Written exam of Condensed Matter Physics - January 20th 2023
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Exercise 1: X-ray scattering and phonons.

The structure of a crystal with cubic symmetry is investigated by means of the Debye-Scherrer method with a radiation of wavelength $\lambda = 0.1\,\mathrm{nm}$. The first nine peaks of the X-ray scattering pattern are observed in correspondence of the following scattering angles ($\varphi = 2\vartheta$):

$$\varphi_1 = 11.5^\circ; \quad \varphi_2 = 16.3^\circ; \quad \varphi_3 = 19.9^\circ; \quad \varphi_4 = 23.1^\circ; \quad \varphi_5 = 25.8^\circ;$$

$$\varphi_6 = 28.4^\circ; \quad \varphi_7 = 32.9^\circ; \quad \varphi_8 = 34.9^\circ; \quad \varphi_9 = 36.9^\circ.$$

1. [8 points] Tell if the structure of the crystal is simple cubic, fcc, bcc, or diamond, motivating your answer, then determine the numerical value of the size a of the (conventional) unit cell, as the average over the values deduced from each of the nine observed peaks, $a_1, ..., a_9$. [The values $a_1, ..., a_9$ and a should be calculated with three significant digits].

2. [2 points] The phonon spectrum of the given crystal is investigated by means of neutron scattering. Tell how many optical branches will be observed if the crystal hosts a two-atom basis, motivating your answer.

3. [5 points] The sound velocities of the given crystal (averaged over the directions) are $c_\ell = 3715\,\mathrm{m/s}$ for the longitudinal mode, $c_{t1} = 1665\,\mathrm{m/s}$ and $c_{t2} = 2025\,\mathrm{m/s}$ for the two transverse modes. Determine the numerical values of the average sound velocity c_D within the Debye model, of the Debye temperature of the sound modes Θ_D, and of the specific heat c_v at a temperature $T = 1\,\mathrm{K}$.

Exercise 2: Semiconductors.

An intrinsic three-dimensional semiconductor has gap energy $E_g = 0.600\,\mathrm{eV}$ and hole effective mass $m_h = 5.01 \times 10^{-31}\,\mathrm{kg} = 0.550\,m_0$, where m_0 is the free electron mass.

1. [5 points] Determine the numerical value of electron effective mass m_e, given that the chemical potential μ_i at a temperature $T = 300\,\mathrm{K}$ is $20\,\mathrm{meV}$ above the middle of the gap.

2. [5 points] Determine the numerical value of the concentration of intrinsic carriers n_i at $T = 300\,\mathrm{K}$.

3. [5 points] If the same semiconductor is doped with a concentration $N_A = 2.00 \times 10^{20}\,\mathrm{m}^{-3}$ of acceptors (no donors are present), determine the numerical values of the electron and hole concentrations in the conduction and valence band, respectively n and p, at $T = 300\,\mathrm{K}$, assuming that all the acceptors are fully ionized. [Notice that the condition $n_i \ll N_A$ is not met for the values of the parameters assigned in this exercise]

[Useful constants and conversion factors: the reduced Planck constant is $\hbar = 1.05 \times 10^{-34}\,\mathrm{J{\cdot}s}$, the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,\mathrm{J{\cdot}K^{-1}}$, the elementary charge is $e = 1.60 \times 10^{-19}\,\mathrm{C}$, the free electron mass is $m_0 = 9.11 \times 10^{-31}\,\mathrm{kg}$; $1\,\mathrm{eV}$ corresponds to a temperature of $1.16 \times 10^4\,\mathrm{K}$ or to an energy of $1.60 \times 10^{-19}\,\mathrm{J}$].

Solution
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Exercise 1.

