Written exam of Condensed Matter Physics - February 12th 2019
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Exercise 1: Phonons.

Consider a model for a linear crystal composed of N units cells of size a, with a two-atom basis. All atoms are constrained to move only along the line that defines the crystal. The two inequivalent atoms have masses M and m, respectively. The spring constant describing the elastic force between neighboring atoms is K (see Fig. 1). Indicate with u_n and w_n the displacement of the two inequivalent atoms in the n-th unit cell, with respect to their equilibrium positions. Adopt Born-von Karman periodic boundary conditions.

1. Assuming traveling-wave solutions $u_n = Ae^{i(qna-\omega t)}$ and $w_n = Be^{i(qna-\omega t)}$, where q is the one-dimensional wave vector, determine the dispersion of the acoustic and optical phonon branches, $\omega_a(q)$ and $\omega_o(q)$.

2. Verify that, for small q, $\omega_a(q) \approx c_s|q|$, and determine the expression of the sound velocity c_s.

3. Let now $a = 0.145\,\text{nm}$, $m = 12\,m_u$, $M = 16\,m_u$, with $m_u = 1.66 \times 10^{-27}\,\text{kg}$, $K = 8.55\,\text{kg/s}^2$. After determining the numerical value of the sound velocity c_s, adopt a Debye model for the acoustic branch, $\omega_a(q) = c_s|q|$, and an Einstein model for the optical branch, with $\omega_E = \omega_o(q = 0)$, to calculate the specific heat c_V of the lattice at very high temperatures ($\kappa_B T \gg \hbar\omega_E$), and at $T = 5\,\text{K}$. Consider that $\int_0^\infty \frac{x}{e^x-1}\,dx = \frac{\pi^2}{6}$.

[Note that the Planck constant is $\hbar = 1.05 \times 10^{-34}\,\text{J·s}$, the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,\text{J·K}^{-1}$].

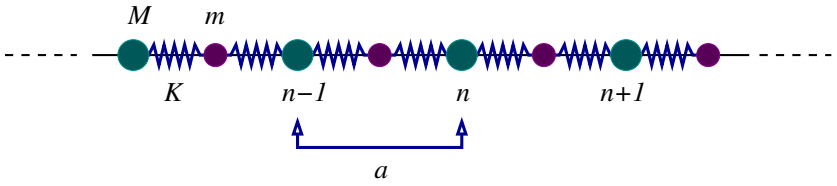

Fig. 1.

Exercise 2: Semiconductors.

Consider an intrinsic semiconductor that can be described as a two band system, with the top of the valence band at $\varepsilon_v = 1.15\,\text{eV}$ and the bottom of the conduction band at $\varepsilon_c = 1.95\,\text{eV}$ (these two values are assumed to be temperature independent). The values of the effective masses along the principal axes of the crystal are: $m_c^{x,y} = 0.2\,m_0$ and $m_c^z = 0.4\,m_0$ for electrons; $m_v^{x,y} = 0.3\,m_0$ and $m_v^z = 0.6\,m_0$ for holes; here, $m_0 = 9.11 \times 10^{-31}\,\text{kg}$ is the free electron mass. The mobilities of electrons and holes along the principal axes are $\mu_e^{x,y} = 4.80 \times 10^{-2}\,\text{m}^2\text{·V}^{-1}\text{·s}^{-1}$, $\mu_e^z = 2.40 \times 10^{-2}\,\text{m}^2\text{·V}^{-1}\text{·s}^{-1}$, $\mu_h^{x,y} = 3.20 \times 10^{-2}\,\text{m}^2\text{·V}^{-1}\text{·s}^{-1}$, $\mu_h^z = 1.60 \times 10^{-2}\,\text{m}^2\text{·V}^{-1}\text{·s}^{-1}$.

1. Calculate the density of electrons in the conduction band n_c, the density of holes in the valence band p_v, at a temperature $T = 300\,\text{K}$.

2. Calculate the components of the conductivity tensor along the principal axes, $\sigma_i^x = \sigma_i^y$ and σ_i^z (in $\Omega^{-1}\text{·m}^{-1}$, the subscript i indicates that the quantity refers to the intrinsic regime) at $T = 300\,\text{K}$.

