam 2005*

## *Part I*

(Lecturer Dr Michael Kuchiev)

## 1. Crystal structure (12%)

**Lattices**

Consider a crystal with the sc lattice; the lattice vectors are $\mathbf{a} = a\,\mathbf{i},\ \mathbf{b} = a\,\mathbf{j},\ \mathbf{c} = a\,\mathbf{k}$, where $a$ is the lattice constant and **i, j, k** are three ortho-normal vectors.

1) Prove that the reciprocal lattice is sc as well.
   Hint: remember that $\mathbf{a}^* = \frac{2\pi}{V_c}\mathbf{b}\times\mathbf{c},\ etc,$ where $V_c = |\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})|$ is the volume of the unit cell.
2) Find separation between closest parallel planes of the lattice, which have the Miller indexes (1,1,0). Compare this separation with the length of the vector $\mathbf{K}$=(1,1,0) in the reciprocal lattice.
3) What orientation has the vector (1,1,0) of the reciprocal lattice in relation to the plane (1,1,0) in the initial lattice.
4) Write down two relations between the orientation and length of the vector ($k,l,m$) of the reciprocal lattice and the orientation and the separation of the planes with the Miller indexes ($k,l,m$) in general case.

**Bragg reflection**

**5)** Write down conditions for the n-th diffraction maximum for scattering of light by a crystal. Present them

- in the Bragg form (i.e. using the Miller indexes)
- in the Laue form (i.e. using the vectors of the reciprocal lattice)

## 2. Phonons (12%)

Consider contribution of phonons to the heat capacity of some solid state.

1) What is the limit of the heat capacity at high temperature?
2) How the heat capacity depends on the temperature in the low-temperature limit ?
   Hint: the main point is whether this behaviour is exponential, or power-type. Why?
   (It may be helpful to remember that the key point here plays the simple fact that the space is three-dimensional.)

## 3. Electron properties (12%)

1) Explain *very* briefly the concept of the Fermi energy for the free electron gas.
2) Express the Fermi wave vector $k_F$ via the electron concentration $n_e = N_e / V$, where $N_e$ is a number of the conducting electrons.
   Hint: you are welcome to either derive this dependence accurately, or to establish it on the basis of simple dimensional counting. (The numerical constant here is not important here.)
3) How the Fermi energy depends on the electron concentration ?
   Hint: again you are welcome to either derive this dependence accurately, or to apply a simple dimensional counting.
4) Consider the classical limit $\hbar \to 0$. Find the Fermi energy in this case. Argue *very* briefly whether quantum effects play a role in metals.

## *Answers*

# 1) Crystal structure

**Lattices**

1)

$$V_c = a^3$$

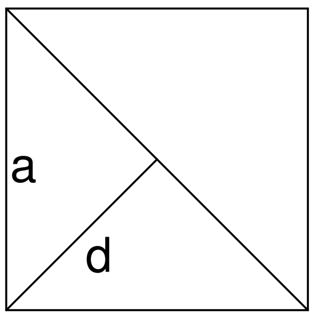
$$\mathbf{a}^* = \frac{2\pi}{a^3} a^2\, \mathbf{j}\times\mathbf{k} = \frac{2\pi}{a}\, \mathbf{i} = a^*\, \mathbf{i},$$

$$\mathbf{b}^* = a^*\, \mathbf{j},$$

$$\mathbf{c}^* = a^*\, \mathbf{k}$$

$$a^* = \frac{2\pi}{a}$$ − is the lattice constant of the reciprocal lattice (1.1)

2)




$d = \frac{a}{\sqrt{2}}$

Fig.1

Figure 1 shows that

$$d_{(1,1,0)} = \frac{a}{\sqrt{2}} \quad (1.2)$$

3) The vector of the reciprocal lattice $\mathbf{K}_{(1,1,0)}$ is perpendicular to the plane (1,1,0). The length of the vector of the reciprocal lattice is

$$|\mathbf{K}_{(1,1,0)}| = \frac{2\pi}{a}\sqrt{1+1} = 2\pi\frac{\sqrt{2}}{a} = \frac{2\pi}{d_{(1,1,0)}} \quad (1.3)$$

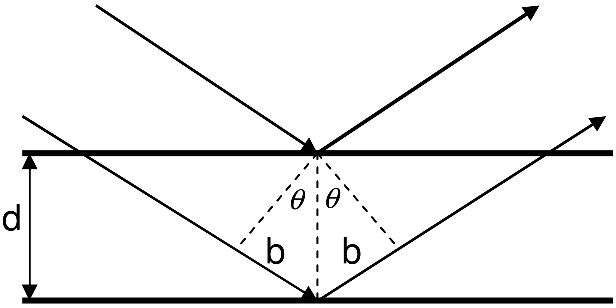
Here Eq.(1.2) was used. Thus, the length of the reciprocal vector is reciprocal to the plane separation.