1. We calculate the ratios $r_i = \sin^2(\varphi_{i+1}/2)/\sin^2(\varphi_i/2)$, with $i = 1, ..., 8$ and find the values

$$r_1 = 2.00; \quad r_2 = 1.49; \quad r_3 = 1.34; \quad r_4 = 1.24; \quad r_5 = 1.21; \quad r_6 = 1.33; \quad r_7 = 1.12; \quad r_8 = 1.11.$$

The values for the diamond are $r_1 = 8/3$, ..., which rules out the diamond; the values for the fcc are $r_1 = 4/3$, ..., which rules out the fcc; the values for the bcc are $r_1 = 2$, $r_2 = 3/2$, $r_3 = 4/3$, $r_4 = 5/4$, $r_5 = 6/5$, $r_6 = 7/6$, ..., which rules out the bcc, while the simple cubic is compatible with all the above values, so the crystal is simple cubic.

Calculating $a_i = \lambda\sqrt{h_i^2 + k_i^2 + \ell_i^2}/[2\sin(\varphi_i/2)]$, with $i = 1, ..., 9$, where h, k, ℓ are the Miller indices of the simple cubic, we find the following values (in nm):

$$a_1 = 0.499; \quad a_2 = 0.499; \quad a_3 = 0.501; \quad a_4 = 0.499; \quad a_5 = 0.501; \quad a_6 = 0.499; \quad a_7 = 0.499; \quad a_8 = 0.500; \quad a_9 = 0.500.$$

The average value is $a = \frac{1}{9}\sum_{i=1}^{9} a_i = 0.500\,\mathrm{nm}$.

2. The crystal is a simple cubic, if it host a p atom basis, the number of optical branches is $3p - 3$. In our case $p = 2$, so three optical branches will be observed.

3. The average sound velocity within the Debye model is

$$c_\mathrm{D} = \left[\frac{1}{3}\left(\frac{1}{c_\ell^3} + \frac{1}{c_{t1}^3} + \frac{1}{c_{t2}^3}\right)\right]^{-1/3} = 2034\,\mathrm{m/s}.$$

The Debye temperature of the sound modes is

$$\Theta_\mathrm{D} = \frac{\hbar c_\mathrm{D} q_\mathrm{D}}{\kappa_B} = \frac{\hbar c_\mathrm{D}(6\pi^2)^{1/3}}{a\kappa_B} = 121\,\mathrm{K}.$$

At $T = 1\,\mathrm{K}$ the temperature is much lower than the Debye temperature, so we can neglect the contribution of the optical modes and use for the sound modes the asymptotic formula

$$c_v = 234\left(\frac{T}{\Theta_\mathrm{D}}\right)^3 n\kappa_B = 234\left(\frac{T}{a\Theta_\mathrm{D}}\right)^3 \kappa_B = 14.6\,\frac{\mathrm{J}}{\mathrm{K}\cdot\mathrm{m}^3}.$$

Exercise 2.

1. We have

$$0.02\,\mathrm{eV} = \delta \equiv \mu_i - \left(E_v + \frac{1}{2}E_g\right) = \frac{3}{4}\kappa_B T \ln\frac{m_h}{m_e} \quad \Rightarrow \quad m_e = m_h\,\mathrm{e}^{-\frac{4\delta}{3\kappa_B T}} = 1.79\times10^{-31}\,\mathrm{kg} = 0.196\,m_0.$$

2. We have

$$n_i = 2.5\left(\frac{m_e m_h}{m_0^2}\right)^{3/4}\left(\frac{T}{300\,\mathrm{K}}\right)^{3/2}\mathrm{e}^{-E_g 2\kappa_B T}\times10^{25}\,\mathrm{m}^{-3} = 4.29\times10^{19}\,\mathrm{m}^{-3}.$$

3. From the charge neutrality condition (with no donors present) and the law of mass action we have

$$\begin{cases} n - p = -N_A \\ np = n_i^2 \end{cases} \quad \Rightarrow \quad \begin{cases} p = \frac{1}{2}\left(\sqrt{N_A^2 + 4n_i^2} + N_A\right) = 2.09\times10^{20}\,\mathrm{m}^{-3}, \\ n = \frac{1}{2}\left(\sqrt{N_A^2 + 4n_i^2} - N_A\right) = 8.81\times10^{18}\,\mathrm{m}^{-3}. \end{cases}$$