3. Suppose now that the system is doped with a density $N_a = 2.45 \times 10^{20}\,\text{m}^{-3}$ of acceptor atoms (each atom accepts one electron). Assuming that the system is in the predominantly extrinsic regime, and that acceptors are fully ionized, calculate the density of electrons in the conduction band n_c, the density of holes in the valence band p_v, and the values of the components of the conductivity tensor along the principal axes, $\sigma^x = \sigma^y$ and σ^z (in $\Omega^{-1}\text{·m}^{-1}$) at $T = 300\,\text{K}$.

[Note that 1 eV corresponds to a temperature of $1.16 \times 10^4\,\text{K}$ or to an energy of $1.60 \times 10^{-19}\,\text{J}$, the Planck constant is $\hbar = 1.05 \times 10^{-34}\,\text{J·s}$, the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,\text{J·K}^{-1}$, the elementary charge is $e = 1.60 \times 10^{-19}\,\text{C}$].

Solution of the mid-term assessment test
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Exercise 1.

1. The equations of motion are

$$\begin{cases} M\ddot{u}_n = -K\left(2u_n - w_n - w_{n-1}\right), \\ m\ddot{w}_n = -K\left(2w_n - u_{n+1} - u_n\right). \end{cases}$$

Substituting the traveling-wave solutions we find

$$\begin{cases} \left(2K - M\omega^2\right) A - K\left(1 + \mathrm{e}^{-iqa}\right) B = 0, \\ -K\left(1 + \mathrm{e}^{iqa}\right) A + \left(2K - m\omega^2\right) B = 0, \end{cases}$$

which admits nontrivial solutions for A, B if and only if the determinant of the matrix associated to the system of linear equations vanishes. Letting in the following $\overline{\Omega} \equiv \sqrt{K(M+m)/(Mm)}$, which is the relevant frequency scale in our problem, and introducing the dimensionless parameter $\lambda \equiv 2Mm/(M+m)^2$, the equation that determines the phonon frequencies reads

$$\omega^4 - 2\overline{\Omega}^2\omega^2 + 2\lambda\overline{\Omega}^4 \sin^2\frac{qa}{2} = 0,$$

whose solutions are

$$\omega_\pm^2(q) = \overline{\Omega}^2\left(1 \pm \sqrt{1 - 2\lambda\sin^2\frac{qa}{2}}\right),$$

with $\omega_a(q) = \omega_-(q)$ and $\omega_o(q) = \omega_+(q)$ describing the acoustic and optical phonon branch, respectively.

2. For the acoustic branch, since for $|q|a \ll 1$ we have $\sin^2\frac{qa}{2} \approx \left(\frac{qa}{2}\right)^2$ and $\sqrt{1 - \frac{1}{2}\lambda(qa)^2} \approx 1 - \frac{1}{4}\lambda(qa)^2$, we find

$$\omega_a(q) \approx c_s|q|, \qquad \text{with } c_s = \frac{\sqrt{\lambda}}{2}\,\overline{\Omega}a.$$

Likewise, for $|q|a \ll 1$, the optical branch approaches $\omega_a(q) \approx \sqrt{2}\,\overline{\Omega}$.

3. Inserting the values given in the text, we find

$$\overline{\Omega} = \sqrt{\frac{7K}{48\,m_u}} = 2.74 \times 10^{13}\,\mathrm{s}^{-1}, \quad \lambda = \frac{24}{49} = 0.490, \qquad \rightarrow \qquad c_s = 1.39 \times 10^3\,\mathrm{m/s}.$$

We set $\omega_E \approx \omega_o(q=0) = \sqrt{2}\,\overline{\Omega}$. Then, the internal energy per unit volume is

$$u = \sum_{s=a,o}\int_{-\pi/a}^{\pi/a}\frac{\mathrm{d}q}{2\pi}\frac{\hbar\omega_s(q)}{\mathrm{e}^{\beta\hbar\omega_s(q)} - 1} \approx \int_0^{q_D}\frac{\mathrm{d}q}{\pi}\frac{\hbar c_s q}{\mathrm{e}^{\beta\hbar c_s q} - 1} + \frac{1}{a}\frac{\hbar\omega_E}{\mathrm{e}^{\beta\hbar\omega_E} - 1},$$

with $\beta = 1/(k_B T)$, and $q_D = \pi/a$, because in one dimension the Debye sphere coincides with the first Brillouin zone.

