**Written exam of Condensed Matter Physics - July 12th 2021**
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**Exercise 1: X-ray scattering and phonons [15 points].**

$ZnSnSb_2$ crystallizes with the chalcopyrite structure, and belongs to the tetragonal system (see Fig. 1), with sides of the primitive cell $a = b = 0.6275\,\mathrm{nm}$ and $c = 1.255\,\mathrm{nm} = 2a$.

1. Determine the fundamental reciprocal lattice vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$ of $ZnSnSb_2$; determine the scattering angles $\varphi = 2\theta$ and the Miller indices $hkl$ of the first 5 peaks that are observed if the crystal structure of $ZnSnSb_2$ is investigated by means of the Debye-Scherrer technique, with X rays of wavelength $\lambda = 0.2\,\mathrm{nm}$ [**7 points**].

2. How many optical phonon branches are expected to be observed in $ZnSnSb_2$? Why? What is the Debye wave-vector $q_\mathrm{D}$ of the sound modes of $ZnSnSb_2$? [**4 points**].

3. The velocity of the longitudinal sound modes of $ZnSnSb_2$ is $v_\ell = 4028\,\mathrm{m/s}$ and the velocity of the transverse sound modes is $v_\mathrm{t} = 2302\,\mathrm{m/s}$. Determine the average sound velocity $\overline{v}$ within the Debye model, and the Debye temperature $\Theta_\mathrm{D}$ of the sound modes of $ZnSnSb_2$. [**4 points**].

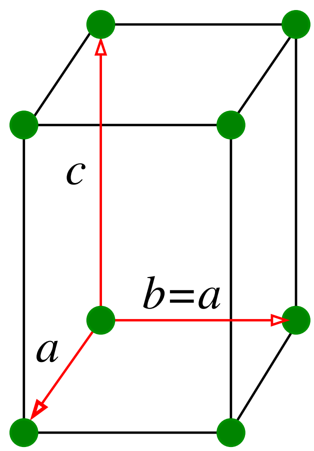


Fig. 1.

**Exercise 2: Bloch electrons [15 points].**

Consider a cubic crystal with lattice constant $a = 0.5\,\mathrm{nm}$ and an even number of valence electrons. The conduction and valence bands ($E_\mathrm{C}$ and $E_\mathrm{V}$, respectively) feature the following dispersion curves

$$E_\mathrm{C} = A\left[\frac{1}{5} - \frac{1}{2}\sin^2\left(\frac{k_x a}{2}\right)\right],$$

$$E_\mathrm{V} = B\left[\cos(k_x a) - 1\right],$$

along the $k_x$ direction, where $A = 0.70\,\mathrm{eV}$ and $B = 0.6\,\mathrm{eV}$.

1. Plot the dispersion curves in the first Brillouin zone along the $k_x$ direction [**4 points**].

2. Say if the crystal is a metal or an insulator [**3 points**].

3. Evaluate the $m_{xx}$ component of the effective mass tensor of the electrons at the conduction band minimum and of the holes at the valence band maximum [**4 points**].

2. For each band, determine at which point of the $k_x$ axis of the first Brillouin zone the velocity is maximum and provide the value [**4 points**].

[Note that 1 eV corresponds to an energy of $1.602\times10^{-19}$ J; the Planck constant is $\hbar = 1.055\times10^{-34}$ J·s; the Boltzmann constant is $\kappa_B = 1.381\times10^{-23}\,\mathrm{J\cdot K^{-1}}$; the free electron mass is $m_0 = 9.109\times10^{-31}$ kg].

**Solution of the written exam**
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**Exercise 1**.

1. Taking the primitive vectors $\boldsymbol{a}_1 = a\,\hat{\boldsymbol{x}}$, $\boldsymbol{a}_2 = a\,\hat{\boldsymbol{y}}$, $\boldsymbol{a}_3 = c\,\hat{\boldsymbol{z}} = 2a\,\hat{\boldsymbol{z}}$, where $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$ and $\hat{\boldsymbol{z}}$ are the unit vectors of the corresponding axes, one has

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\,\hat{\boldsymbol{x}}, \qquad \boldsymbol{b}_2 = \frac{2\pi}{a}\,\hat{\boldsymbol{y}}, \qquad \boldsymbol{b}_2 = \frac{\pi}{a}\,\hat{\boldsymbol{z}}.$$