4) In general, the plane, which has the Miller indexes (*k*, *l*, *m*), is perpendicular to the vector (*k*, *l*, *m*) of the reciprocal lattice. The separation $d_{(k,l,m)}$ between nearest planes (*k*,*l*,*m*) and the length of the reciprocal vector $\mathbf{K}_{(k,l,m)}$ are reciprocal

$$\mathbf{K}_{(k,l,m)} = \frac{2\pi}{d_{(k.l.m)}} \qquad (1.4)$$

Eq. (1.3) presents a particular example of a general rule Eq.(1.4).

**Bragg's reflection**




5)

Fig.2

Fig.2 shows that:

- Phase differnence ~ $2b = 2d_{(k,l,m)} \sin\theta$ (1.5)

  Bragg's law $2d_{(k,l,m)} \sin\theta = n\lambda$

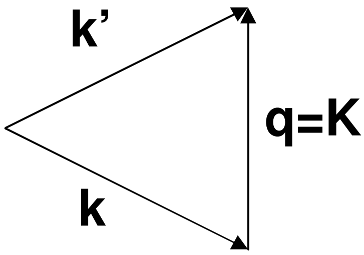
- 


Fig.3

$$\mathbf{q} = \mathbf{k}' - \mathbf{k} = \mathbf{K}_{(n,l,m)} \qquad (1.6)$$

Here **k** and **k'** are the wave vectors of the incident and scattered beams of light.

6)

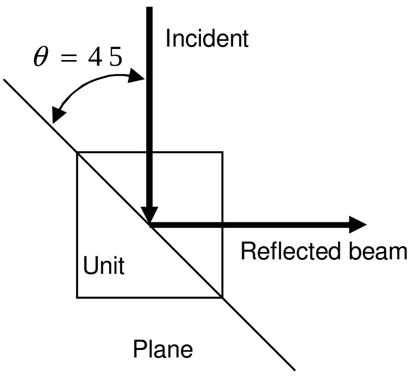



Fig.4

Fig.4 shows that $\theta = \pi / 4$

$$\lambda = 2d\sin\theta = 2\frac{a}{\sqrt{2}}\frac{1}{\sqrt{2}} = a = 1\text{Å} \tag{1.7}$$

Here Eq.(1.2) was used. From Eq.(1.7) one finds

$$\hbar\omega = 12.4\,\text{Kev} \tag{1.8}$$

Fig.4 shows that the reflected beam moves along (0,1,0).

## 2) Phonons

**Oscillator**

1)

$$\bar{\varepsilon} = \left( n(\omega) + \frac{1}{2} \right)\hbar\omega$$
$$n(\omega) = \frac{1}{\exp(\hbar\omega / k_B T) - 1} \tag{2.1}$$

2)

High-temperature limit: $k_B T \gg \hbar\omega$
Low-temperature limit: $k_B T \ll \hbar\omega$ (2.2)

3)

$$C = \frac{d\bar{\varepsilon}}{dT} \to k_B \quad \text{when } k_B T \gg \hbar\omega \tag{2.3}$$

4) $$C \cong k_B \exp\left(-\frac{\hbar\omega}{k_B T}\right), \text{ when } k_B T \ll \hbar\omega$$

$$\text{more accurately } C \approx k_B \exp\left(-\frac{\hbar\omega}{k_B T}\right)\left(\frac{\hbar\omega}{k_B T}\right)^2, \quad (2.4)$$

but the main point is the exponential reduction anyway

**Solid state**

5) $$C = 3N k_B \quad \text{when } T > \Theta_D \quad (2.5)$$

6) $$C \propto N\left(\frac{T}{\Theta_D}\right)^3, \text{ when } T \ll \Theta_D \quad (2.6)$$

7) For an oscillator the low-temperature limit is always valid when temperature is sufficiently low, which makes the heat capacity exponentially small, see Eq. (2.4). In contrast, for a solid state, even for low temperatures there exist the phonons that satisfy the high-temperature limit, in which the heat capacity is large, see Eq.(2.3). Eq.(2.6) counts the number of these phonons.

## 3) Electron properties

1) The Fermi energy is an energy level below which all states in metal at *T=0* are occupied while all states above it are empty.

2)

$$2\int \frac{V d^3k}{(2\pi)^3} = 2\frac{V 4\pi}{(2\pi)^3}\int_0^{k_F} k^2 dk = \frac{V k_F^3}{3\pi^2} = N_e$$

$$k_F = \left(3\pi^2 n\right)^{1/3} \quad (3.1)$$

Dimension counting gives $k_F = const\ n^{1/3}$, where *const* is a just numerical coefficient.

3)

$$E_F = \frac{p_F^2}{2m} = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3}$$

Dimensional counting gives (3.2)

$$E_F = const\ \frac{\hbar^2}{m} n^{2/3}$$

where *const* is just a number

4) $$E_F \to 0 \text{ when } \hbar \to 0 \tag{3.3}$$

which shows that the Fermi energy is a purely quantum quantity. Thus the quantum effects play a major role in many effects in metals.