EXAM on WBPH030 “Solid State Physics”

Content: 5 pages (including this cover page)

Thursday 26 January 2023

ANSWERSHEET

1. Crystal Structure and X-ray scattering

1.1. (2p) How to form a crystal using the concepts of lattice and a basis?

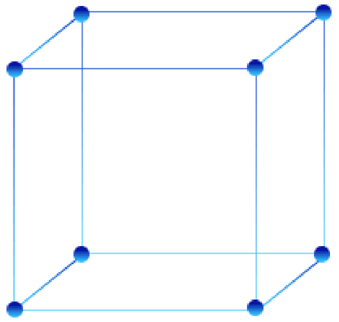
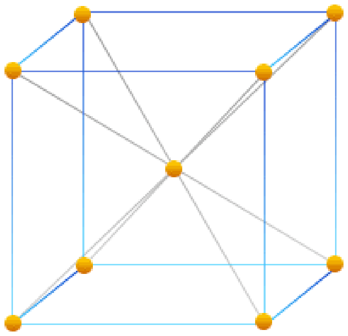
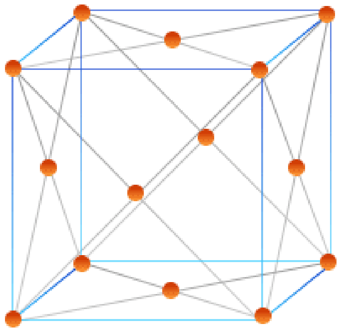
Answer:

- Basis – group of atoms, which being periodically repeated, will recover all the crystal.
- Lattice – is a mathematical construction defining the position of this group in space.

To form a crystal one needs to put a basis in each lattice point.

1.2. (3p) There are 3 space lattices of cubic type. Name and sketch them (rough sketches without using rulers are acceptable).

Answer:

Simple cubic	Face centered cubic	Base centered cubic
		
$\begin{cases} \boldsymbol{a}_1 = (100) \times a \\ \boldsymbol{a}_2 = (010) \times a \\ \boldsymbol{a}_3 = (001) \times a \end{cases}$	$\begin{cases} \boldsymbol{a}_1 = (\frac{1}{2}\,\frac{1}{2} - \frac{1}{2}) \times a \\ \boldsymbol{a}_2 = (-\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}) \times a \\ \boldsymbol{a}_3 = (\frac{1}{2} - \frac{1}{2}\,\frac{1}{2}) \times a \end{cases}$	$\begin{cases} \boldsymbol{a}_1 = (0\,\frac{1}{2}\,\frac{1}{2}) \times a \\ \boldsymbol{a}_2 = (\frac{1}{2}\,0\,\frac{1}{2}) \times a \\ \boldsymbol{a}_3 = (\frac{1}{2}\,\frac{1}{2}\,0) \times a \end{cases}$

1.3. (6p) a) Define the NaCl lattice type and b) coordinates of its basis in terms of $\boldsymbol{r_j} = x_j\boldsymbol{a_1} + y_j\boldsymbol{a_2} + z_j\boldsymbol{a_3}$, where the $\boldsymbol{a}_i$ are vectors in the Cartesian coordinate system. c) What is the maximal packing fraction for this lattice type (considering all the atoms to be of the same radius)? d) What are Miller's indices of the most densely packed plane?

Answer:

a) Once one defines a basis, which is a repetitive atomic group, it becomes visible that the basises lay in lattice points of fcc. (1p)

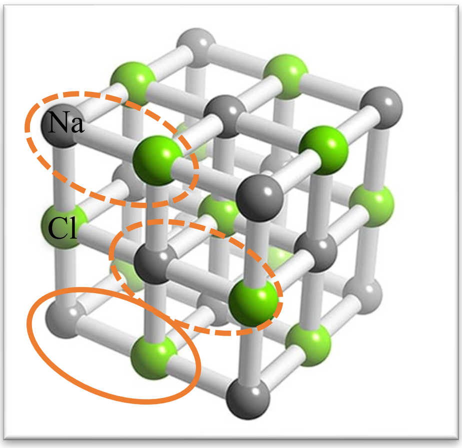


Figure 1. NaCl crystal structure

b) Basis of NaCl consist of 2 atoms, 1 Na (in the vertex) and 1Cl (in the half side) atoms. It`s asked to give coordinates of atoms of a basis in Cartesian coordinate system, meaning in orthogonal one. The conventional lattice vectors can be chosen as $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$. $\begin{cases} \boldsymbol{a}_1 = (100) \times a \\ \boldsymbol{a}_2 = (010) \times a \\ \boldsymbol{a}_3 = (001) \times a \end{cases}$;

$$\boldsymbol{r_j} = x_j \boldsymbol{a_1} + y_j \boldsymbol{a_2} + z_j \boldsymbol{a_3} \quad \begin{cases} \boldsymbol{r}_{Na} = 0 \cdot \boldsymbol{a}_1 + 0 \cdot \boldsymbol{a}_2 + 0 \cdot \boldsymbol{a}_3 \\ \boldsymbol{r}_{Cl} = \frac{1}{2} \cdot \boldsymbol{a}_1 + 0 \cdot \boldsymbol{a}_2 + 0 \cdot \boldsymbol{a}_3 \end{cases};$$

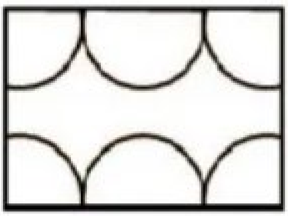
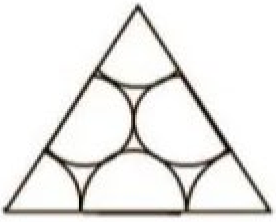
(1p)

c) In fcc the closest atoms are laying on the face diagonal, means, if r is the radius of the atom, $4r = a\sqrt{2}$, then

$$p_{fcc} = \frac{NV_a}{V_{cell}} = \frac{V_a(\overset{\text{vertex}}{\frac{1}{8} \cdot 8} + \overset{\text{face}}{\frac{1}{2} \cdot 6})}{a^3}; \; V_a = \frac{4}{3}\pi r^3; \; p_{fcc} = \frac{\frac{4}{3}\pi r^3}{(\frac{4r}{\sqrt{2}})^3} = \frac{\pi\sqrt{2}}{6} = 73\%$$

(2p)

d) Compare 3 planes of fcc: (100), (110), (111).

