Course 406, Midterm I, 02/28/2019

Problem 1. (3 points)

Consider a 2D crystal with the in-plane dimensions $1 \times 1 \mu m^2$ and the speed of sound $c = 3,000 m/s$. Assume that only the phonon modes with $\hbar \omega < k_B T$ are excited. How many longitudinal modes are excited in this crystal at $T = 1K$?

Each mode in the $k$-space occupies the area $\frac{(2\pi)^2}{1 \times 1 \mu m^2}$

Maximum $k_{max}$ that corresponds to the condition $\hbar \omega_{max} = k_B T$ is $k_{max} = \frac{k_B T}{\hbar c}$

The total number of modes within the circle of radius $k_{max}$ is

$$N = \frac{\pi k_{max}^2}{(2\pi)^2} = \frac{(k_B T)^2}{\hbar c} \frac{1}{4\pi} (1 \times 1 \mu m^2) = 157$$
Problem 2. The phonon spectrum of a 2D crystal is shown in the Figure (consider just one acoustic and one optical branches of the spectrum).

(a) (2 points) Estimate the sound velocity for \( k \) far away from the boundary of the Brillouin zone. \( 1 \) THz = \( 10^{12} \) Hz.

\[
c = \frac{\omega}{k} = \frac{2\pi \times 25 \times 10^{12}}{3 \times 10^{10}} = 5.2 \text{ km/s}
\]

(b) (2 points) What is the occupancy (the average number of phonons) of the acoustic mode with \( f = 5 \) THz at \( T = 30 K \)?

\[
\langle n \rangle = \frac{1}{e^{\hbar \omega / k_B T} - 1} = \frac{1}{e^{\hbar \omega / k_B T} - 1} \approx 0.00024
\]

(c) Consider the energy dependence of the phonon density of states \( g_{2D}(\epsilon) \) for this crystal.

(2 points) What is the asymptotic behavior of \( g_{2D}(\epsilon) \) for the acoustic branch near the center of the Brillouin zone?

(3 points) What is the asymptotic behavior of \( g_{2D}(\epsilon) \) for the optical branch near the center of the Brillouin zone?

Hint: approximate the optical branch near the center of the Brillouin zone as \( (\epsilon_{\text{max}} - \epsilon) = A k^2 \).
\[ g_{2D}(\varepsilon) = g_{2D}(k) \frac{dk}{d\varepsilon} \quad g_{2D}(k) \propto k \]

The asymptotic behavior of \( g_{2D}(\varepsilon) \) at \( \varepsilon \to 0 \) (the acoustic branch):

The dispersion relation is linear, \( \frac{dk}{d\varepsilon} = \frac{1}{hc} \).

Thus, \( g_{2D}(\varepsilon) \propto \varepsilon \)

The asymptotic behavior of \( g_{2D}(\varepsilon) \) for the optical branch near the center of Brillouin zone:

\[ (\varepsilon_{\text{max}} - \varepsilon) = Ak^2 \quad \frac{d\varepsilon}{dk} \propto k \quad g_{2D}(\varepsilon) = \text{const} \]
Problem 3. (3 points) Consider a (hypothetical) 3D metal with a cubic crystal lattice. Using the free electron model, find the number of electrons per atom (could be non-integer) at which the Fermi sphere begins to touch the faces of the first Brillouin zone.

\[ k_{3D}(E_F) = (3\pi^2 n)^{1/3} \]
\[ k_{3D}(BZ \text{ boundary}) = \frac{\pi}{a} = \frac{\pi}{\sqrt[3]{\frac{1m^3}{N}}} \]
\[ 3\pi^2 n = \pi^3 N \]
\[ \frac{n}{N} = \frac{\pi}{3} \approx 1 \]

\( n \) – the electron density

\( N \) – the atom density
Problem 4.

The plot shows two electron bands in the first Brillouin zone of a 1D metal.

(a) (2 point) Schematically plot the effective electron mass as a function of energy.

(b) (3 points) Estimate the effective mass (in units of the bare electron mass, \( m_e = 9 \times 10^{-31} kg \)) at \( k = 0 \) in the lower band if \( a = 0.3 nm \).

(c) (2 points) Assume that the Fermi energy is 0.3eV. At room temperature (\( T = 300K \)), what is the probability that a state 0.01eV above the Fermi level is occupied by an electron?

\[
\begin{align*}
\text{(b)} & \quad m^* = \frac{\hbar^2}{2m_e} \left[ \frac{\partial^2 \varepsilon_f(k)}{\partial k^2} \right]^{-1} \quad E = \frac{(\hbar k)^2}{2m^*} \\
& \quad m^* \approx \frac{(\hbar k)^2}{2E} = 3.8m_e \\
\text{(c)} & \quad f(\varepsilon) = \frac{1}{1 + e^{\frac{\varepsilon-E_F}{k_BT}}} = \frac{1}{1 + e^{\frac{0.01eV}{0.026eV}}} = 0.4
\end{align*}
\]
Problem 5 (3 points).

Consider a 2D square crystal lattice with a unit cell size $a$. There are two electrons per unit cell. Assume that the electron dispersion relation looks like $\varepsilon(k) = 1eV \sin\left(\frac{ak}{2}\right)$ along direction 1 and $\varepsilon(k) = 1.5eV \sin\left(\frac{ak}{2\sqrt{2}}\right)$ along direction 2 in the $k$-space. Find the minimal band gap along direction 1 required for this crystal to be an insulator. Provide essential plots and explanations.

The crystal is an insulator (i.e. not a metal) if the bottom of the second band in direction 1 is higher than the top of the first band in direction 2. Thus, the minimal gap is 0.5 eV.