Written exam of Condensed Matter Physics - June 20th 2022
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Exercise 1. A binary insulating compound with chemical formula AM crystallizes in the cubic system. The crystal is ground into a powder and its structure is investigated by means of X-ray diffraction, using a radiation with wavelength $\lambda = 0.125\,\text{nm}$. The first eight diffraction peaks are observed at the Bragg angles

$$\theta = \varphi/2 = 12.77^\circ,\ 18.21^\circ,\ 22.50^\circ,\ 26.23^\circ,\ 29.61^\circ,\ 32.77^\circ,\ 35.78^\circ,\ 38.68^\circ.$$

1. [8 points] Determine the crystal structure (simple cubic, fcc, bcc, or diamond?) of the given compound; attribute each peak to the families of lattice planes that produce it and determine the side a of the (conventional) cubic unit cell, taken as the average of the values determined from each peak.

2. [2 points] If the phonon spectrum of the crystal is investigated by neutron scattering, how many acoustic and optical phonon branches would be observed at a generic (i.e., not high-symmetry) point of the first Brillouin zone? Motivate your answer.

3. [5 points] A measure of the specific heat of the given compound at a temperature $T = 1\,\text{K}$ (where one can safely assume that only acoustic phonons contribute) yields $c_v = 6.461\,\text{J}/(\text{K}\cdot\text{m}^3)$, determine the average sound velocity c_{D} within the Debye model for acoustic phonons.

Exercise 2. Consider a semiconductor whose crystal structure is simple cubic. The principal axes of the crystal are taken as the x, y and z axes. The dispersion curves of the conduction and valence bands (E_{C} and E_{V}, respectively) along the k_z direction are

$$E_{\text{C}} = A\,[2 - \cos(k_z a)]\,, \qquad E_{\text{V}} = B\,[\cos(k_z a) - 1]\,,$$

where the lattice constant is $a = 0.5\,\text{nm}$, $A = 1.0\,\text{eV}$, and $B = 0.5\,\text{eV}$.

1. [3 points] Plot the dispersion curves in the first Brillouin zone along the k_z direction and say whether the given crystal is a direct- or an indirect-band gap semiconductor.

2. [5 points] Evaluate the element m_{zz} of the effective mass tensor of the electrons at the conduction band minimum (m^{e}_{zz}) and of the holes at the valence band maximum (m^{h}_{zz}).

3. [5 points] Evaluate the concentration of electrons n and holes p in the conduction and valence bands, respectively, at $T = 300\,\text{K}$ (the semiconductor is intrinsic, i.e., no impurity is present in the lattice; assume that the conduction and valence band can be described within the effective mass approximation, with the mass tensor calculated at the bottom of the conduction band for electrons and at the top of the valence band for holes).

4. [2 points] Evaluate the binding energy of a donor, E_{d}, assuming that the relative dielectric constant of the semiconductor is $\varepsilon_r = 15$ and that the donor state formed below the bottom of the conduction band is hydrogenoid.

[Note that 1 eV corresponds to an energy of 1.602×10^{-19} J; the Planck constant is $\hbar = 1.055\times10^{-34}$ J·s; the Boltzmann constant is $\kappa_{\text{B}} = 1.381\times10^{-23}\,\text{J/K}$; the free electron mass is $m_0 = 9.109\times10^{-31}\,\text{kg}$; the absolute value of the electron charge is $e = 1.602\times10^{-19}\,\text{C}$; the vacuum electric permittivity is $\varepsilon_0 = 8.854\times10^{-12}\,\text{F/m}$; the binding energy of the electron in a hydrogen atom is $E_0 \approx m_0 e^4/(32\pi^2\varepsilon_0^2\hbar^2) = 13.61\,\text{eV}$].

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Exercise 1.

1. For two consecutive peaks, $i+1$ and i, in the cubic system one has

$$\left(\frac{\sin\theta_{i+1}}{\sin\theta_i}\right)^2 = \frac{h_{i+1}^2+k_{i+1}^2+\ell_{i+1}^2}{h_i^2+k_i^2+\ell_i^2},$$

where h, k, ℓ are the Miller indices. From the data, one finds for the ratio on the left-hand side the values

$$1.999,\ 1.500,\ 1.334,\ 1.250,\ 2.200,\ 1.167,\ 1.143.$$

According to the selection rules for the cubic system, for the fcc lattice one expects the ratios $\frac{4}{3}$, 2, $\frac{11}{8}$, ... which rules out this lattice; for the diamond lattice one expects the ratios $\frac{8}{3}$, $\frac{11}{8}$, $\frac{16}{11}$, ... which rules out this lattice; for the simple cubic lattice one expects the ratios 2, $\frac{3}{2}$, $\frac{4}{3}$, $\frac{5}{4}$, $\frac{6}{5}$, $\frac{4}{3}$, ... which rules out this lattice; for the bcc lattice one expects the ratios 2, $\frac{3}{2}$, $\frac{4}{3}$, $\frac{5}{4}$, $\frac{6}{5}$, $\frac{7}{6}$, $\frac{8}{7}$, which are all compatible with the experimental data, so the crystal is a bcc. The families of lattice planes giving rise to the first eight peaks in a bcc crystal are 110, 200, 211, 220, 310, 222, 321, 400, and all the families equivalent to them under permutations of different indices, and change of sign of all but one nonzero indices.