	(100)	(110)	(111)
			
N	$4 * \frac{1}{4} + 1 = 2$	$2 * \frac{1}{2} + 4 * \frac{1}{4} = 2$	$3 * \frac{1}{2} + 3 * \frac{1}{6} = 2$

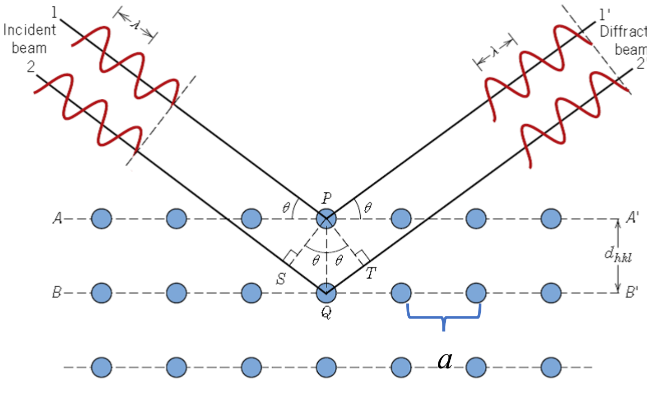
A	a^2	$a * a\sqrt{2} = a^2\sqrt{2}$	$\frac{a\sqrt{2} * a\sqrt{2} * sin60°}{2} = \frac{a^2\sqrt{3}}{2}$
p_{fr}	2atoms/a^2	$\sqrt{2}/a^2 =$ $1.4atoms/a^2$	$\frac{4}{\sqrt{3}}/a^2 = 2.31atoms/a^2$

(111) plane is the most densely packed plane.

(2p)

1.4. (5p) Briefly discuss the Bragg diffraction. What is the requirement for the wavelength of the radiation to be diffracted on a crystal?

Answer:



Path difference between 1`and 2`is:

$$\Delta = SQ + QT$$

$$SQ = QT = 2 * d_{hkl} * sin\theta$$

constructive interference of 1`and 2`is possible, if this path difference is equal to any integer value of the wavelength:

$$\Delta = n\lambda, n = 1,2 \dots$$

Thus the Braggs law is:

$$2d_{hkl}sin\theta = n\lambda$$

So the requirement for a wavelength is:

$$\lambda \sim d_{hkl} \sim a$$

If the formula is not mentioned, but the discussion is correct, one gets 3p

1.5. (10p) Determine the structural factor of the FCC lattice of KCl.

If the atomic form factors of both K and Cl are the same, one will obtain the *x*-ray diffraction pattern similar to simple cubic. Explain why.

The structural factor is given by:

$$S_G = \sum_j e^{-i\mathbf{G}\mathbf{r}_j} \int dV\, n_j(\boldsymbol{\rho})\, e^{-i\mathbf{G}\boldsymbol{\rho}}.$$

Answer:

One can consider KCl as 2 fcc monoatomic lattices (one for K and other for Cl), shifted by $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ relatively to each other.

There are 4 atoms in conventional fcc cell. 1 in the vertex and 3 on faces. If the K atom will be taken as the origin, coordinates r_j of K atoms in convencional fcc lattice will be: (000), $(\frac{1}{2}\frac{1}{2}0)$, $(\frac{1}{2}0\frac{1}{2})$, $(0\frac{1}{2}\frac{1}{2})$, so the 1st term in structural factor will be:

$$S_{G,K} = \sum_{j,K} e^{-i\boldsymbol{G}\boldsymbol{r}_{j,K}} f_{j,K}$$

$$= f_K \cdot \left(e^{-i\boldsymbol{G}(\boldsymbol{0},\boldsymbol{0},\boldsymbol{0})} + e^{-i\boldsymbol{G}\left(\frac{1}{2},\frac{1}{2},0\right)} + e^{-i\boldsymbol{G}\left(\frac{1}{2},0,\frac{1}{2}\right)} + e^{-i\boldsymbol{G}\left(0,\frac{1}{2},\frac{1}{2}\right)}\right);$$

$$G = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3; \boldsymbol{b}_i \cdot \boldsymbol{a}_j = 2\pi\delta_{ij}$$

$$f_K \cdot \left(e^{-i(hb_1,kb_2,lb_3)(\boldsymbol{0},\boldsymbol{0},\boldsymbol{0})} + e^{-i(hb_1,kb_2,lb_3)\left(\frac{1}{2},\frac{1}{2},0\right)} + e^{-i(hb_1,kb_2,lb_3)\left(\frac{1}{2},0,\frac{1}{2}\right)} + e^{-i(hb_1,kb_2,lb_3)\left(0,\frac{1}{2},\frac{1}{2}\right)}\right)$$

$$= f_K \cdot \left(1 + e^{-i\pi(h+k)} + e^{-i(h+l)} + e^{-i(k+l)}\right) =$$

$$= \begin{cases} 4f_K, & h,k,l\ even \\ 4f_K & h,k,l\ odd \\ 0, & 2\ odd\ 1\ even \\ 0, & 1\ odd\ 2\ even \end{cases};$$

The 2nd term in structural factor, associated with Cl fcc sublattice, will be the same but multiplied by $e^{-i\boldsymbol{\pi}(h+k+l)}$:

$$S_{G,Cl} = f_{Cl} \cdot e^{-i\boldsymbol{\pi}(h+k+l)} \cdot \left(1 + e^{-i\pi(h+k)} + e^{-i(h+l)} + e^{-i(k+l)}\right) =$$

