Written exam of Condensed Matter Physics
September 7th 2020
Prof.s S. Caprara and A. Polimeni

Exercise 1.

Sodium Chloride (NaCl) crystals can be described as a FCC Bravais Lattice with a two-atom basis, the side of the conventional unit cell being a=0.564 nm.

1. How many optical and sound modes are found in NaCl if its phonon spectrum is investigated by neutron scattering?
2. The velocity of longitudinal sound modes of NaCl is $c_L = 4.55 \times 10^3$ m/s, the velocity of transverse sound modes is $c_T = 2.61 \times 10^3$ m/s. Assuming that the dependence of the velocity of sound on the direction of propagation can be neglected, determine the average sound velocity c within the Debye scheme; hence, determine the Debye temperature Θ_D.
3. Determine the specific heat of NaCl at a temperature T=5 K, assuming that the contribution of optical modes can be neglected.

NOTE: The Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}$ J/K, the Planck constant is $\hbar = 1.05 \times 10^{-34}$ J·s.

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Exercise 2.

Consider two samples of the same semiconductor, labeled as A and B. Sample A is pure, sample B is doped with a density N_d of donors. The top of the valence band is taken as the origin of the energy scale, ε_v=0. The bottom of the conduction band is located at ε_c=0.366 eV. At a temperature T=300 K, the density of intrinsic carriers of sample A is $n_i = 1.1 \times 10^{22}$ m^{-3}, the chemical potential of sample A is $\mu_i = 0.186$ eV, the chemical potential of sample B is $\mu = 0.294$ eV.

1. Determine the average mass of electrons in the conduction band, m_c, and the average mass of holes in the valence band, m_v.
2. Assuming that the donor levels are fully ionized at the given temperature, determine the density of donors N_d in sample B.
3. Based on the previous result, is sample B in the predominantly intrinsic or predominantly extrinsic regime?

NOTE: The Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}$ J/K, the Planck constant is $\hbar = 1.05 \times 10^{-34}$ J·s, the free electron mass is $m_0 = 9.11 \times 10^{-31}$ kg, 1 eV is equivalent to 1.60×10^{-19} J.

Solution.

Exercise 1.

1. Since there are p=2 atoms in the basis, NaCl hosts 3 sound modes (two transverse and one longitudinal) and $3p$–3=3 optical modes.

2. Within the Debye scheme, the average sound velocity is

$$c = \left[\frac{1}{3}\left(\frac{1}{c_L^3} + \frac{2}{c_T^3}\right)\right]^{-1/3} = 2.90 \times 10^3 \text{ m/s}.$$

The Debye temperature is

$$\Theta_D = \frac{\hbar c}{\kappa_B}(6\pi^2 n)^{1/3} = 243 \text{ K},$$

where we have used

$$n = \frac{N}{V} = \frac{4}{a^3} = 2.23 \times 10^{28} \text{ m}^{-3},$$

for the density of lattice points in a FCC lattice.

3. At temperatures much lower than Θ_D, the specific heat is

$$c_V = \frac{2\pi^2}{5}\kappa_B\left(\frac{\kappa_B T}{\hbar c}\right)^3 = 627 \text{ J/(K·m}^3\text{)}.$$

Exercise 2.

1. The gap is $E_g = \varepsilon_c - \varepsilon_v = 0.366$ eV. Let us write $m_{c,v} = \widetilde{m}_{c,v} m_0$, measuring the masses in units of the free electron mass. Then we have the system of two equations

$$\widetilde{m}_c \widetilde{m}_v = \left[\frac{4 n_i \mathrm{e}^{E_g/2\kappa_B T}}{\left(\frac{2 m_0 \kappa_B T}{\pi \hbar^2}\right)^{3/2}}\right]^{4/3} = 0.418,$$

$$\frac{\widetilde{m}_v}{\widetilde{m}_c} = \exp\left(\frac{4\mu_i - 2E_g}{3\kappa_B T}\right) = 1.17,$$

whose solution is $\widetilde{m}_c = 0.598, \widetilde{m}_v = 0.699$, i.e., $m_c = 5.45 \times 10^{-31}$ kg, $m_v = 6.37 \times 10^{-31}$ kg.

2. Under the given assumptions, we have

$$N_d \approx \Delta n = 2 n_i \sinh\frac{\mu - \mu_i}{\kappa_B T} = 7.17 \times 10^{23} \text{ m}^{-3}.$$

3. Since $N_d \approx \Delta n \gg n_i$, the system is in the predominantly extrinsic regime.