To determine the size of the conventional unit cell form the i-th diffraction peak one can use the formula

$$a_i = \frac{\lambda\sqrt{h_i^2+k_i^2+\ell_i^2}}{2\sin\theta_i},$$

extracting from the data the values (in nm) 0.3999, 0.4000, 0.4001, 0.4000, 0.4000, 0.4000, 0.4000, 0.4000, so the average value is $a = 0.4000\,\text{nm}$.

2. The crystal hosts a two atom basis ($p = 2$), so one expects to observe 3 acoustic phonon branches and $3p-3 = 3$ optical phonon branches.

3. The low-temperature specific heat of the crystal is dominated by the sound modes, and can be written as

$$c_v = 234\left(\frac{T}{\Theta_{\rm D}}\right)^3 n\kappa_{\rm B},$$

where $n = 2/a^3 = 3.125\times10^{28}\,\text{m}^{-3}$ is the density of Bravais lattice points in the given bcc lattice. Hence, putting $T = 1\,\text{K}$ and $c_v = 6.461\,\text{J}/(\text{K}\cdot\text{m}^3)$, one deduces

$$\Theta_{\rm D} = \left(\frac{234\,n\kappa_{\rm B}}{c_v}\right)^{1/3} T = 250.0\,\text{K}.$$

But

$$\Theta_{\rm D} = \frac{\hbar c_{\rm D} q_{\rm D}}{\kappa_{\rm B}},$$

where $q_{\rm D} = (6\pi^2 n)^{1/3} = (12\pi^2)^{1/3}/a = 1.226\times10^{10}\,\text{m}^{-3}$ is the he Debye wavevector of the sound modes. Hence, one obtains

$$c_{\rm D} = \frac{\kappa_{\rm B}\Theta_{\rm D}}{\hbar q_{\rm D}} = 2670\,\text{m/s}.$$

Exercise 2.

1. The dispersions are plotted in Fig. 1, where the conduction band is the uppermost curve and the valence band is the lowermost curve. The gap is direct and is located at the Γ point of the first Brillouin zone.

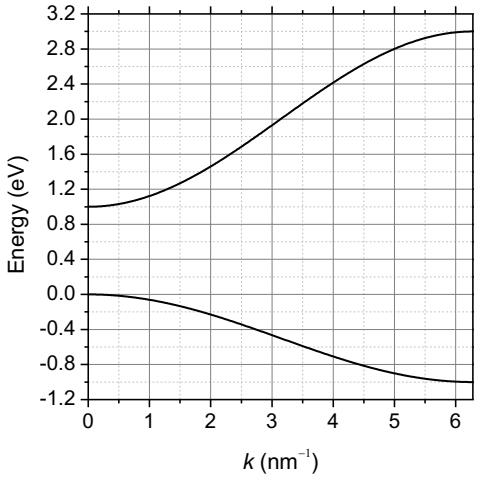

Fig. 1.

2. The requested elements of the effective mass tensor are

$$m^{\mathrm{e}}_{zz} = \frac{\hbar^2}{Aa^2} = 2.777 \times 10^{-31}\,\mathrm{kg} = 0.3048\,m_0, \qquad m^{\mathrm{h}}_{zz} = -\frac{\hbar^2}{Ba^2} = -5.553 \times 10^{-31}\,\mathrm{kg} = -0.6096\,m_0.$$

Due to the cubic symmetry, the masses along the other principal axes are the same.

3. The energy gap of the given semiconductor is $E_g = 1.0\,\mathrm{eV}$ and the mass tensor is isotropic, because of the cubic symmetry, hence the mass of carriers in the conduction and valence band is, respectively, $m_c = m^{\mathrm{e}}_{zz} = 0.3048\,m_0$ and $m_v = -m^{\mathrm{h}}_{zz} = 0.6096\,m_0$. In the intrinsic case

$$n = p = n_i = 2\left(\frac{\kappa_{\mathrm{B}} T\, m_0}{2\pi\hbar^2}\right)^{3/2}\left(\frac{m_c m_v}{m_0^2}\right)^{3/4} \mathrm{e}^{-E_g/(2\kappa_{\mathrm{B}}T)} = 2.831 \times 10^{16}\,\mathrm{m}^{-3}.$$

4. Under the given assumptions,

$$E_{\mathrm{d}} = \frac{m^{\mathrm{e}}_{zz}}{m_0 \varepsilon_r^2} E_0 = 18.45\,\mathrm{meV}.$$