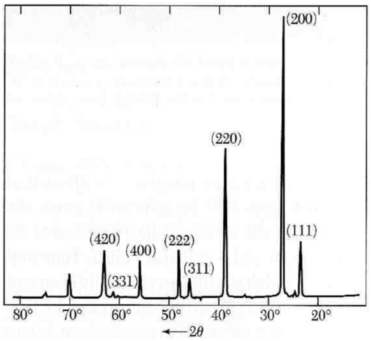
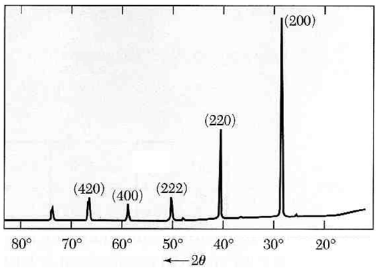
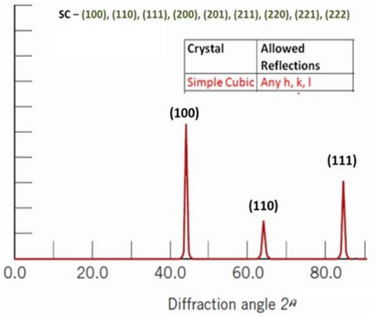
$$= \begin{cases} 4f_{Cl}, & h,k,l\ even \\ -4f_{Cl} & h,k,l\ odd \\ 0, & 2\ odd\ 1\ even \\ 0, & 1\ odd\ 2\ even \end{cases};$$

Finally, $S_G = \begin{cases} 4(f_K + f_{Cl}), & h,k,l\ even \\ 4(f_K - f_{Cl}), & h,k,l\ odd \end{cases}$, and one will obtain 2 sets of X-ray diffraction peaks, higher peaks with intensity ~ $(f_K + f_{Cl})^2$ for planes with all even indices and lower peaks with intensity ~ $(f_K - f_{Cl})^2$ for with planes all odd indices.

If $f_K = f_{Cl}$, $S_G = \begin{cases} 8f, & h,k,l\ even \\ 0, & h,k,l\ odd \end{cases}$, then the X-ray diffraction pattern will contain only peaks with all even indices, which is equivalent to the pattern of SC X-ray diffraction, but for a lattice constant 2 times smaller.

End of an answer

Sample X-ray diffraction patterns:

If $f_i > f_j$	If $f_i = f_j$	SC
		

2. Phonons and Electrons

2.1. (4p) Write down the Newtonian equation of a 1D chain made of monoatomic harmonic oscillators.

Answer:

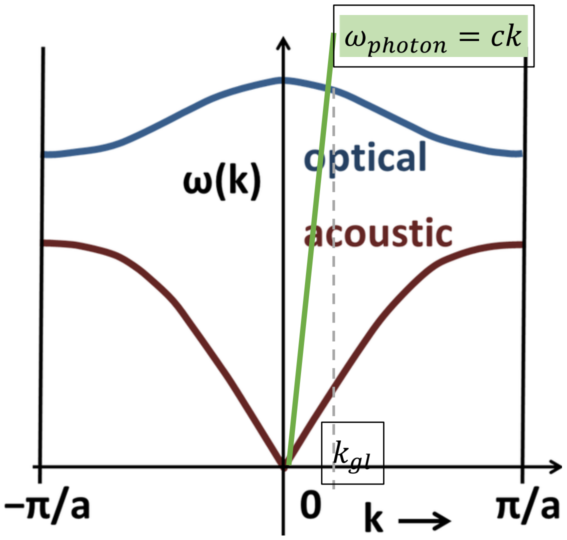
If M is mass of an oscillator, C is a force constant and u_i is a displacement of i^{th}oscillator, the Newtonian eq. is:

$$M\ddot{u}_i = C(u_{i+1} + u_{i-1} - 2u_i)$$

2.2. (4p) Discuss what will happen if there are two types of atoms. Sketch the dispersion relation for phonons in this chain. Discuss the interaction of such a lattice with visible light.

Answer:

In a monoatomic chain, all the masses are the same, so they will response identically to the perturbation. When the masses differ from each other, the response is different and eventually there will be a situation, when heavier, more inert atoms, are still moving in the initial direction, while lighter are already moving backwards, creating a mode, in which atoms with different masses are oscillating in opposite directions. Thus in dispersion relation, one will have to branches, lower one corresponding to a case, when all the atoms are moving in the same direction (acoustic branch) and the upper one for the case of opposite direction movement (optical branch).



Let`s discuss the interaction of light with $\lambda = 500\,nm$ with the phonons in such a chain. Knowing λ one can estimate the value of k_{gl} for such a photon: $k_{gl} = \frac{2\pi}{\lambda} \sim 1 \times 10^{7}[m^{-1}]$ At the zone boundary $k_{ph} \sim \frac{\pi}{\alpha} = \frac{\pi}{1nm} \sim 10^{9}[m^{-1}]$, which is 100 times larger. So one can imagine the relative position of k_{gl} on the k axis. Thus, due to momenta and energy conservation phonons can excite only optical phonons.

Here k_{gl} is referred to wavevector of a green light and k_{ph} is a wavevector of a phonon.

2.3. Consider **a 3D simple cubic** lattice of a metal.

2.3.1. (9p) Determine the phononic heat capacity, at low temperature, in Debye approximation if the dispersion relation is assumed to be:

$\omega = v_s|\boldsymbol{k}|$.