A reciprocal lattice vector $\boldsymbol{K} = h\,\boldsymbol{b}_1 + k\,\boldsymbol{b}_2 + l\,\boldsymbol{b}_3$ has magnitude

$$K = |\boldsymbol{K}| = \frac{\pi}{a}\sqrt{4(h^2+k^2)+l^2}.$$

According to the Debye-Scherrer formula,

$$\sin\frac{\varphi}{2} = \frac{\lambda}{4\pi}K = \frac{\lambda}{4a}\sqrt{4(h^2+k^2)+l^2},$$

with $\frac{\lambda}{4a} = 0.07968$. The first peak corresponds to the Miller indices 001 and $\varphi_1 = 9.14°$; the second peak corresponds to the Miller indices 002, 100, 010, and $\varphi_2 = 18.34°$; the third peak corresponds to the Miller indices 011, 101, and $\varphi_3 = 20.53°$; the fourth peak corresponds to the Miller indices 110, 102, 012, and $\varphi_4 = 26.05°$; the fifth peak corresponds to the Miller indices 003, 111 and $\varphi_5 = 27.66°$.

2. Since there are $p = 4$ atoms in the primitive cell, the number of optical modes is $3p-3 = 9$. The Debye wave-vector of sound modes is

$$q_{\rm D} = (6\pi^2 n)^{1/3} = \left(\frac{6\pi^2}{a^2 c}\right)^{1/3} = 4.930\times 10^9\,{\rm m}^{-1}.$$

3. The average sound velocity is

$$\overline{v} = \left[\frac{1}{3}\left(\frac{1}{v_\ell^3} + \frac{2}{v_{\rm t}^3}\right)\right]^{-1/3} = 2558\,{\rm m/s}.$$

The Debye temperature of the sound modes is

$$\Theta_{\rm D} = \frac{\hbar\,\overline{v}\,q_{\rm D}}{\kappa_B} = 96.32\,{\rm K}.$$

**Exercise 2**.

1. The band structure is shown in Fig. 2.

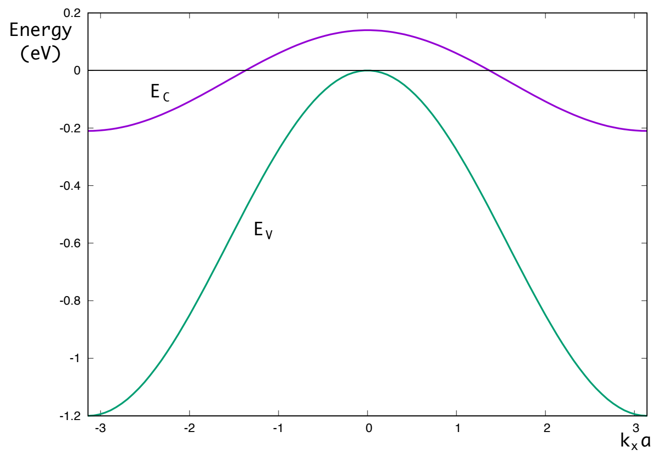


Fig. 2.

2. The system is a metal, because the conduction band is partially overlapped with the valence band so that part of the valence electrons will be transferred from the latter to the former, to reach lower energy states. As a consequence, even at $T = 0$, there will be a finite density of holes near the top of the valence band and a finite density of electrons near the bottom of the conduction band, and a well defined Fermi energy.

3. Expanding the dispersion relation near the bottom of the conduction band one finds

$$m^{\mathrm{C}}_{xx} = \frac{4\hbar^2}{Aa^2} = 1.57 \times 10^{-30}\,\mathrm{kg} = 1.71\, m_0.$$

Similarly, expanding the dispersion relation near the top of the valence band one finds

$$m^{\mathrm{V}}_{xx} = -\frac{\hbar^2}{Ba^2} = -4.7 \times 10^{-31}\,\mathrm{kg} = -0.51\, m_0.$$

4. The absolute value of the velocity along $k_x$, $v_{\mathrm{V,C}} = \frac{1}{\hbar}\frac{\partial E_{\mathrm{V,C}}}{\partial k_x}$, is maximum at $k_x = \pm\frac{\pi}{2a}$ in both bands. There, one finds

$$v_{\mathrm{V;max}} = \frac{Ba}{\hbar} = 4.55 \times 10^5\,\mathrm{m/s}, \qquad v_{\mathrm{C;max}} = \frac{Aa}{4\hbar} = 1.33 \times 10^5\,\mathrm{m/s}.$$