At high temperature, $k_B T \gg \hbar\omega_D, \hbar\omega_E$, with $\omega_D \equiv c_s q_D$, the exponentials in the denominators can be expanded to first order, the two phonon modes give the same contribution (equipartition), and

$$u \approx \frac{2k_B T}{a} \quad \Rightarrow \quad c_V = \frac{2k_B}{a} \equiv c_V^{DP},$$

i.e., we recover the Dulong-Petit (DP) value for a one-dimensional crystal with two atoms per unit cell. For the given set of parameters $c_V \approx 1.90 \times 10^{-13}\,\mathrm{J/(K{\cdot}m)}$.

At low temperature, $k_B T \ll \hbar\omega_D, \hbar\omega_E$,

$$u \approx \frac{\hbar c_s}{\pi}\left(\frac{k_B T}{\hbar c_s}\right)^2\int_0^\infty \frac{x}{\mathrm{e}^x - 1}\,\mathrm{d}x + \frac{\hbar\omega_E}{a}\mathrm{e}^{-\beta\hbar\omega_E} \approx \frac{\pi^2\hbar\omega_D}{6a}\left(\frac{k_B T}{\hbar\omega_D}\right)^2 \quad \Rightarrow \quad c_V = \frac{\pi^2 k_B}{3a}\left(\frac{k_B T}{\hbar\omega_D}\right),$$

where we adopted the change of variable $x = \beta\hbar c_s q$ in the integral over q, and extended the integration limit to infinity, to extract the leading behavior at small T. In the final expression for u, we neglected the exponentially small contribution of the optical branch, since the numerical estimate gives $\Theta_E \equiv \hbar\omega_E/k_B = 296\,\mathrm{K}$, i.e., at $T = 5\,\mathrm{K}$, $\mathrm{e}^{-\beta\hbar\omega_E} \approx \mathrm{e}^{-59.2} \approx 1.96 \times 10^{-26}$. Thus, at $T = 5\,\mathrm{K}$, $c_V \approx 0.0715\, k_B/a \approx 0.0357\, c_V^{DP} = 6.80 \times 10^{-15}\,\mathrm{J/(K{\cdot}m)}$, where we used the numerical value of the Debye temperature $\Theta_D \equiv \hbar\omega_D/k_B = 230\,\mathrm{K}$.

Exercise 2.

1. The gap is $E_g = 1.28 \times 10^{-19}\,\mathrm{J}$, hence $E_g/\kappa_B = 9.28 \times 10^3\,\mathrm{K}$. The thermal energy is $\kappa_B T = 4.14 \times 10^{-21}\,\mathrm{J} = 2.58 \times 10^{-2}\,\mathrm{eV}$, hence $E_g/2\kappa_B T = 15.5$. The average effective masses are $m_c = (m_c^x\, m_c^y\, m_c^z)^{1/3} = 0.252\, m_0$ and $m_v = (m_v^x\, m_v^y\, m_v^z)^{1/3} = 0.378\, m_0$. Then, the number of intrinsic carriers at $T = 300\,\mathrm{K}$ is

$$n_i = \frac{1}{4}\left(\frac{2\kappa_B T}{\pi\hbar^2}\right)^{3/2} (m_c m_v)^{3/4}\, \mathrm{e}^{-E_g/2\kappa_B T} = 7.98 \times 10^{17}\,\mathrm{m}^{-3}$$

and in the intrinsic regime $n_c = p_v = n_i$.
2. In the intrinsic regime, the components of the conductivity tensor along the principal axes are

$$\sigma^x = \sigma^y = e\, n_i(\mu_e^x + \mu_h^x) = 1.02 \times 10^{-2}\,\Omega^{-1}\cdot\mathrm{m}^{-1}, \qquad \sigma^z = e\, n_i(\mu_e^z + \mu_h^z) = 5.11\ \times 10^{-3}\,\Omega^{-1}\cdot\mathrm{m}^{-1},$$

3. The doped semiconductor is p-type. If the dopants are fully ionized

$$n_c \approx \frac{n_i^2}{N_a} = 2.60 \times 10^{15}\,\mathrm{m}^{-3}, \qquad p_v \approx N_a = 2.45 \times 10^{20}\,\mathrm{m}^{-3}.$$

In the predominantly extrinsic regime the contribution of minority carriers can be safely neglected, and the components of the conductivity tensor along the principal axes are

$$\sigma^x = \sigma^y = e\, p_v\, \mu_h^x = 1.26\,\Omega^{-1}\cdot\mathrm{m}^{-1}, \qquad \sigma^z = e\, p_v\, \mu_h^z = 0.628\,\Omega^{-1}\cdot\mathrm{m}^{-1}.$$