(*Hint: use formulas (5,6) or (7)*)

Answer:

We start from the definition of a heat capacity: $C_v = (\frac{\partial U}{\partial T})_v$. As this is a derivative of a total energy of a lattice, we need to obtain this energy. We know that lattice vibrations can be represented as independent quantum oscillators, means the total energy will be the energy of an ensemble of quantum oscillators: $U = \sum_k \sum_p \hbar\omega_k(\langle n_k\rangle + \frac{1}{2})$, where first sum is over all possible wavevectors and second is a sum for all polarizations. We can turn this sum to the integral, using following: $\sum_k \cdot\, \Delta_k = \int_{k_{min}}^{k_{max}} d^3k \rightarrow$, which simply means summing all the primitive volumes Δ_k. And the summation over p gives us a factor of 3, $\langle n_k\rangle$ – is an average number of phonons with a wavevector k (there is different number of phonons with different k, and this relation of how many oscillators one has per unit value of k is given by density of states, $D(\omega)$). Then,

$$U = \sum_k \sum_p \hbar\omega_k\left(\langle n_k\rangle + \frac{1}{2}\right) = 3\int_{k_{min}}^{k_{max}} \frac{1}{\Delta_k}\left(\hbar\omega_k\left(\langle n_k\rangle + \frac{1}{2}\right)\right) d^3k =$$

$$= 3\int_{k_{min}}^{k_{max}} \frac{1}{\Delta_k}\hbar\omega_k\langle n_k\rangle d^3k + \cdots \xRightarrow{d^3k\to d\omega} = 3\int_{\omega_{min}}^{\omega_{max}} \hbar\omega_k\langle n_\omega\rangle\cdot D(\omega)d\omega$$

$$|D(\omega) = \frac{dN}{d\omega} = \frac{dN}{dk}\frac{dk}{d\omega} = \left(\frac{V_k}{\Delta_k}\right)\frac{dk}{d\omega} = \frac{d}{dk}\left(\frac{4}{3}(\pi k^3)\cdot\frac{V}{(2\pi)^3}\right)\cdot\frac{dk}{d\omega} = \frac{4\pi k^2 V}{(2\pi)^3}\cdot\frac{dk}{d\omega};$$

$$\langle n_\omega\rangle = \frac{1}{e^{\frac{\hbar\omega_k}{k_BT}}-1}|$$

$$U = \frac{12\pi V}{(2\pi)^3}\int_{\omega_{min}}^{\omega_{max}} \frac{\hbar\omega_k k^2\cdot\frac{dk}{d\omega}}{e^{\frac{\hbar\omega_k}{k_BT}}-1}d\omega.$$

It was asked to obtain a heat capacity in Debye approximation, which gives us dispersion relation: $\omega = v_s|\mathbf{k}|, \frac{dk}{d\omega} \to \frac{1}{v_s}$

$$U = \frac{12\pi V}{(2\pi v_s)^3}\int_0^{\omega_D} \frac{\hbar\omega^3}{e^{\frac{\hbar\omega}{k_BT}}-1}d\omega = \left| d\omega \to d\left(\frac{\hbar\omega}{k_BT}\right) = d\chi, \chi_{max} = \frac{\hbar\omega_D}{k_BT} \right| =$$

$$= \frac{12\pi V\hbar}{(2\pi v_s)^3}\int_{\omega_{min}}^{\omega_{max}} \frac{\left(\frac{\hbar\omega}{k_BT}\right)^3 * \left(\frac{k_BT}{\hbar}\right)^3}{e^{\frac{\hbar\omega}{k_BT}}-1}\cdot\left(\frac{k_BT}{\hbar}\right)\cdot d\left(\frac{\hbar\omega}{k_BT}\right)$$

$$= \frac{12\pi V\hbar}{(2\pi v_s)^3}\cdot\left(\frac{k_BT}{\hbar}\right)^4\cdot\int_0^{\chi_{max}} \frac{\chi^3}{e^\chi-1}\cdot d(\chi)$$

The other condition, that simplifies the model – is the limit of low T:

$$k_BT \ll \hbar\omega_D \ \to \frac{\hbar\omega_D}{k_BT} \to \infty \ \to \int_0^\infty \frac{\chi^3}{e^\chi-1}\cdot d(\chi) = \frac{\pi^4}{15}$$

Thus, $U = \frac{12\pi V\hbar}{(2\pi v_s)^3}\cdot\left(\frac{k_BT}{\hbar}\right)^4\cdot\frac{\pi^4}{15}$ and

$$C_v = \left(\frac{\partial U}{\partial T}\right)_v = \frac{16\pi V\hbar}{5(2v_s)^3}\cdot\left(\frac{k_B}{\hbar}\right)^4\cdot T^3$$

The final formula without derivation cost (3p). If the derivations are reasonable, but answer has small mistakes, answer costs (8p)

2.3.2. (9p) Derive the density of electronic orbitals in this lattice if the dispersion relation for the free electron is given as:

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

Answer:

$$D(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{d}{d\varepsilon}\left(\frac{2(4V\pi k^3)}{3(2\pi)^3}\right) = \frac{d}{d\varepsilon}\left(\frac{8V\pi}{3(2\pi)^3}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\varepsilon^{\frac{3}{2}}\right)$$

$$= \frac{V}{2(\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\varepsilon^{\frac{1}{2}}$$

Derive the expression for the radius of a Fermi surface if the density of electron is n.

$$N_{tot} = NZ = \frac{(Vk_F{}^3)}{3(\pi)^2} \rightarrow k_F = \left(3\pi^2 Z\left(\frac{N}{V}\right)\right)^{\frac{1}{3}} = (3\pi^2 Zn)^{1/3}$$

The final formulas without derivation cost (2p) each. If the derivations are reasonable, but answer has small mistakes, answer costs (8p)

2.4. (*5p* bonus*) Discuss how the electric conductivity of metals will depend on temperature.

