Written exam of Condensed Matter Physics - May 10th 2023
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Exercise 1: Phonons.

A monoatomic substance forms a crystal with fcc structure.

1. [2 points] How many phonon branches are present in the given crystal? Motivate your answer.

2. [4 points] A measurement of the specific heat of the crystal at a temperature $T = 1\,\mathrm{K}$ yields the value $c_V = 8.256\,\mathrm{J{\cdot}K^{-1}{\cdot}m^{-3}}$. Assuming that c_V can be calculated within the Debye model for the acoustic branches, determine the numerical value of the average Debye sound velocity v_D.

3. [6 points] The cumulative density of states of the three acoustic branches calculated at the Debye frequency ω_D is $\mathcal{D}(\omega_\mathrm{D}) = 1.053 \times 10^{17}\,\mathrm{s/m^3}$. Determine the numerical values of the Debye frequency ω_D, of the Debye wave vector q_D, and of the side of the conventional cubic unit cell a.

4. [3 points] The transverse sound velocity in the given crystal, averaged over the various directions, is $v_t = 2266\,\mathrm{m/s}$. Determine the numerical value of the longitudinal sound velocity, averaged over the various directions, v_ℓ.

Exercise 2: Semiconductors

The conduction and valence band energies [respectively, $E_c(\boldsymbol{k})$ and $E_v(\boldsymbol{k})$, with $\boldsymbol{k}$ the Bloch wave vector] of an intrinsic three-dimensional semiconductor can be approximated close to the band extrema by the expressions

$$E_c(\boldsymbol{k}) = E_g + C\,k^2,$$
$$E_v(\boldsymbol{k}) = -V\,k^2,$$

where E_g is the band gap energy, $C = 2.54 \times 10^{-19}\,\mathrm{eV{\cdot}m^2}$, $V = 6.35 \times 10^{-20}\,\mathrm{eV{\cdot}m^2}$, and $k^2 \equiv |\boldsymbol{k}|^2$. The carrier concentration is $n_i(T_1) = 2.526 \times 10^{13}\,\mathrm{cm^{-3}}$ and $n_i(T_2) = 2.787 \times 10^{14}\,\mathrm{cm^{-3}}$, at the temperatures $T_1 = 500\,\mathrm{K}$ and $T_2 = 600\,\mathrm{K}$.

1. [6 points] Assuming that the band gap energy E_g does not depend on the temperature in the given interval ($500-600\,\mathrm{K}$), determine its numerical value.

2. [6 points] Determine the carrier concentration at the temperature $T = 550\,\mathrm{K}$.

3. [3 points] Determine the electrical conductivity σ of the semiconductor at the temperature $T = 550\,\mathrm{K}$, knowing the electron and hole relaxation times, respectively, $\tau_e = 4.0 \times 10^{-13}\,\mathrm{s}$ and $\tau_h = 2.0 \times 10^{-13}\,\mathrm{s}$.

[Useful constants and conversion factors: the reduced Planck constant is $\hbar = 1.05 \times 10^{-34}\,\mathrm{J{\cdot}s}$, the Boltzmann constant is $\kappa_\mathrm{B} = 1.38 \times 10^{-23}\,\mathrm{J{\cdot}K^{-1}}$, 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. The crystal is a three-dimensional Bravais lattice, the substance is monoatomic, so there are three acoustic branches and no optical branches.

2. One has

$$c_V = \frac{2\pi^2}{5}\kappa_B \left(\frac{\kappa_B T}{\hbar v_D}\right)^3 \qquad \Rightarrow \qquad v_D = \left(\frac{2\pi^2 \kappa_B}{5\, c_V}\right)^{1/3} \frac{\kappa_B T}{\hbar} = 2456\,\mathrm{m/s}.$$

3. One has

$$\mathcal{D}(\omega_D) = \frac{3}{2\pi^2}\frac{\omega_D^2}{v_D^3} \qquad \Rightarrow \qquad \omega_D = \left[\frac{2\pi^2}{3} v_D^3 \mathcal{D}(\omega_D)\right]^{1/2} = 1.013 \times 10^{14}\,\mathrm{s}^{-1}.$$

Then, since $\omega_D = v_D q_D$, one finds

$$q_D = \frac{\omega_D}{v_D} = 4.125 \times 10^{10}\,\mathrm{m}^{-1}.$$

Finally, since the density of lattice points in a fcc lattice is $n = 4/a^3$, one has

$$q_D = \frac{2(3\pi^2)^{1/3}}{a} \qquad \Rightarrow \qquad a = \frac{2(3\pi^2)^{1/3}}{q_D} = 0.15\,\mathrm{nm}.$$

4. The average Debye sound velocity v_D obeys the relation

$$\frac{1}{v_D^3} = \frac{1}{3}\left(\frac{1}{v_\ell^3} + \frac{2}{v_t^3}\right),$$

hence,

$$v_\ell = \left(\frac{3}{v_D^3} - \frac{2}{v_t^3}\right)^{-1/3} = 3197\,\mathrm{m/s}.$$

Exercise 2.

1. For an intrinsic semiconductor the intrinsic carrier concentration is $n_i = n_e = n_h$ (n_e and n_h being the density of electrons in the conduction band and the density of holes in the valence band, respectively). Using the law of mass action, the band gap energy can be determined by the carrier concentration ratio for the two temperatures considered

$$E_g = \frac{2\kappa_B}{\frac{1}{T_2} - \frac{1}{T_1}} \ln\left[\left(\frac{T_2}{T_1}\right)^{3/2} \frac{n_i(T_1)}{n_i(T_2)}\right] = 1.1\,\mathrm{eV}.$$

2. The masses of electrons and holes are, respectively,

$$m_e = \frac{\hbar^2}{2C} = 0.15\, m_0, \qquad m_h = \frac{\hbar^2}{2V} = 0.60\, m_0,$$

where m_0 is the free electron mass. Then

$$n_i(T = 550\,\mathrm{K}) = 2.5\left(\frac{m_e m_h}{m_0^2}\right)^{3/4}\left(\frac{T}{300\,\mathrm{K}}\right)^{3/2} \mathrm{e}^{-E_g/2\kappa_B T} \times 10^{19}\,\mathrm{cm}^{-3} = 9.305 \times 10^{13}\,\mathrm{cm}^{-3}.$$

3. The conductivity is

$$\sigma = e^2 n_i \left(\frac{\tau_e}{m_e} + \frac{\tau_h}{m_h}\right) = 7.866\,\Omega^{-1}\cdot\mathrm{m}^{-1}.$$