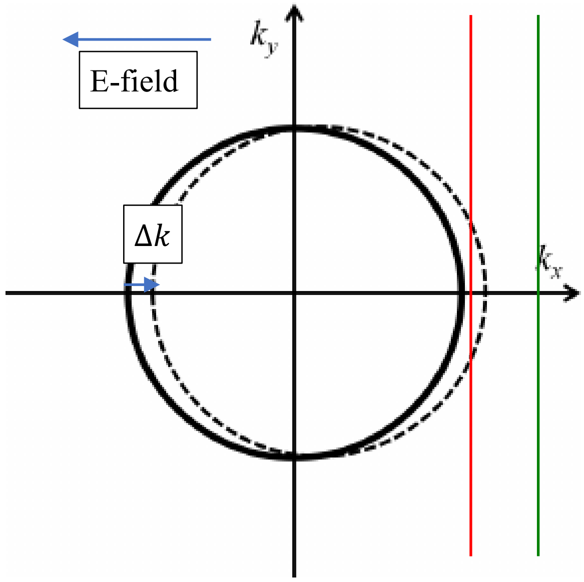
3. Nearly free electrons, intrinsic and impurity conductivity of semiconductors

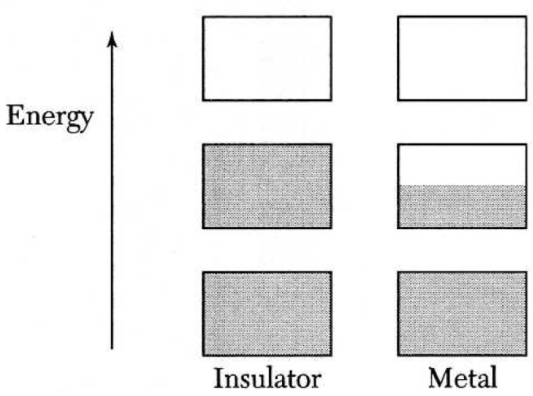
3.1. (4p) a) Discuss the reason for forming energy gaps at the Brillouin zone (BZ) boundary (2p). b) Sketch and explain the difference between the metal, semiconductor, and insulator (2p).

Answer:

a) Energy gaps results from the interaction of a conduction electron wave with the potential of the lattice, formed by ions. When the value of a wavevector of the electron approaches the BZ edge, the wavelength becomes comparable with the lattice constant and the scattering of the electron on the ionic cores becomes more significant, causing the energy loses. So for the electrons with such a k_e, energies will be significantly smaller than the one of a free electron. In the limiting case, when the $k_e = k_{BZ}$, the electron is "captured" in a resonator, forming a standing wave.

b) When the electric field is applied, electrons will start to move along the field, which means that E field adds a term to a k_e.





As was discussed in a) and shown on a Fig.2, in any real material there will be energy gaps, leading to formation of allowed energy bands. What defines whether the material is insulating or conducting under the electric field is whether there are any electrons, that can move.

If k_{BZ}, BZ boundary, lays on a green line, there are allowed k_e values and electron can move, if BZ boundary lays on a red line, one can see, that there will be no allowed states, so the electron can **not** move.

It`s common to say, that the crystal is metallic if band is from 10 to 90 % full, so E_F is still away from the boundary, and as insulator, if bands are either full or empty.

3.2. (6p) Compare the bands folded to the first BZ by $\boldsymbol{k}_{1BZ} = \boldsymbol{k} \pm n\boldsymbol{G}$, where n is an integer

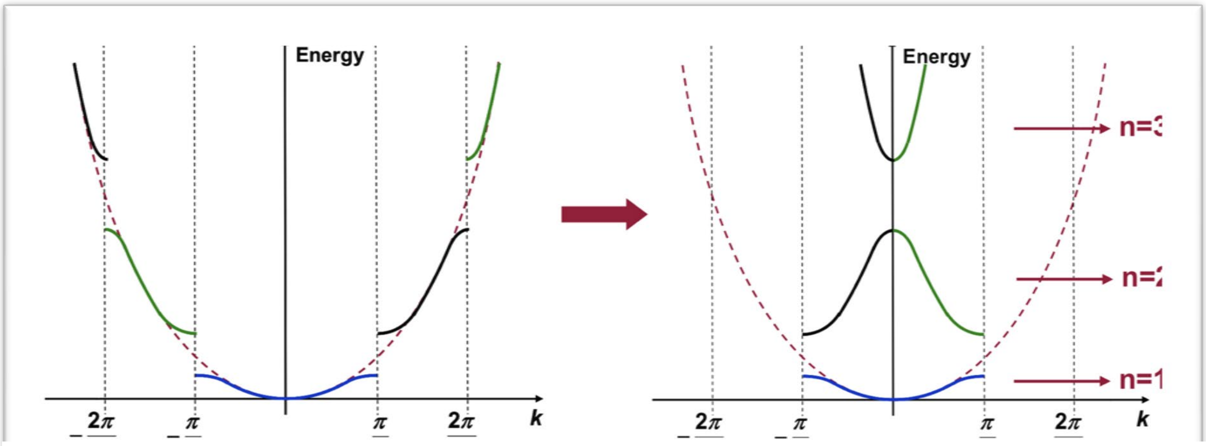


Figure 2 Schematics of the zone folding

Which band (n = 0, 1, or 2 …) could have the smallest effective mass?

Answer:

Effective mass is defined as:

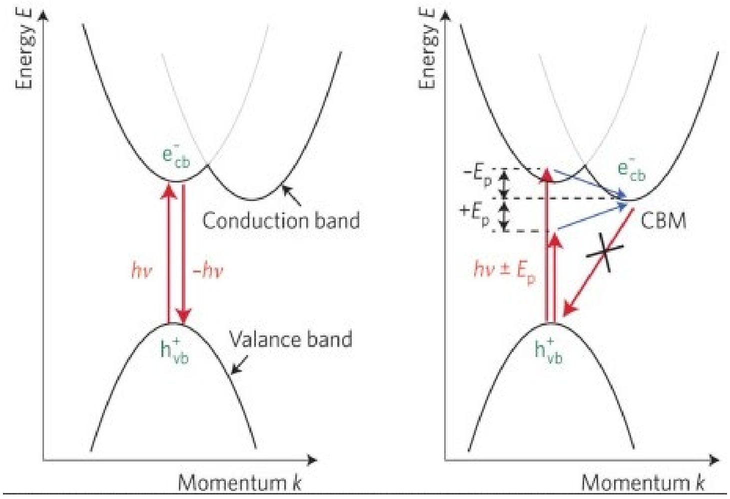
$$m^* = \hbar^2 \left(\frac{d^2E}{dk^2}\right)^{-1},$$

So the smallest effective mass will belong to electrons with largest $\left(\frac{d^2E}{dk^2}\right)^{-1}$, means the most narrow band. In our case, $n = 3$.

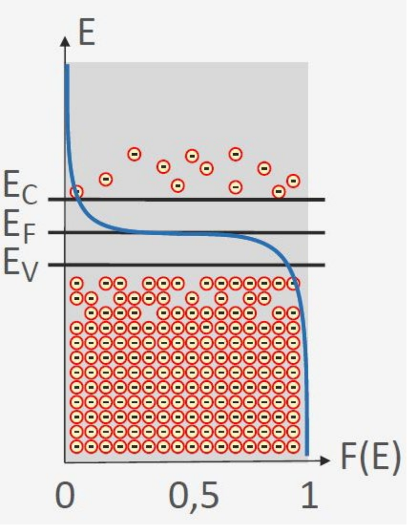
3.3. (6p) How to excite carriers in an intrinsic semiconductor?

Answer: There are several ways, 2 of them were discussed in this course:

Photoexcitation



Thermal excitation

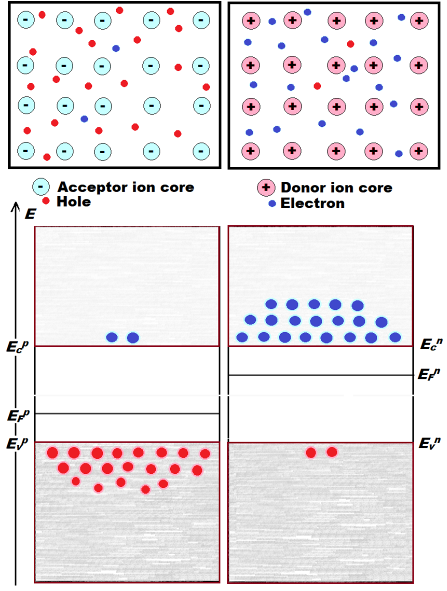


We can excite carriers in a semiconductor material by increasing the temperature. Doing so we provide electrons with extra energy and due to F-D distribution at finite temperature rise the probability of the electrons to occupy some states in a bottom of the conduction band. Other way, which is possible even at $T = 0$ is to excite electrons with phonons whose energy is the same or larger than the band gap.

3.4. (6p) a) Contacting semiconductor, say Si with *n*- and *p*-type impurities, one can form a ***p-n*** junction. Show the processes of band realignment at thermal equilibrium. . b) How will the energy bands conductivity change at positive and negative biases (positive bias *V* is applied from the *p*- to the *n*- side).

Answer:

a) *See on the next page*

<table>
<tr><th colspan="2">Before contact</th><th colspan="2">Before thermal equilibrium</th><th colspan="2">At equilibrium</th></tr>
<tr><td><i>p</i>-type</td><td><i>n</i>-type</td><td><i>p</i>-type</td><td><i>n</i>-type</td><td><i>p</i>-type</td><td><i>n</i>-type</td></tr>
<tr><td colspan="2">
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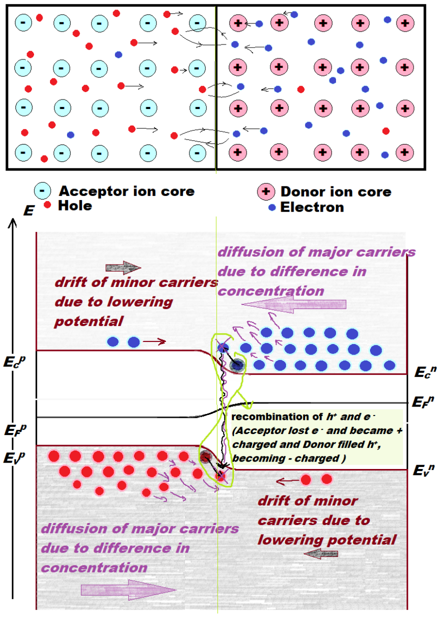
<td colspan="2">
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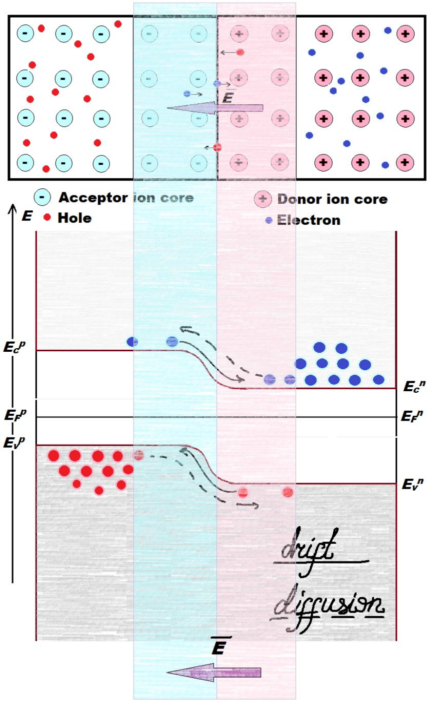
<td colspan="2" rowspan="2">
</td></tr>
<tr><td colspan="4"><i>The aim of any thermodynamic system is to reach an equilibrium, which among other requirements needs equal chemical potentials in all parts of the system.</i></td></tr>
<tr><td colspan="2">We suppose that the gap is intrinsically the same, but for <i>p</i>-type the Fermi level lays closer to the valence band and for the <i>n</i>-type – closer to conduction band. Both semiconductors are neutral.</td>
<td colspan="2">When <i>p</i>- and <i>n</i>-type sc are brought to contact, the free electrons from n-type start to diffuse to <i>p</i>-type, driven by a gradient in chemical potential. This current is called <i>“diffusive current”.</i> When electrons from n-type reach p-type, they recombine with holes, so the Acceptor in <i>p</i>-type becomes negatively charged and the Donor, whose electron left <i>n</i>-type, becomes positively charged. The internal electric field is build up due to local charging of contact region, - (negative) on <i>p</i>-side and + (positive) on <i>n</i>-side. Due to this potential difference, minor carriers, e^- in <i>p</i>-type and h^+ in <i>n</i>-type move towards potential lowering, creating a <i>drift current.</i></td>
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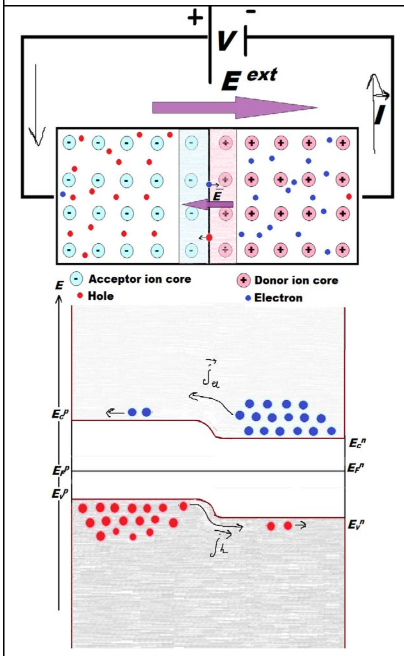
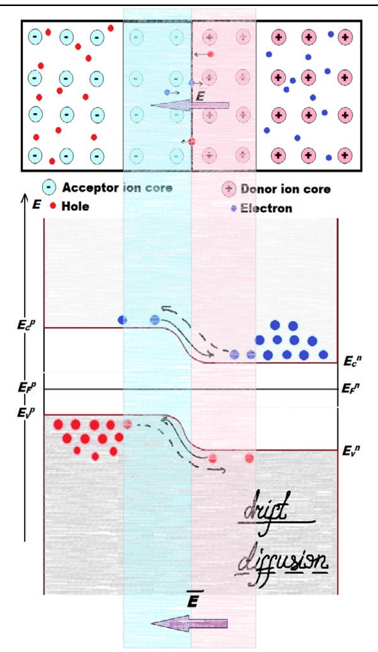
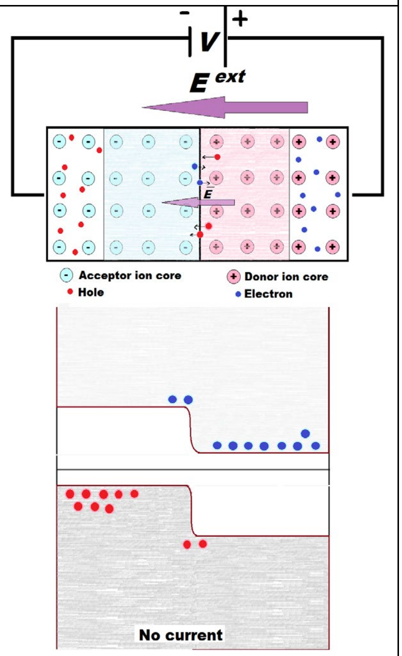
</table>

b)

Positive bias	Unbiased	Negative bias
 	 	

4. **Crystals in a magnetic field**

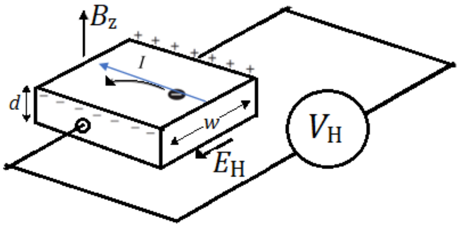
4.1. (6p) Using Drudes` model, briefly explain the Hall effect in metals.

Answer:

Drudes assumptions:

- Electrons in a metal - ideal gas.
- The electrons do not experience coulombic interaction with the ions, but do collide with a change in direction and velocity.
- Electrons reach thermal equilibrium by collisions with the ions. Their mean kinetic energy is: $\frac{m_e v_T^2}{2} = \frac{3}{2} k_B T$
- The average distance of an electron's free movement between collisions is called the mean free path λ and a time between 2 collisions is τ – relaxation time.

From Drude model, current density: $\boldsymbol{j} = -en\boldsymbol{v}$.



Hall effect:

The Hall effect occurs when a current flows through a conductor under a magnetic field. As a result of the Lorenz force, negative charges accumulate on one side of the conductor and positive (if they are) on the other side, so the voltage perpendicular to the channel appears, we call it Hall voltage.

Lorenz force: $\boldsymbol{F} = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})$, we suppose the steady state, means, $F = 0$, then

$$-q\boldsymbol{E} = \boldsymbol{v} \times \boldsymbol{B}. \qquad (1)$$

Let us simplify the problem letting the current pass by $\boldsymbol{x}$ axis, means electrons ($q = -e$) have the largest velocity in this direction, $-v_x$ and $\boldsymbol{B}$ to have only z component, so $\boldsymbol{B} = (0,0,B_z)$, so (1) becomes:

$$E_y = -v_x B_z, \qquad \text{then we use } E_y = -\frac{V_H}{w} \text{ to get}$$

$$V_H = w v_x B_z$$

We express v_x from Drudes` expression for current density: $v_x = \frac{j_x}{en} = \frac{I_x}{enS} = \frac{I_x}{endw}$,

$$\text{so } V_H = \frac{I_x B_z}{end} \ .$$

4.2. (4p) a) Which physical parameter defines para- or diamagnetic? (1p)

Answer:

This parameter is a magnetic permeability (μ) and it is the measure of magnetization of a material in response to an applied magnetic field.

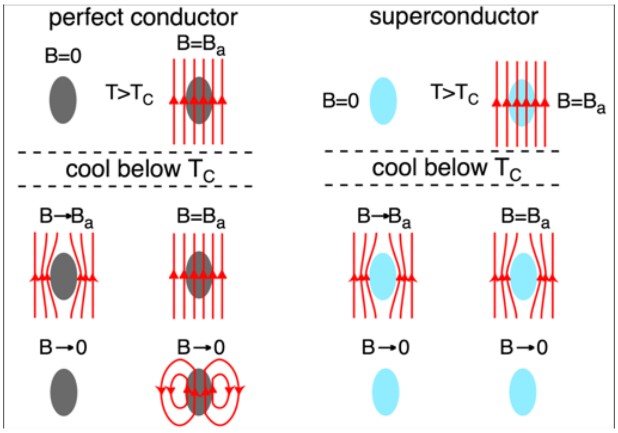
b) How do those two types of materials behave in a magnetic field? (3p)

Answer:

Diamagnetic materials are repelled by a magnetic field, as an applied magnetic field creates an induced magnetic field in opposite direction, causing a repulsive force. Diamagnetism occurs in **all** materials but in diamagnets this is **the only** magnetic effect. In paramagnets and ferromagnets, the weak diamagnetic force is **overcome** by the attractive force of magnetic dipoles in the material, so paramagnetic and ferromagnetic materials are attracted by a magnetic field.

- Diamagnets are materials with a magnetic permeability **less** than magnetic permeability of free space μ_0.
- Paramagnets are materials with a magnetic permeability **larger** than magnetic permeability of free space μ_0.

4.3. (6p) Some materials demonstrate a superconducting transition at a critical temperature. Describe the difference in magnetization between a superconductor and a perfect conductor under an external magnetic field.



Answer: the Meissner effect:

The perfect conductor will prevent any change in magnetic flux by EM induction, whereas SC expels external b-field with generated surface currents, so under T_c/B_c, there will be no magnetization in a SC.

4.4. (10p) For the system shown on right, write down the expression for the magnetic moment of a system subjected to a magnetic field ***B***.

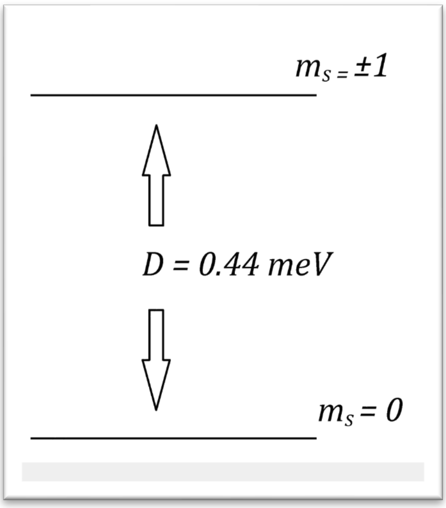
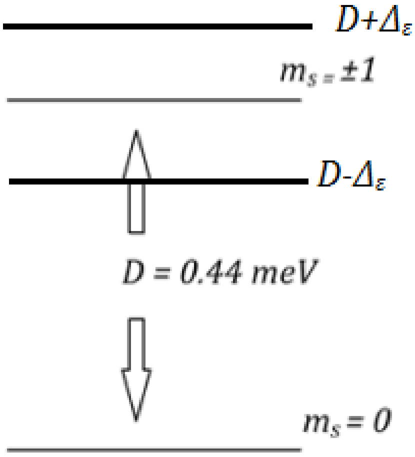


Figure 3. Triplet state system, for example, the ground state of O_2.

Answer: Such a triplet state has 2 electrons in the same orientation. When such a system is subjected to magnetic field, there will be 3 ways of how those electrons may respond: both spins aligned with B, both electrons aligned against B, and one spin up, one spin down. First possibility lowers the energy, second raises and in the third option there will be no response to a magnetic field. So the electronic system under the magnetic field is transformed:



$|\Delta_\varepsilon| = \mu B$ is an energy term, gained in a magnetic field. $\mu = -g m_s \mu_B B$ So the relative occupacies of this levels will be:

$$e^{-\frac{(D+\mu B)}{k_B T}} \text{ for spins alligned against}$$

$$e^{-\frac{(D-\mu B)}{k_B T}} \text{ for spins aligned with B}$$

$$e^{-\frac{D}{k_B T}} \text{for spin up} - \text{down and}$$

$$1 \text{ for ground s state.}$$

So, according to (4) given in FORMULA LIST, one can get an expression:

$$\langle \mu \rangle = \frac{-\mu e^{-(D+\mu B)} + \mu e^{-(D-\mu B)}}{1 + e^{-\frac{D}{k_B T}} + e^{-\frac{(D+\mu B)}{k_B T}} + e^{-\frac{(D-\mu B)}{k_B T}}}.$$

-------------------------------- End of Questions --------------------------------

FORMULA LIST

The density of states is defined by:

$$D(\omega) = \frac{dN}{d\omega} \,. \tag{1}$$

Fermi-Dirac distribution:

$$f(\varepsilon)_{FD} = \frac{1}{e^{\frac{\varepsilon-\mu}{k_B T}} + 1} \,. \tag{2}$$

Bose-Einstein distribution:

$$f(\varepsilon)_{BE} = \frac{1}{e^{\frac{\varepsilon-\mu}{k_B T}} - 1} \,. \tag{3}$$

Quantum statistical average:

$$< A > = \frac{\sum_i A_i e^{-\frac{E_i}{k_B T}}}{\sum_i e^{-\frac{E_i}{k_B T}}} \,. \tag{4}$$

Taylor series of exponential:

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \,, \qquad -\infty < x < \infty \,. \tag{5}$$

Exponential integral:

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}} \,. \tag{6}$$

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15} \,. \tag{7}$$